



Full wwPDB EM Validation Report ⓘ

Jan 9, 2023 – 04:37 PM JST

PDB ID : 7W1V
EMDB ID : EMD-32257
Title : Active state CI from Rotenone-NADH dataset, Subclass 1
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-20
Resolution : 3.00 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:

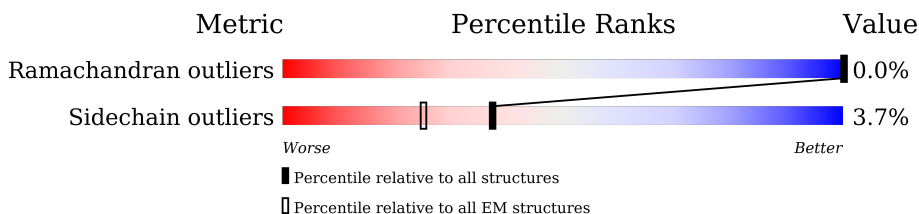
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 3.00 Å.

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



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

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

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

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Mol	Chain	Length	Quality of chain
9	J	342	97%
10	K	43	98%
11	L	125	98%
12	M	690	97%
13	N	144	93%
14	O	217	98%
15	P	208	99%
16	Q	430	96%
17	S	70	100%
18	T	96	94%
19	U	83	96%
20	V	140	98%
21	W	142	96%
22	Y	67	93%
23	Z	80	95%
24	a	138	95%
25	b	126	73%
26	c	156	99%
27	d	175	98%
28	e	104	94%
29	f	49	94%
30	g	122	97%
31	h	105	95%
32	i	347	99%
33	j	115	95%

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Mol	Chain	Length	Quality of chain
34	k	98	 94% 6%
35	l	606	 98%
36	m	175	 15% 97%
37	n	56	 32% 98%
38	o	128	 6% 95% 5%
39	p	178	 8% 95% 5%
40	r	459	 98%
41	s	318	 97%
42	u	171	 5% 98%
43	v	124	 19% 96%
44	w	320	 9% 98%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 68209 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	433	3330	2103	593	614	20	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	176	1411	887	243	268	13	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	86	684	431	129	122	2	0	0

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			693	447	102	139	5		
6	X	88	Total	C	N	O	S	0	0
			693	448	103	137	5		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	690	Total	C	N	O	S	0	0
			5284	3314	923	1008	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	144	1200	767	217	212	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	217	1667	1062	280	315	10	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	e	104	856	548	142	162	4	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	f	49	377	246	65	66	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	g	122	1005	653	174	172	6	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	606	Total	C	N	O	S	0	0
			4797	3181	743	822	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	175	Total	C	N	O	S	0	0
			1276	850	187	226	13		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	178	Total	C	N	O	S	0	0
			1530	979	278	265	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
			3624	2406	572	608	38		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			1036	646	196	185	9		

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

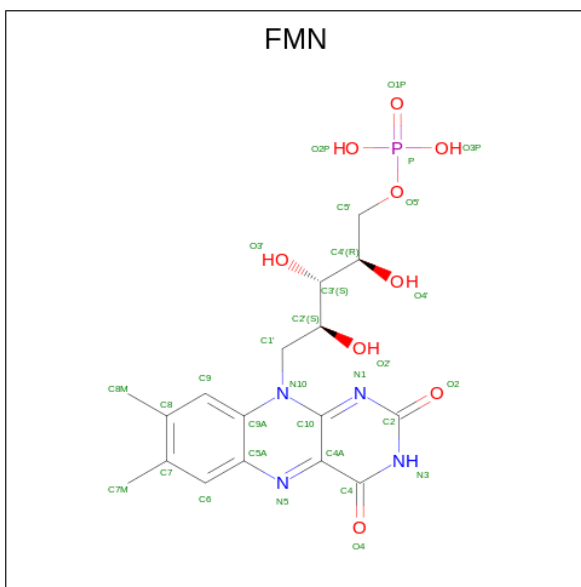
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2586	1646	439	491	10		

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



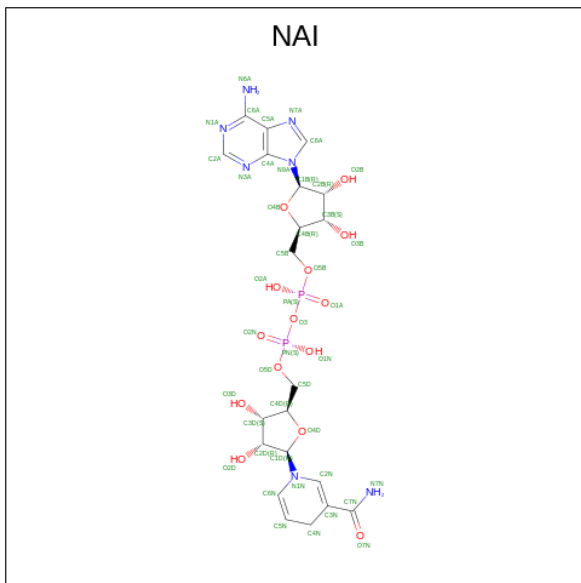
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	A	1	8	4	4	0
45	B	1	16	8	8	0
45	B	1	16	8	8	0
45	C	1	8	4	4	0
45	M	1	16	8	8	0
45	M	1	16	8	8	0

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



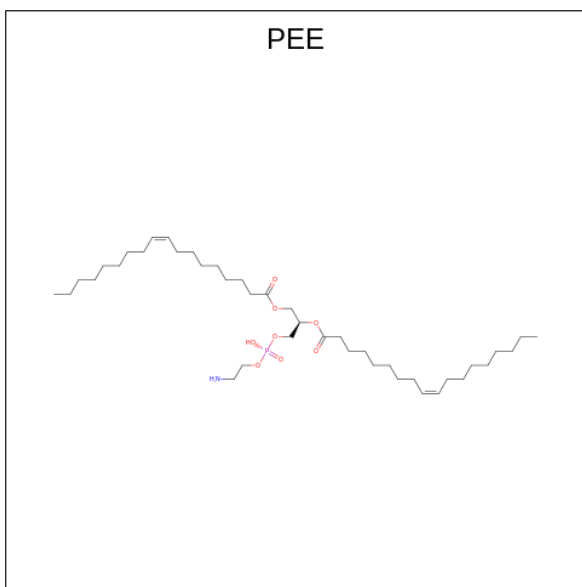
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	A	1	31	17	4	9	1	0

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



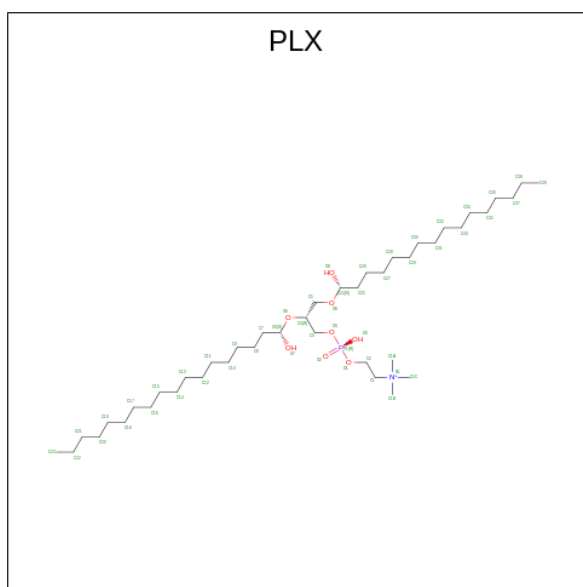
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	A	1	44	21	7	14	2	0

- Molecule 48 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



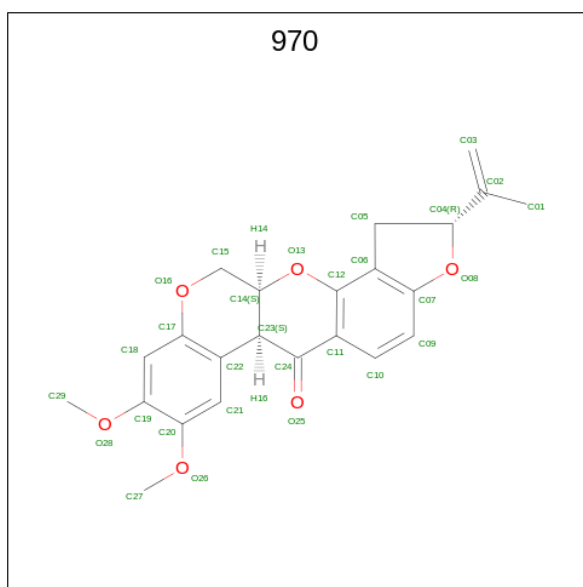
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	B	1	Total 51	C 41	N 1	O 8	P 1	0
48	C	1	Total 47	C 37	N 1	O 8	P 1	0
48	U	1	Total 51	C 41	N 1	O 8	P 1	0
48	W	1	Total 41	C 31	N 1	O 8	P 1	0
48	i	1	Total 47	C 37	N 1	O 8	P 1	0
48	j	1	Total 41	C 31	N 1	O 8	P 1	0
48	l	1	Total 96	C 76	N 2	O 16	P 2	0
48	l	1	Total 96	C 76	N 2	O 16	P 2	0
48	r	1	Total 51	C 41	N 1	O 8	P 1	0

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



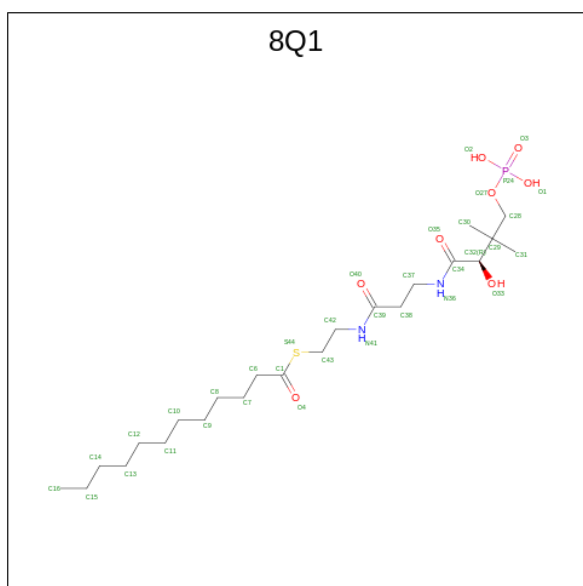
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	C	1	52	42	1	8	1	0
49	J	1	52	42	1	8	1	0
49	a	1	52	42	1	8	1	0
49	g	1	52	42	1	8	1	0
49	j	1	52	42	1	8	1	0
49	r	1	104	84	2	16	2	0
49	r	1	104	84	2	16	2	0

- Molecule 50 is (2R,6aS,12aS)-8,9-dimethoxy-2-(prop-1-en-2-yl)-1,2,12,12a-tetrahydrofuro[2',3':7,8][1]benzopyrano[2,3-c][1]benzopyran-6(6aH)-one (three-letter code: 970) (formula: C₂₃H₂₂O₆) (labeled as "Ligand of Interest" by depositor).



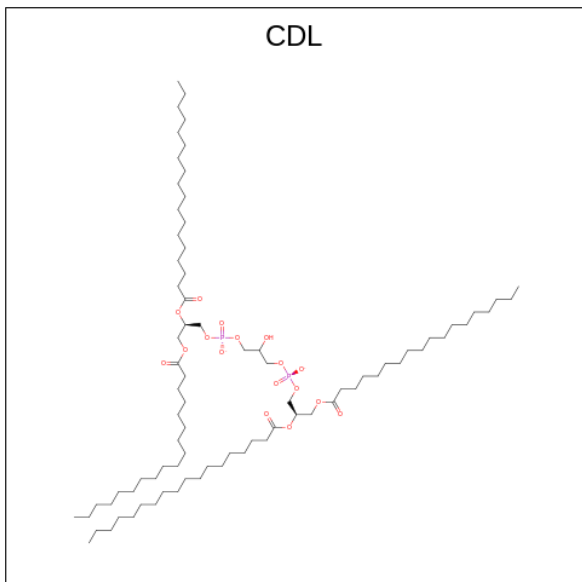
Mol	Chain	Residues	Atoms			AltConf
50	C	1	Total	C	O	0
			29	23	6	

- Molecule 51 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 52 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



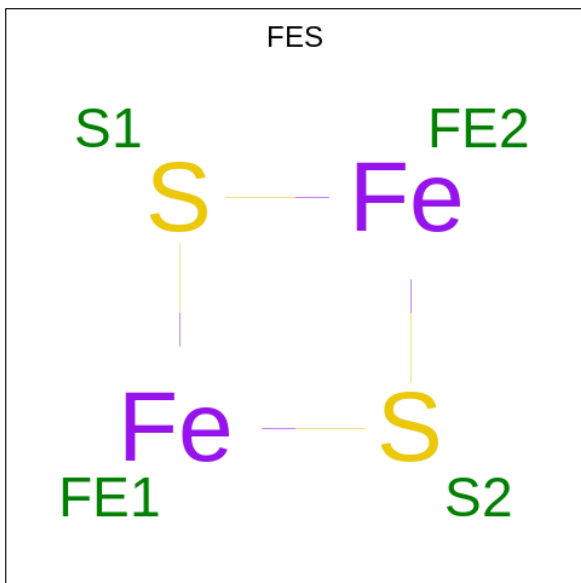
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
52	I	1	Total 51	C 32	O 17	P 2	0
52	V	1	Total 172	C 134	O 34	P 4	0
52	V	1	Total 172	C 134	O 34	P 4	0
52	a	1	Total 100	C 81	O 17	P 2	0
52	g	1	Total 55	C 36	O 17	P 2	0
52	i	1	Total 199	C 161	O 34	P 4	0
52	i	1	Total 199	C 161	O 34	P 4	0
52	l	1	Total 199	C 161	O 34	P 4	0
52	l	1	Total 199	C 161	O 34	P 4	0
52	o	1	Total 100	C 81	O 17	P 2	0
52	s	1	Total 89	C 70	O 17	P 2	0

- Molecule 53 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
54	s	1	38	34	4	0

- Molecule 55 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



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

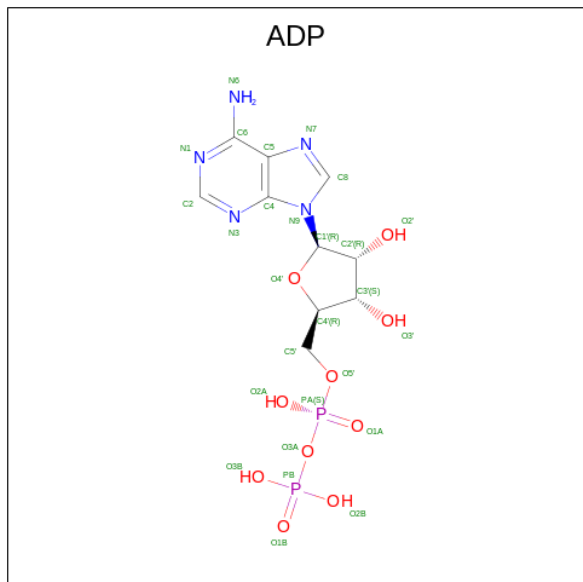
- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

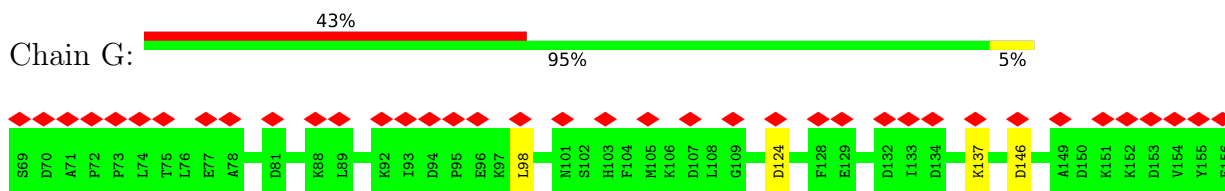
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
57	T	1	1	1	0

- Molecule 58 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).

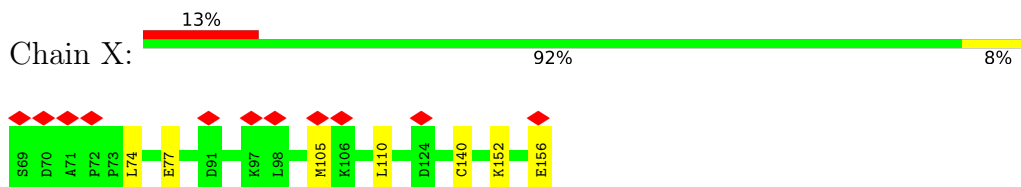


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	w	1	27	10	5	10	2	0

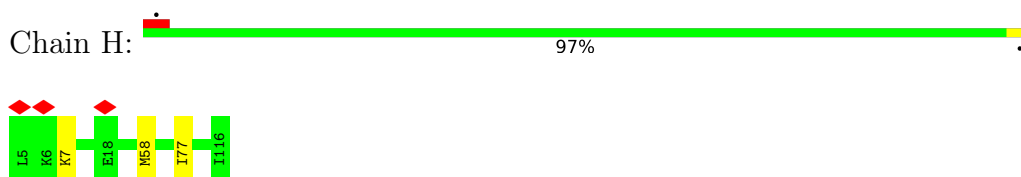
- Molecule 6: Acyl carrier protein



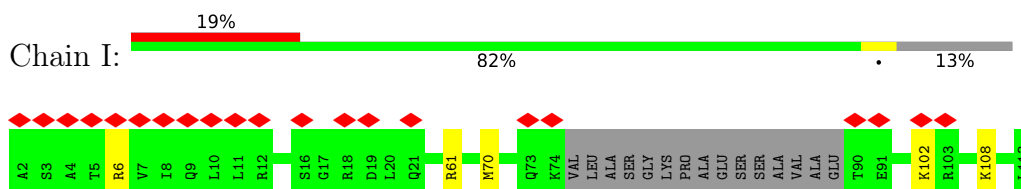
- Molecule 6: Acyl carrier protein



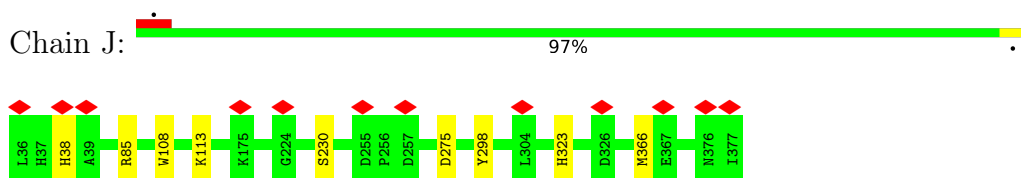
- Molecule 7: Complex I subunit B13



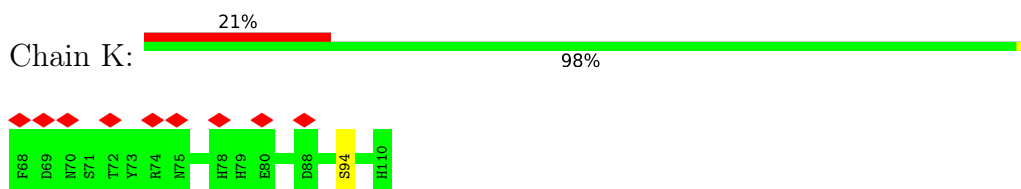
- Molecule 8: Complex I-B14.5a



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

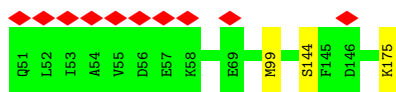


- Molecule 10: Complex I-9kD

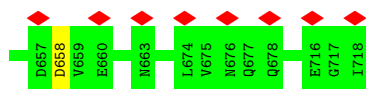
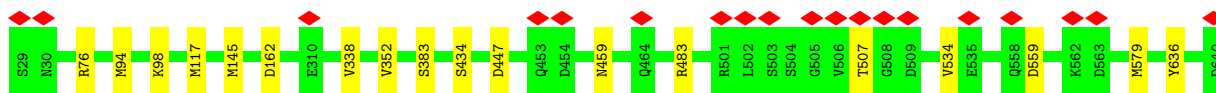


- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

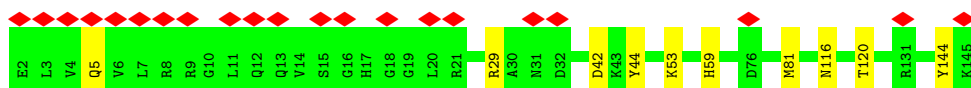
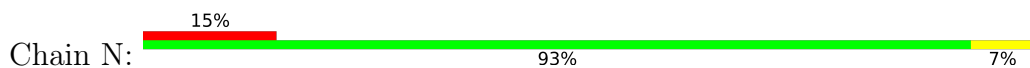




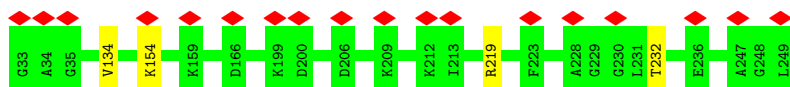
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



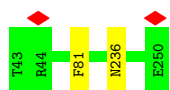
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



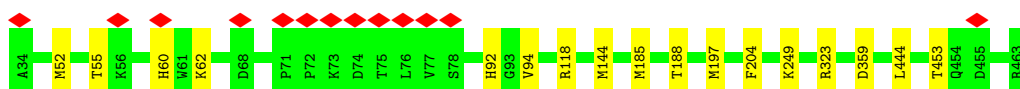
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 15: Complex I-30kD



- Molecule 16: Complex I-49kD

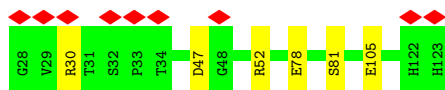


- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

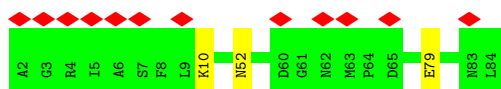




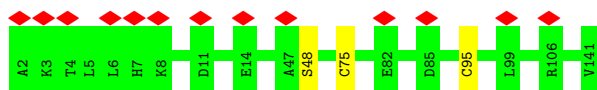
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



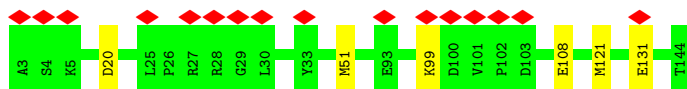
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



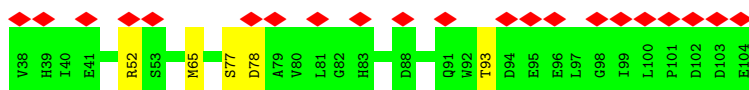
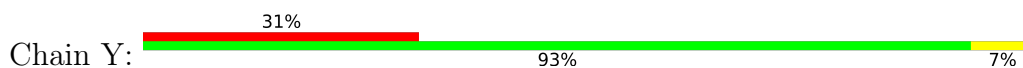
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



- Molecule 21: Complex I-B16.6



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



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




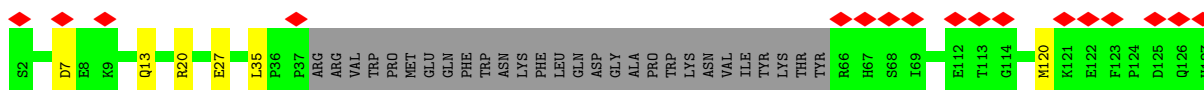
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:  95% 5%



- Molecule 25: Complex I-B17

Chain b:  13% 73% 5% 22%



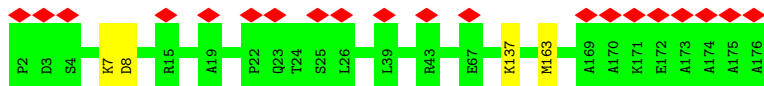
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c:  12% 99%



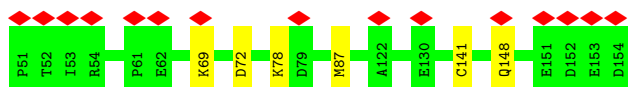
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d:  11% 98%

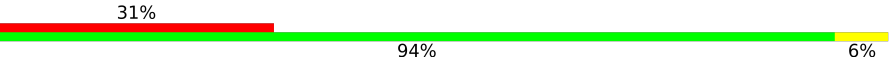


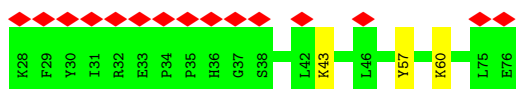
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e:  14% 94% 6%

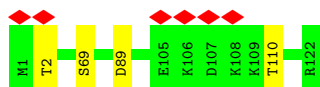


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

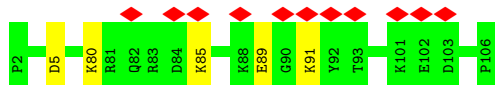
Chain f:  31% 94% 6%



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



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



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



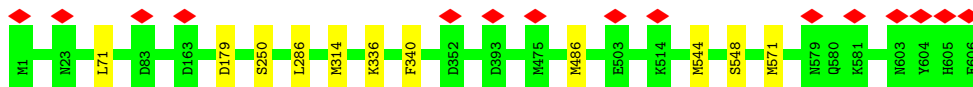
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3



- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L



- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

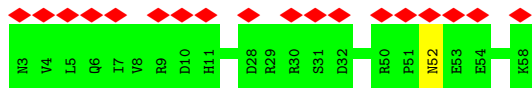


- Molecule 36: NADH-ubiquinone oxidoreductase chain 6





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



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



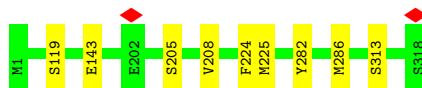
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



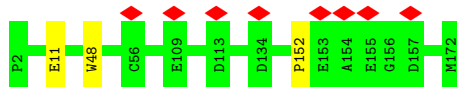
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4



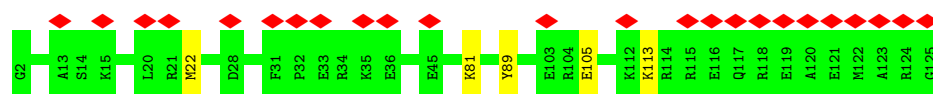
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1



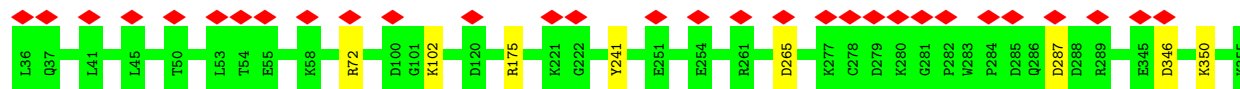
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 43: Complex I-B18



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63357	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	0.204	Depositor
Minimum map value	-0.134	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0336	Depositor
Map size (\AA)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, 970, ZN, NAI, PEE, 2MR, SF4, PLX, ADP, FES, CDL, NDP, MG, 8Q1, UQ

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	0/3406	0.50	0/4603
2	B	0.25	0/1442	0.50	0/1951
3	C	0.25	0/1279	0.51	0/1730
4	E	0.24	0/995	0.52	0/1340
5	F	0.27	0/695	0.61	0/936
6	G	0.25	0/705	0.47	0/956
6	X	0.25	0/705	0.42	0/955
7	H	0.23	0/929	0.42	0/1258
8	I	0.25	0/798	0.54	0/1079
9	J	0.25	0/2828	0.48	0/3834
10	K	0.24	0/377	0.48	0/509
11	L	0.25	0/1039	0.49	0/1403
12	M	0.24	0/5372	0.49	0/7279
13	N	0.24	0/1241	0.51	0/1690
14	O	0.24	0/1707	0.46	0/2324
15	P	0.25	0/1789	0.50	0/2436
16	Q	0.26	0/3538	0.48	0/4796
17	S	0.24	0/581	0.52	0/781
18	T	0.24	0/755	0.52	0/1018
19	U	0.25	0/664	0.44	0/912
20	V	0.24	0/1042	0.45	0/1411
21	W	0.26	0/1192	0.51	0/1610
22	Y	0.25	0/610	0.46	0/836
23	Z	0.27	0/660	0.49	0/892
24	a	0.26	0/1184	0.47	0/1603
25	b	0.26	0/844	0.51	0/1149
26	c	0.26	0/1371	0.48	0/1875
27	d	0.25	0/1494	0.50	0/2015
28	e	0.26	0/880	0.54	0/1196
29	f	0.24	0/385	0.42	0/522
30	g	0.25	0/1036	0.46	0/1401
31	h	0.24	0/889	0.49	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.25	0/2773	0.45	0/3768
33	j	0.25	0/938	0.42	0/1281
34	k	0.24	0/759	0.41	0/1029
35	l	0.26	0/4926	0.46	0/6700
36	m	0.27	0/1307	0.49	0/1777
37	n	0.24	0/491	0.49	0/663
38	o	0.25	0/1092	0.50	0/1481
39	p	0.25	0/1586	0.50	1/2151 (0.0%)
40	r	0.24	0/3715	0.42	0/5067
41	s	0.26	0/2581	0.45	0/3529
42	u	0.26	0/1436	0.48	0/1938
43	v	0.28	0/1060	0.53	0/1421
44	w	0.25	0/2646	0.47	0/3584
All	All	0.25	0/67742	0.48	1/91879 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	p	109	PRO	CA-N-CD	-5.54	103.75	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/433 (100%)	418 (97%)	13 (3%)	0	100	100
2	B	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
3	C	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
4	E	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
5	F	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
6	G	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
6	X	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
7	H	110/112 (98%)	104 (94%)	5 (4%)	1 (1%)	17	55
8	I	93/112 (83%)	83 (89%)	10 (11%)	0	100	100
9	J	340/342 (99%)	330 (97%)	9 (3%)	1 (0%)	41	76
10	K	41/43 (95%)	41 (100%)	0	0	100	100
11	L	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
12	M	688/690 (100%)	672 (98%)	16 (2%)	0	100	100
13	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
14	O	215/217 (99%)	205 (95%)	10 (5%)	0	100	100
15	P	206/208 (99%)	199 (97%)	7 (3%)	0	100	100
16	Q	427/430 (99%)	411 (96%)	16 (4%)	0	100	100
17	S	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
18	T	94/96 (98%)	94 (100%)	0	0	100	100
19	U	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
20	V	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
21	W	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
22	Y	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
23	Z	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
24	a	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
25	b	94/126 (75%)	89 (95%)	5 (5%)	0	100	100
26	c	154/156 (99%)	142 (92%)	12 (8%)	0	100	100
27	d	173/175 (99%)	171 (99%)	2 (1%)	0	100	100
28	e	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
29	f	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
30	g	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
31	h	103/105 (98%)	100 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	i	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
33	j	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
34	k	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
35	l	604/606 (100%)	588 (97%)	16 (3%)	0	100	100
36	m	173/175 (99%)	162 (94%)	11 (6%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
39	p	176/178 (99%)	170 (97%)	6 (3%)	0	100	100
40	r	457/459 (100%)	454 (99%)	3 (1%)	0	100	100
41	s	316/318 (99%)	308 (98%)	7 (2%)	1 (0%)	41	76
42	u	169/171 (99%)	166 (98%)	2 (1%)	1 (1%)	25	64
43	v	122/124 (98%)	118 (97%)	4 (3%)	0	100	100
44	w	318/320 (99%)	307 (96%)	11 (4%)	0	100	100
All	All	8175/8313 (98%)	7919 (97%)	252 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	38	HIS
7	H	77	ILE
41	s	208	VAL
42	u	152	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/346 (100%)	332 (96%)	14 (4%)	31	68
2	B	150/151 (99%)	146 (97%)	4 (3%)	44	77
3	C	132/132 (100%)	124 (94%)	8 (6%)	18	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	107/107 (100%)	102 (95%)	5 (5%)	26	63
5	F	74/76 (97%)	68 (92%)	6 (8%)	11	40
6	G	76/81 (94%)	72 (95%)	4 (5%)	22	58
6	X	76/81 (94%)	69 (91%)	7 (9%)	9	34
7	H	99/99 (100%)	97 (98%)	2 (2%)	55	83
8	I	87/97 (90%)	82 (94%)	5 (6%)	20	56
9	J	296/296 (100%)	288 (97%)	8 (3%)	44	77
10	K	42/42 (100%)	41 (98%)	1 (2%)	49	79
11	L	113/113 (100%)	110 (97%)	3 (3%)	44	77
12	M	576/580 (99%)	557 (97%)	19 (3%)	38	73
13	N	129/130 (99%)	119 (92%)	10 (8%)	12	42
14	O	182/183 (100%)	178 (98%)	4 (2%)	52	81
15	P	190/190 (100%)	188 (99%)	2 (1%)	73	90
16	Q	370/370 (100%)	354 (96%)	16 (4%)	29	66
17	S	57/58 (98%)	57 (100%)	0	100	100
18	T	79/79 (100%)	73 (92%)	6 (8%)	13	43
19	U	69/69 (100%)	66 (96%)	3 (4%)	29	66
20	V	101/101 (100%)	98 (97%)	3 (3%)	41	75
21	W	121/123 (98%)	115 (95%)	6 (5%)	24	60
22	Y	62/62 (100%)	57 (92%)	5 (8%)	11	40
23	Z	62/62 (100%)	58 (94%)	4 (6%)	17	50
24	a	121/121 (100%)	114 (94%)	7 (6%)	20	55
25	b	90/119 (76%)	84 (93%)	6 (7%)	16	49
26	c	141/141 (100%)	139 (99%)	2 (1%)	67	88
27	d	155/155 (100%)	151 (97%)	4 (3%)	46	78
28	e	93/96 (97%)	87 (94%)	6 (6%)	17	50
29	f	35/45 (78%)	32 (91%)	3 (9%)	10	37
30	g	108/109 (99%)	104 (96%)	4 (4%)	34	70
31	h	93/93 (100%)	88 (95%)	5 (5%)	22	57
32	i	311/311 (100%)	306 (98%)	5 (2%)	62	86
33	j	100/100 (100%)	94 (94%)	6 (6%)	19	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	k	85/85 (100%)	79 (93%)	6 (7%)	14	46
35	l	536/540 (99%)	525 (98%)	11 (2%)	53	82
36	m	127/141 (90%)	121 (95%)	6 (5%)	26	63
37	n	53/53 (100%)	52 (98%)	1 (2%)	57	84
38	o	113/113 (100%)	106 (94%)	7 (6%)	18	52
39	p	158/159 (99%)	150 (95%)	8 (5%)	24	60
40	r	409/410 (100%)	400 (98%)	9 (2%)	52	81
41	s	275/275 (100%)	267 (97%)	8 (3%)	42	76
42	u	153/153 (100%)	151 (99%)	2 (1%)	69	89
43	v	106/111 (96%)	101 (95%)	5 (5%)	26	63
44	w	282/283 (100%)	274 (97%)	8 (3%)	43	77
All	All	7140/7241 (99%)	6876 (96%)	264 (4%)	37	70

All (264) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	52	ARG
1	A	61	ASP
1	A	74	ASP
1	A	106	SER
1	A	119	GLU
1	A	125	CYS
1	A	174	ARG
1	A	334	THR
1	A	357	MET
1	A	403	ASP
1	A	425	CYS
1	A	448	GLU
1	A	456	GLN
2	B	44	ARG
2	B	50	MET
2	B	68	ARG
2	B	75	SER
3	C	49	LYS
3	C	66	THR
3	C	71	CYS
3	C	79	MET

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Mol	Chain	Res	Type
3	C	86	MET
3	C	142	TYR
3	C	154	ASP
3	C	195	ARG
4	E	57	LYS
4	E	80	ASP
4	E	89	GLU
4	E	100	ARG
4	E	116	THR
5	F	27	SER
5	F	46	LYS
5	F	57	GLU
5	F	64	LYS
5	F	65	LEU
5	F	89	ARG
6	G	98	LEU
6	G	124	ASP
6	G	137	LYS
6	G	146	ASP
7	H	7	LYS
7	H	58	MET
8	I	6	ARG
8	I	61	ARG
8	I	70	MET
8	I	102	LYS
8	I	108	LYS
9	J	85	ARG
9	J	108	TRP
9	J	113	LYS
9	J	230	SER
9	J	275	ASP
9	J	298	TYR
9	J	323	HIS
9	J	366	MET
10	K	94	SER
11	L	99	MET
11	L	144	SER
11	L	175	LYS
12	M	76	ARG
12	M	94	MET
12	M	98	LYS
12	M	117	MET

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Mol	Chain	Res	Type
12	M	145	MET
12	M	162	ASP
12	M	338	VAL
12	M	352	VAL
12	M	383	SER
12	M	434	SER
12	M	447	ASP
12	M	459	ASN
12	M	483	ARG
12	M	507	THR
12	M	534	VAL
12	M	559	ASP
12	M	579	MET
12	M	636	TYR
12	M	658	ASP
13	N	5	GLN
13	N	29	ARG
13	N	42	ASP
13	N	44	TYR
13	N	53	LYS
13	N	59	HIS
13	N	81	MET
13	N	116	ASN
13	N	120	THR
13	N	144	TYR
14	O	134	VAL
14	O	154	LYS
14	O	219	ARG
14	O	232	THR
15	P	81	PHE
15	P	236	ASN
16	Q	52	MET
16	Q	55	THR
16	Q	60	HIS
16	Q	62	LYS
16	Q	92	HIS
16	Q	94	VAL
16	Q	144	MET
16	Q	185	MET
16	Q	188	THR
16	Q	197	MET
16	Q	204	PHE

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Mol	Chain	Res	Type
16	Q	249	LYS
16	Q	323	ARG
16	Q	359	ASP
16	Q	444	LEU
16	Q	453	THR
18	T	30	ARG
18	T	47	ASP
18	T	52	ARG
18	T	78	GLU
18	T	81	SER
18	T	105	GLU
19	U	10	LYS
19	U	52	ASN
19	U	79	GLU
20	V	48	SER
20	V	75	CYS
20	V	95	CYS
21	W	20	ASP
21	W	51	MET
21	W	99	LYS
21	W	108	GLU
21	W	121	MET
21	W	131	GLU
6	X	74	LEU
6	X	77	GLU
6	X	105	MET
6	X	110	LEU
6	X	140	CYS
6	X	152	LYS
6	X	156	GLU
22	Y	52	ARG
22	Y	65	MET
22	Y	77	SER
22	Y	78	ASP
22	Y	93	THR
23	Z	14	MET
23	Z	30	GLU
23	Z	42	ARG
23	Z	73	TRP
24	a	52	LYS
24	a	98	LEU
24	a	100	ASP

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Mol	Chain	Res	Type
24	a	103	GLU
24	a	127	ASP
24	a	158	ARG
24	a	176	LYS
25	b	7	ASP
25	b	13	GLN
25	b	20	ARG
25	b	27	GLU
25	b	35	LEU
25	b	120	MET
26	c	96	ASP
26	c	156	VAL
27	d	7	LYS
27	d	8	ASP
27	d	137	LYS
27	d	163	MET
28	e	69	LYS
28	e	72	ASP
28	e	78	LYS
28	e	87	MET
28	e	141	CYS
28	e	148	GLN
29	f	43	LYS
29	f	57	TYR
29	f	60	LYS
30	g	2	THR
30	g	69	SER
30	g	89	ASP
30	g	110	THR
31	h	5	ASP
31	h	80	LYS
31	h	85	LYS
31	h	89	GLU
31	h	91	LYS
32	i	159	MET
32	i	194	LEU
32	i	244	MET
32	i	313	MET
32	i	323	MET
33	j	1	MET
33	j	44	MET
33	j	82	ASN

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Mol	Chain	Res	Type
33	j	83	ASN
33	j	87	MET
33	j	101	SER
34	k	10	MET
34	k	24	SER
34	k	37	MET
34	k	53	PHE
34	k	59	MET
34	k	76	SER
35	l	71	LEU
35	l	179	ASP
35	l	250	SER
35	l	286	LEU
35	l	314	MET
35	l	336	LYS
35	l	340	PHE
35	l	486	MET
35	l	544	MET
35	l	548	SER
35	l	571	MET
36	m	1	MET
36	m	85	SER
36	m	87	LYS
36	m	98	MET
36	m	135	PHE
36	m	169	MET
37	n	52	ASN
38	o	30	ARG
38	o	37	LEU
38	o	41	SER
38	o	44	LYS
38	o	85	LYS
38	o	106	LYS
38	o	121	LEU
39	p	38	ARG
39	p	54	GLU
39	p	110	SER
39	p	115	TYR
39	p	132	SER
39	p	138	LYS
39	p	141	GLN
39	p	150	ARG

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Mol	Chain	Res	Type
40	r	60	SER
40	r	130	LEU
40	r	139	GLN
40	r	140	THR
40	r	248	THR
40	r	263	MET
40	r	290	SER
40	r	304	GLN
40	r	420	THR
41	s	119	SER
41	s	143	GLU
41	s	205	SER
41	s	224	PHE
41	s	225	MET
41	s	282	TYR
41	s	286	MET
41	s	313	SER
42	u	11	GLU
42	u	48	TRP
43	v	22	MET
43	v	81	LYS
43	v	89	TYR
43	v	105	GLU
43	v	113	LYS
44	w	72	ARG
44	w	102	LYS
44	w	175	ARG
44	w	241	TYR
44	w	265	ASP
44	w	287	ASP
44	w	346	ASP
44	w	350	LYS

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

Mol	Chain	Res	Type
12	M	278	HIS
18	T	123	HIS
22	Y	83	HIS
31	h	97	HIS
31	h	98	HIS
32	i	204	ASN

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Mol	Chain	Res	Type
35	l	59	GLN
37	n	14	HIS
40	r	251	ASN
44	w	132	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	2MR	Q	118	16	10,12,13	1.99	1 (10%)	5,13,15	5.82	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	5.75	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	11.89	130.38	119.48
16	Q	118	2MR	CD-NE-CZ	4.07	131.03	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.20	130.94	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 46 ligands modelled in this entry, 2 are monoatomic - leaving 44 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	$\# Z > 2$
51	8Q1	X	201	-	31,34,34	1.70	6 (19%)	40,43,43	1.52	4 (10%)
49	PLX	a	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.61	1 (1%)
48	PEE	B	303	-	50,50,50	1.17	6 (12%)	53,55,55	0.97	2 (3%)
48	PEE	l	703	-	49,49,50	1.17	6 (12%)	52,54,55	0.95	2 (3%)
45	SF4	C	301	3	0,12,12	-	-	-	-	-
47	NAI	A	503	-	42,48,48	4.94	19 (45%)	47,73,73	1.32	7 (14%)
52	CDL	I	201	-	50,50,99	1.41	8 (16%)	56,62,111	1.12	4 (7%)
48	PEE	l	704	-	45,45,50	1.22	6 (13%)	48,50,55	1.00	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	PLX	r	503	-	51,51,51	1.15	4 (7%)	55,59,59	0.55	1 (1%)
53	NDP	J	401	-	45,52,52	4.56	20 (44%)	53,80,80	2.04	7 (13%)
51	8Q1	G	201	6	31,34,34	1.70	6 (19%)	40,43,43	1.55	6 (15%)
49	PLX	J	403	-	51,51,51	1.14	4 (7%)	55,59,59	0.61	1 (1%)
50	970	C	304	-	33,33,33	4.92	16 (48%)	48,50,50	2.53	18 (37%)
48	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	0.96	2 (3%)
48	PEE	C	302	-	46,46,50	1.21	6 (13%)	49,51,55	0.97	2 (4%)
48	PEE	i	402	-	46,46,50	1.21	6 (13%)	49,51,55	0.97	2 (4%)
52	CDL	V	201	-	93,93,99	1.12	9 (9%)	99,105,111	0.85	4 (4%)
49	PLX	r	502	-	51,51,51	1.16	5 (9%)	55,59,59	0.59	1 (1%)
52	CDL	o	201	-	99,99,99	1.09	9 (9%)	105,111,111	0.87	4 (3%)
52	CDL	a	201	-	99,99,99	1.09	8 (8%)	105,111,111	0.84	4 (3%)
52	CDL	s	401	-	88,88,99	1.14	9 (10%)	94,100,111	0.91	4 (4%)
52	CDL	i	401	-	99,99,99	1.10	9 (9%)	105,111,111	0.84	4 (3%)
48	PEE	j	201	-	40,40,50	1.15	5 (12%)	43,45,55	1.01	2 (4%)
52	CDL	l	702	-	99,99,99	1.09	9 (9%)	105,111,111	0.89	4 (3%)
49	PLX	j	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.60	1 (1%)
55	FES	M	803	12	0,4,4	-	-	-	-	-
45	SF4	M	802	12	0,12,12	-	-	-	-	-
45	SF4	A	501	1	0,12,12	-	-	-	-	-
45	SF4	B	302	2	0,12,12	-	-	-	-	-
52	CDL	l	701	-	98,98,99	1.09	8 (8%)	104,110,111	0.88	4 (3%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
54	UQ	J	402	-	33,33,63	3.47	8 (24%)	40,43,79	2.70	14 (35%)
48	PEE	U	101	-	50,50,50	1.16	6 (12%)	53,55,55	0.91	2 (3%)
49	PLX	g	201	-	51,51,51	1.14	4 (7%)	55,59,59	0.62	1 (1%)
52	CDL	i	403	-	98,98,99	1.10	9 (9%)	104,110,111	0.86	4 (3%)
54	UQ	s	402	-	38,38,63	3.54	9 (23%)	46,49,79	2.85	16 (34%)
46	FMN	A	502	-	33,33,33	1.07	2 (6%)	48,50,50	1.22	7 (14%)
52	CDL	V	202	-	77,77,99	1.20	7 (9%)	83,89,111	0.97	4 (4%)
55	FES	O	301	14	0,4,4	-	-	-	-	-
49	PLX	C	303	-	51,51,51	1.16	4 (7%)	55,59,59	0.60	1 (1%)
58	ADP	w	401	-	24,29,29	3.12	6 (25%)	29,45,45	1.46	4 (13%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-
48	PEE	W	201	-	40,40,50	1.16	5 (12%)	43,45,55	0.97	2 (4%)
52	CDL	g	202	-	54,54,99	1.37	8 (14%)	60,66,111	1.13	4 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	8Q1	X	201	-	-	16/41/41/41	-
49	PLX	a	202	-	-	32/55/55/55	-
48	PEE	B	303	-	-	26/54/54/54	-
48	PEE	l	703	-	-	27/53/53/54	-
45	SF4	C	301	3	-	-	0/6/5/5
47	NAI	A	503	-	-	10/25/72/72	0/5/5/5
52	CDL	I	201	-	-	32/61/61/110	-
48	PEE	l	704	-	-	20/49/49/54	-
49	PLX	r	503	-	-	34/55/55/55	-
53	NDP	J	401	-	-	9/30/77/77	0/4/5/5
51	8Q1	G	201	6	-	16/41/41/41	-
49	PLX	J	403	-	-	29/55/55/55	-
50	970	C	304	-	-	2/8/41/41	0/5/5/5
48	PEE	r	501	-	-	32/54/54/54	-
48	PEE	C	302	-	-	29/50/50/54	-
48	PEE	i	402	-	-	29/50/50/54	-
52	CDL	V	201	-	-	55/104/104/110	-
49	PLX	r	502	-	-	32/55/55/55	-
52	CDL	o	201	-	-	56/110/110/110	-
52	CDL	a	201	-	-	64/110/110/110	-
52	CDL	s	401	-	-	50/99/99/110	-
52	CDL	i	401	-	-	56/110/110/110	-
48	PEE	j	201	-	-	24/44/44/54	-
52	CDL	l	702	-	-	54/110/110/110	-
49	PLX	j	202	-	-	31/55/55/55	-
55	FES	M	803	12	-	-	0/1/1/1
45	SF4	A	501	1	-	-	0/6/5/5
45	SF4	M	802	12	-	-	0/6/5/5
45	SF4	B	302	2	-	-	0/6/5/5
52	CDL	l	701	-	-	52/109/109/110	-
45	SF4	B	301	2	-	-	0/6/5/5
54	UQ	J	402	-	-	10/27/51/87	0/1/1/1
48	PEE	U	101	-	-	22/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	PLX	g	201	-	-	37/55/55/55	-
52	CDL	i	403	-	-	62/109/109/110	-
54	UQ	s	402	-	-	12/33/57/87	0/1/1/1
46	FMN	A	502	-	-	6/18/18/18	0/3/3/3
52	CDL	V	202	-	-	51/88/88/110	-
55	FES	O	301	14	-	-	0/1/1/1
49	PLX	C	303	-	-	23/55/55/55	-
58	ADP	w	401	-	-	3/12/32/32	0/3/3/3
45	SF4	M	801	12	-	-	0/6/5/5
48	PEE	W	201	-	-	20/44/44/54	-
52	CDL	g	202	-	-	34/65/65/110	-

All (266) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	C	304	970	O16-C17	17.90	1.57	1.37
47	A	503	NAI	O4B-C1B	16.27	1.63	1.41
47	A	503	NAI	C2B-C1B	-15.37	1.30	1.53
53	J	401	NDP	C3B-C2B	-12.77	1.24	1.52
53	J	401	NDP	C6N-C5N	12.48	1.55	1.33
50	C	304	970	O25-C24	11.10	1.37	1.22
53	J	401	NDP	O4D-C4D	10.66	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.27	1.26	1.53
50	C	304	970	C23-C24	10.19	1.63	1.52
53	J	401	NDP	C3D-C4D	-9.82	1.27	1.53
54	J	402	UQ	C18-C19	9.67	1.56	1.33
54	s	402	UQ	C18-C19	9.60	1.56	1.33
54	J	402	UQ	C13-C14	9.39	1.55	1.33
54	s	402	UQ	C13-C14	9.30	1.55	1.33
54	s	402	UQ	C23-C24	9.01	1.54	1.33
54	s	402	UQ	C8-C9	8.95	1.54	1.33
58	w	401	ADP	C3'-C4'	-8.90	1.30	1.53
54	J	402	UQ	C8-C9	8.90	1.54	1.33
53	J	401	NDP	O4B-C1B	8.35	1.52	1.41
47	A	503	NAI	O4B-C4B	-8.18	1.26	1.45
53	J	401	NDP	O4B-C4B	-7.93	1.27	1.45
54	J	402	UQ	C23-C24	7.80	1.54	1.32
58	w	401	ADP	O4'-C4'	7.75	1.62	1.45
54	s	402	UQ	C28-C29	7.69	1.54	1.32
47	A	503	NAI	C2D-C1D	-7.46	1.29	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	J	401	NDP	C2N-C3N	7.34	1.55	1.34
50	C	304	970	C14-C23	-6.97	1.46	1.52
47	A	503	NAI	O4D-C4D	6.94	1.60	1.45
58	w	401	ADP	O4'-C1'	-6.87	1.31	1.41
50	C	304	970	O08-C07	6.42	1.47	1.37
47	A	503	NAI	C2D-C3D	5.96	1.69	1.53
47	A	503	NAI	C7N-N7N	5.74	1.48	1.33
53	J	401	NDP	P2B-O2B	5.71	1.70	1.59
47	A	503	NAI	O4D-C1D	5.53	1.55	1.42
53	J	401	NDP	C3B-C4B	5.53	1.67	1.53
51	G	201	8Q1	C34-N36	5.48	1.45	1.33
51	X	201	8Q1	C34-N36	5.46	1.45	1.33
51	X	201	8Q1	C39-N41	5.38	1.45	1.33
51	G	201	8Q1	C39-N41	5.36	1.45	1.33
50	C	304	970	O13-C12	5.23	1.45	1.37
47	A	503	NAI	C4N-C3N	-5.03	1.40	1.49
50	C	304	970	C05-C04	-4.99	1.47	1.54
53	J	401	NDP	O4D-C1D	-4.94	1.30	1.42
53	J	401	NDP	C6N-N1N	4.86	1.49	1.37
50	C	304	970	C03-C02	4.72	1.53	1.34
47	A	503	NAI	O2B-C2B	4.57	1.53	1.43
53	J	401	NDP	C7N-N7N	4.22	1.44	1.33
53	J	401	NDP	O2D-C2D	-4.15	1.33	1.43
53	J	401	NDP	C6A-N6A	4.12	1.49	1.34
47	A	503	NAI	C6N-C5N	3.99	1.40	1.33
46	A	502	FMN	C4A-N5	3.86	1.38	1.30
58	w	401	ADP	C6-N6	3.85	1.48	1.34
48	B	303	PEE	C18-C19	3.74	1.53	1.31
48	l	703	PEE	C18-C19	3.74	1.53	1.31
48	W	201	PEE	C18-C19	3.74	1.53	1.31
48	j	201	PEE	C18-C19	3.74	1.53	1.31
48	r	501	PEE	C18-C19	3.74	1.53	1.31
48	C	302	PEE	C18-C19	3.74	1.53	1.31
48	i	402	PEE	C18-C19	3.74	1.53	1.31
48	U	101	PEE	C18-C19	3.73	1.53	1.31
48	l	704	PEE	C18-C19	3.72	1.53	1.31
48	U	101	PEE	C39-C38	3.67	1.53	1.31
48	r	501	PEE	C39-C38	3.67	1.53	1.31
48	B	303	PEE	C39-C38	3.65	1.53	1.31
48	l	704	PEE	C39-C38	3.65	1.53	1.31
48	C	302	PEE	C39-C38	3.65	1.52	1.31
48	l	703	PEE	C39-C38	3.65	1.52	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	i	402	PEE	C39-C38	3.64	1.52	1.31
47	A	503	NAI	C7N-C3N	3.61	1.56	1.48
47	A	503	NAI	C6A-N6A	3.61	1.47	1.34
52	V	202	CDL	OA8-CA7	3.50	1.43	1.33
52	I	201	CDL	OA8-CA7	3.49	1.43	1.33
52	i	401	CDL	OA8-CA7	3.49	1.43	1.33
52	g	202	CDL	OA8-CA7	3.47	1.43	1.33
52	V	201	CDL	OA8-CA7	3.46	1.43	1.33
52	a	201	CDL	OA8-CA7	3.44	1.43	1.33
52	o	201	CDL	OA8-CA7	3.44	1.43	1.33
52	i	403	CDL	OA8-CA7	3.42	1.43	1.33
52	l	701	CDL	OA8-CA7	3.42	1.43	1.33
52	s	401	CDL	OA8-CA7	3.42	1.43	1.33
52	l	702	CDL	OA8-CA7	3.39	1.43	1.33
50	C	304	970	C15-C14	3.38	1.57	1.51
50	C	304	970	C11-C24	3.33	1.54	1.48
47	A	503	NAI	C4N-C5N	-3.32	1.40	1.48
58	w	401	ADP	O2'-C2'	-3.30	1.35	1.43
52	V	202	CDL	OA6-CA5	3.27	1.43	1.34
50	C	304	970	O16-C15	3.13	1.52	1.44
52	V	201	CDL	OA6-CA5	3.13	1.43	1.34
58	w	401	ADP	O3'-C3'	3.12	1.50	1.43
53	J	401	NDP	O3D-C3D	3.10	1.50	1.43
52	s	401	CDL	OB6-CB5	3.10	1.43	1.34
52	l	701	CDL	OB6-CB5	3.08	1.43	1.34
52	l	702	CDL	OB8-CB7	3.07	1.42	1.33
52	i	403	CDL	OB6-CB5	3.07	1.43	1.34
52	V	202	CDL	OB6-CB5	3.06	1.42	1.34
52	l	702	CDL	OB6-CB5	3.05	1.42	1.34
52	l	701	CDL	OB8-CB7	3.05	1.42	1.33
52	i	403	CDL	OB8-CB7	3.04	1.42	1.33
53	J	401	NDP	C7N-C3N	3.04	1.55	1.48
52	g	202	CDL	OB8-CB7	3.04	1.42	1.33
52	I	201	CDL	OB8-CB7	3.03	1.42	1.33
52	i	401	CDL	OB8-CB7	3.03	1.42	1.33
52	V	202	CDL	OB8-CB7	3.02	1.42	1.33
52	a	201	CDL	OB6-CB5	3.02	1.42	1.34
52	a	201	CDL	OB8-CB7	3.02	1.42	1.33
52	o	201	CDL	OB6-CB5	3.02	1.42	1.34
52	s	401	CDL	OB8-CB7	3.02	1.42	1.33
52	o	201	CDL	OB8-CB7	3.01	1.42	1.33
52	V	201	CDL	OB6-CB5	3.00	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	V	201	CDL	OB8-CB7	3.00	1.42	1.33
52	l	702	CDL	OA6-CA5	3.00	1.42	1.34
52	I	201	CDL	OB6-CB5	2.99	1.42	1.34
52	g	202	CDL	OB6-CB5	2.99	1.42	1.34
52	i	401	CDL	OB6-CB5	2.99	1.42	1.34
52	o	201	CDL	OA6-CA5	2.99	1.42	1.34
52	s	401	CDL	OA6-CA5	2.98	1.42	1.34
52	i	401	CDL	OA6-CA5	2.98	1.42	1.34
52	i	403	CDL	OA6-CA5	2.97	1.42	1.34
52	a	201	CDL	OA6-CA5	2.95	1.42	1.34
52	g	202	CDL	OA6-CA5	2.94	1.42	1.34
52	I	201	CDL	OA6-CA5	2.92	1.42	1.34
52	l	701	CDL	OA6-CA5	2.88	1.42	1.34
50	C	304	970	C12-C06	2.86	1.44	1.39
54	J	402	UQ	C6-C1	2.81	1.54	1.46
54	s	402	UQ	C6-C1	2.77	1.54	1.46
49	C	303	PLX	O6-C4	-2.73	1.41	1.44
49	g	201	PLX	O6-C4	-2.72	1.41	1.44
49	r	503	PLX	O6-C4	-2.69	1.41	1.44
49	a	202	PLX	O6-C4	-2.66	1.41	1.44
50	C	304	970	C09-C07	2.64	1.45	1.39
49	r	502	PLX	O6-C4	-2.54	1.41	1.44
46	A	502	FMN	C10-N1	2.54	1.38	1.33
48	B	303	PEE	O3-C30	2.52	1.40	1.33
48	U	101	PEE	O3-C30	2.51	1.40	1.33
47	A	503	NAI	O3B-C3B	-2.50	1.37	1.43
49	j	202	PLX	O6-C4	-2.50	1.41	1.44
49	j	202	PLX	C7-C6	2.49	1.56	1.50
48	l	704	PEE	O3-C30	2.49	1.40	1.33
48	j	201	PEE	O3-C30	2.49	1.40	1.33
54	J	402	UQ	C7-C8	2.49	1.54	1.50
48	C	302	PEE	O3-C30	2.48	1.40	1.33
47	A	503	NAI	PN-O5D	2.47	1.69	1.59
48	l	703	PEE	O3-C30	2.47	1.40	1.33
54	s	402	UQ	C7-C8	2.47	1.54	1.50
49	J	403	PLX	O6-C4	-2.46	1.41	1.44
53	J	401	NDP	O2B-C2B	2.46	1.53	1.44
48	i	402	PEE	O3-C30	2.45	1.40	1.33
51	X	201	8Q1	C1-S44	2.45	1.82	1.76
48	W	201	PEE	O3-C30	2.44	1.40	1.33
48	r	501	PEE	O3-C30	2.44	1.40	1.33
48	C	302	PEE	O2-C2	-2.44	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	G	201	8Q1	C1-S44	2.42	1.82	1.76
52	l	701	CDL	OA6-CA4	-2.42	1.40	1.46
52	a	201	CDL	OA6-CA4	-2.42	1.40	1.46
48	j	201	PEE	O2-C2	-2.41	1.40	1.46
48	U	101	PEE	O2-C2	-2.40	1.40	1.46
48	i	402	PEE	O2-C2	-2.39	1.40	1.46
48	B	303	PEE	O2-C10	2.38	1.41	1.34
48	r	501	PEE	O2-C2	-2.37	1.40	1.46
52	i	401	CDL	OA6-CA4	-2.37	1.40	1.46
52	I	201	CDL	OA6-CA4	-2.37	1.40	1.46
52	g	202	CDL	OA6-CA4	-2.37	1.40	1.46
53	J	401	NDP	C2D-C3D	2.36	1.59	1.53
52	o	201	CDL	OA6-CA4	-2.36	1.40	1.46
48	l	704	PEE	O2-C2	-2.35	1.40	1.46
49	a	202	PLX	C7-C6	2.35	1.55	1.50
49	r	502	PLX	C7-C6	2.35	1.55	1.50
48	l	703	PEE	O2-C2	-2.34	1.40	1.46
48	W	201	PEE	O2-C2	-2.34	1.40	1.46
48	W	201	PEE	O2-C10	2.34	1.40	1.34
52	i	403	CDL	OA6-CA4	-2.34	1.40	1.46
52	l	702	CDL	OA6-CA4	-2.34	1.40	1.46
52	s	401	CDL	OA6-CA4	-2.32	1.40	1.46
49	r	503	PLX	C7-C6	2.32	1.55	1.50
49	C	303	PLX	C7-C6	2.32	1.55	1.50
48	B	303	PEE	O2-C2	-2.32	1.40	1.46
48	l	704	PEE	O2-C10	2.31	1.40	1.34
49	J	403	PLX	C7-C6	2.31	1.55	1.50
48	l	703	PEE	O2-C10	2.31	1.40	1.34
47	A	503	NAI	C5B-C4B	2.30	1.58	1.51
49	g	201	PLX	C7-C6	2.30	1.55	1.50
48	r	501	PEE	O2-C10	2.28	1.40	1.34
48	i	402	PEE	O2-C10	2.27	1.40	1.34
51	G	201	8Q1	C6-C1	2.26	1.53	1.50
52	g	202	CDL	PB2-OB2	2.25	1.68	1.59
52	o	201	CDL	PB2-OB2	2.25	1.68	1.59
52	V	201	CDL	PB2-OB2	2.23	1.68	1.59
52	i	401	CDL	PB2-OB2	2.23	1.68	1.59
52	a	201	CDL	PB2-OB2	2.23	1.68	1.59
48	C	302	PEE	O2-C10	2.22	1.40	1.34
52	i	401	CDL	OB6-CB4	-2.22	1.41	1.46
51	G	201	8Q1	O35-C34	-2.22	1.19	1.23
48	U	101	PEE	O2-C10	2.22	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	i	403	CDL	PB2-OB2	2.22	1.68	1.59
52	V	201	CDL	OB6-CB4	-2.22	1.41	1.46
52	V	201	CDL	PB2-OB5	2.21	1.68	1.59
51	G	201	8Q1	O40-C39	-2.21	1.18	1.23
52	l	702	CDL	PB2-OB5	2.21	1.68	1.59
52	l	701	CDL	PB2-OB2	2.21	1.68	1.59
52	a	201	CDL	PB2-OB5	2.21	1.68	1.59
52	l	702	CDL	PB2-OB2	2.21	1.68	1.59
52	l	701	CDL	PB2-OB5	2.21	1.68	1.59
52	s	401	CDL	PB2-OB5	2.21	1.68	1.59
52	V	202	CDL	PB2-OB2	2.20	1.68	1.59
52	g	202	CDL	PB2-OB5	2.20	1.68	1.59
48	j	201	PEE	O2-C10	2.20	1.40	1.34
52	s	401	CDL	PB2-OB2	2.19	1.68	1.59
52	i	401	CDL	PB2-OB5	2.19	1.68	1.59
51	X	201	8Q1	O40-C39	-2.19	1.18	1.23
52	I	201	CDL	PB2-OB2	2.19	1.68	1.59
51	X	201	8Q1	O35-C34	-2.19	1.19	1.23
50	C	304	970	O28-C19	2.18	1.40	1.37
52	V	202	CDL	OB6-CB4	-2.18	1.41	1.46
53	J	401	NDP	PA-O5B	2.18	1.68	1.59
52	i	403	CDL	PB2-OB5	2.18	1.68	1.59
52	I	201	CDL	PB2-OB5	2.18	1.68	1.59
49	r	502	PLX	P1-O4	2.17	1.68	1.59
54	s	402	UQ	O4-C4	-2.17	1.18	1.23
52	o	201	CDL	PB2-OB5	2.17	1.68	1.59
52	V	202	CDL	PB2-OB5	2.16	1.68	1.59
52	g	202	CDL	OB6-CB4	-2.16	1.41	1.46
52	I	201	CDL	OB6-CB4	-2.16	1.41	1.46
52	o	201	CDL	OB6-CB4	-2.16	1.41	1.46
49	C	303	PLX	P1-O4	2.16	1.68	1.59
49	j	202	PLX	P1-O4	2.16	1.68	1.59
54	J	402	UQ	O4-C4	-2.15	1.18	1.23
51	X	201	8Q1	C6-C1	2.15	1.53	1.50
52	a	201	CDL	OB6-CB4	-2.15	1.41	1.46
50	C	304	970	C04-C02	2.15	1.53	1.50
52	l	702	CDL	OB6-CB4	-2.14	1.41	1.46
49	J	403	PLX	P1-O4	2.14	1.67	1.59
49	g	201	PLX	P1-O4	2.13	1.67	1.59
49	a	202	PLX	P1-O4	2.13	1.67	1.59
52	l	701	CDL	OB6-CB4	-2.13	1.41	1.46
49	r	503	PLX	P1-O4	2.13	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	i	403	CDL	OB6-CB4	-2.11	1.41	1.46
53	J	401	NDP	O7N-C7N	-2.11	1.19	1.24
50	C	304	970	O26-C20	2.10	1.40	1.37
52	V	201	CDL	OA6-CA4	-2.10	1.41	1.46
48	W	201	PEE	O3-C3	-2.10	1.40	1.45
48	l	703	PEE	O3-C3	-2.09	1.40	1.45
48	l	704	PEE	O3-C3	-2.08	1.40	1.45
48	i	402	PEE	O3-C3	-2.08	1.40	1.45
48	C	302	PEE	O3-C3	-2.07	1.40	1.45
52	s	401	CDL	OB6-CB4	-2.07	1.41	1.46
49	r	502	PLX	P1-O1	2.06	1.67	1.59
49	j	202	PLX	P1-O1	2.06	1.67	1.59
48	r	501	PEE	O3-C3	-2.06	1.40	1.45
48	B	303	PEE	O3-C3	-2.05	1.40	1.45
49	J	403	PLX	P1-O1	2.05	1.67	1.59
49	r	502	PLX	C25-C24	2.05	1.55	1.50
49	r	503	PLX	P1-O1	2.05	1.67	1.59
49	a	202	PLX	P1-O1	2.04	1.67	1.59
49	g	201	PLX	P1-O1	2.04	1.67	1.59
48	j	201	PEE	O3-C3	-2.03	1.40	1.45
52	V	201	CDL	C11-CA5	2.03	1.56	1.50
52	l	702	CDL	C11-CA5	2.03	1.56	1.50
54	s	402	UQ	O1-C1	-2.02	1.19	1.23
49	C	303	PLX	P1-O1	2.02	1.67	1.59
52	i	403	CDL	C11-CA5	2.02	1.56	1.50
48	U	101	PEE	O3-C3	-2.02	1.40	1.45
54	J	402	UQ	C21-C19	2.02	1.55	1.51
52	s	401	CDL	C11-CA5	2.01	1.56	1.50
52	o	201	CDL	C11-CA5	2.01	1.56	1.50
47	A	503	NAI	C2N-C3N	2.01	1.40	1.34
52	i	401	CDL	C11-CA5	2.01	1.56	1.50

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	J	401	NDP	C3N-C2N-N1N	-8.97	110.30	123.10
54	s	402	UQ	C7-C8-C9	-8.13	113.26	126.79
50	C	304	970	O25-C24-C11	-7.98	109.19	121.98
54	J	402	UQ	C7-C8-C9	-7.12	114.94	126.79
50	C	304	970	O08-C07-C06	-6.85	108.82	113.00
53	J	401	NDP	C1D-N1N-C2N	-6.75	109.87	121.11
54	s	402	UQ	C22-C23-C24	-6.08	113.01	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	J	402	UQ	C17-C18-C19	-5.96	113.32	127.66
54	s	402	UQ	C17-C18-C19	-5.91	113.44	127.66
54	s	402	UQ	C12-C13-C14	-5.81	113.68	127.66
51	G	201	8Q1	C6-C1-S44	5.80	120.20	113.46
54	J	402	UQ	C12-C13-C14	-5.78	113.74	127.66
51	X	201	8Q1	C6-C1-S44	5.53	119.89	113.46
50	C	304	970	C06-C05-C04	5.49	106.37	101.45
53	J	401	NDP	C1D-N1N-C6N	-4.97	110.12	120.83
54	J	402	UQ	C10-C9-C8	-4.86	111.20	123.68
58	w	401	ADP	N3-C2-N1	-4.53	121.59	128.68
54	s	402	UQ	C10-C9-C8	-4.50	112.13	123.68
54	J	402	UQ	C22-C23-C24	-4.45	112.52	127.75
54	s	402	UQ	C27-C28-C29	-4.40	112.70	127.75
47	A	503	NAI	N3A-C2A-N1A	-4.35	121.88	128.68
50	C	304	970	C01-C02-C03	-4.24	111.18	121.38
52	l	702	CDL	OA6-CA5-C11	4.19	120.53	111.50
54	s	402	UQ	C26-C24-C23	-4.17	112.67	121.12
54	s	402	UQ	C25-C24-C23	-4.17	112.98	123.68
53	J	401	NDP	N3A-C2A-N1A	-4.15	122.20	128.68
48	j	201	PEE	O2-C10-C11	4.12	120.38	111.50
52	g	202	CDL	OB6-CB5-C51	4.11	120.37	111.50
54	J	402	UQ	C21-C19-C18	-4.11	112.81	121.12
52	l	702	CDL	OB6-CB5-C51	4.09	120.32	111.50
52	s	401	CDL	OA6-CA5-C11	4.07	120.27	111.50
48	l	704	PEE	O2-C10-C11	4.06	120.26	111.50
52	l	701	CDL	OB6-CB5-C51	4.06	120.25	111.50
54	J	402	UQ	C11-C9-C8	-4.05	112.92	121.12
48	B	303	PEE	O2-C10-C11	4.04	120.21	111.50
52	s	401	CDL	OB6-CB5-C51	4.04	120.21	111.50
54	s	402	UQ	C21-C19-C18	-4.02	112.98	121.12
48	r	501	PEE	O2-C10-C11	4.01	120.14	111.50
52	V	202	CDL	OB6-CB5-C51	3.99	120.11	111.50
52	g	202	CDL	OA6-CA5-C11	3.99	120.09	111.50
54	J	402	UQ	C20-C19-C18	-3.99	113.45	123.68
52	o	201	CDL	OA6-CA5-C11	3.98	120.08	111.50
52	l	701	CDL	OA6-CA5-C11	3.97	120.06	111.50
54	s	402	UQ	C20-C19-C18	-3.97	113.50	123.68
52	I	201	CDL	OB6-CB5-C51	3.96	120.04	111.50
52	i	401	CDL	OA6-CA5-C11	3.95	120.02	111.50
54	s	402	UQ	C16-C14-C13	-3.93	113.17	121.12
52	o	201	CDL	OB6-CB5-C51	3.92	119.95	111.50
52	i	403	CDL	OA6-CA5-C11	3.92	119.95	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	W	201	PEE	O2-C10-C11	3.92	119.94	111.50
48	C	302	PEE	O2-C10-C11	3.91	119.93	111.50
52	I	201	CDL	OA6-CA5-C11	3.90	119.90	111.50
52	i	403	CDL	OB6-CB5-C51	3.89	119.88	111.50
48	l	703	PEE	O2-C10-C11	3.88	119.86	111.50
52	a	201	CDL	OB6-CB5-C51	3.88	119.86	111.50
51	X	201	8Q1	C37-C38-C39	3.87	118.81	112.36
52	V	201	CDL	OB6-CB5-C51	3.82	119.73	111.50
48	i	402	PEE	O2-C10-C11	3.79	119.66	111.50
54	s	402	UQ	C15-C14-C13	-3.78	113.98	123.68
54	J	402	UQ	C15-C14-C13	-3.75	114.05	123.68
52	a	201	CDL	OA6-CA5-C11	3.75	119.58	111.50
50	C	304	970	O25-C24-C23	-3.74	115.62	121.00
52	V	201	CDL	OA6-CA5-C11	3.73	119.54	111.50
50	C	304	970	O08-C07-C09	3.71	131.44	123.89
54	s	402	UQ	C11-C9-C8	-3.67	113.69	121.12
52	i	401	CDL	OB6-CB5-C51	3.64	119.34	111.50
48	U	101	PEE	O2-C10-C11	3.57	119.19	111.50
52	V	202	CDL	OA6-CA5-C11	3.41	118.85	111.50
51	G	201	8Q1	O4-C1-C6	-3.40	119.98	123.99
47	A	503	NAI	C3D-C2D-C1D	3.39	107.86	101.43
54	J	402	UQ	C25-C24-C23	-3.35	112.95	122.65
54	s	402	UQ	C30-C29-C28	-3.35	112.96	122.65
54	J	402	UQ	C16-C14-C13	-3.35	114.34	121.12
54	J	402	UQ	C26-C24-C23	-3.34	112.98	122.65
51	X	201	8Q1	O4-C1-C6	-3.31	120.08	123.99
51	G	201	8Q1	C37-C38-C39	3.28	117.83	112.36
52	g	202	CDL	OA8-CA7-C31	3.28	119.98	111.38
50	C	304	970	C04-C02-C03	-3.27	112.94	120.31
50	C	304	970	C09-C07-C06	-3.23	119.74	123.20
54	s	402	UQ	C31-C29-C28	-3.22	113.34	122.65
50	C	304	970	O28-C19-C20	3.05	119.66	115.41
50	C	304	970	O26-C20-C19	3.04	119.64	115.41
46	A	502	FMN	C4-N3-C2	-3.01	120.07	125.64
52	V	202	CDL	OB8-CB7-C71	2.89	120.98	111.91
50	C	304	970	O13-C14-C23	2.84	115.27	112.40
50	C	304	970	C22-C23-C14	2.75	113.41	109.56
47	A	503	NAI	C4D-O4D-C1D	-2.74	103.43	109.47
50	C	304	970	C05-C04-C02	-2.73	111.62	115.62
52	l	702	CDL	OB8-CB7-C71	2.72	120.43	111.91
48	B	303	PEE	O3-C30-C31	2.71	120.43	111.91
58	w	401	ADP	O4'-C1'-C2'	-2.70	102.98	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	502	FMN	C4A-C4-N3	2.69	120.01	113.19
52	o	201	CDL	OB8-CB7-C71	2.68	120.32	111.91
52	V	202	CDL	OA8-CA7-C31	2.67	120.30	111.91
52	V	201	CDL	OB8-CB7-C71	2.67	120.28	111.91
52	I	201	CDL	OB8-CB7-C71	2.65	120.22	111.91
52	o	201	CDL	OA8-CA7-C31	2.65	120.22	111.91
48	r	501	PEE	O3-C30-C31	2.65	120.21	111.91
52	l	701	CDL	OA8-CA7-C31	2.65	120.21	111.91
53	J	401	NDP	PN-O3-PA	-2.64	123.78	132.83
48	l	703	PEE	O3-C30-C31	2.63	120.16	111.91
52	a	201	CDL	OB8-CB7-C71	2.63	120.15	111.91
52	I	201	CDL	OA8-CA7-C31	2.63	120.15	111.91
58	w	401	ADP	PA-O3A-PB	-2.61	123.86	132.83
52	s	401	CDL	OA8-CA7-C31	2.61	120.09	111.91
52	s	401	CDL	OB8-CB7-C71	2.61	120.09	111.91
48	U	101	PEE	O3-C30-C31	2.61	120.08	111.91
48	i	402	PEE	O3-C30-C31	2.60	120.06	111.91
52	i	401	CDL	OB8-CB7-C71	2.60	120.06	111.91
52	i	401	CDL	OA8-CA7-C31	2.60	120.05	111.91
52	i	403	CDL	OB8-CB7-C71	2.60	120.05	111.91
52	l	701	CDL	OB8-CB7-C71	2.58	120.01	111.91
48	l	704	PEE	O3-C30-C31	2.58	120.00	111.91
47	A	503	NAI	C4A-C5A-N7A	-2.58	106.71	109.40
52	i	403	CDL	OA8-CA7-C31	2.58	120.00	111.91
52	l	702	CDL	OA8-CA7-C31	2.57	119.98	111.91
48	j	201	PEE	O3-C30-C31	2.57	119.98	111.91
48	C	302	PEE	O3-C30-C31	2.57	119.96	111.91
47	A	503	NAI	C3B-C2B-C1B	2.55	104.81	100.98
53	J	401	NDP	C2B-C3B-C4B	2.54	107.52	101.99
52	a	201	CDL	OA8-CA7-C31	2.53	119.86	111.91
46	A	502	FMN	O4-C4-C4A	-2.52	119.91	126.60
52	V	201	CDL	OA8-CA7-C31	2.52	119.83	111.91
54	J	402	UQ	CM5-C5-C6	-2.52	120.29	124.40
52	g	202	CDL	OB8-CB7-C71	2.49	119.73	111.91
48	W	201	PEE	O3-C30-C31	2.48	119.70	111.91
50	C	304	970	C11-C12-C06	-2.48	119.15	123.16
47	A	503	NAI	C2D-C3D-C4D	2.47	107.43	102.64
49	a	202	PLX	C1A-N1-C1	2.45	119.95	109.92
49	g	201	PLX	C1A-N1-C1	2.44	119.89	109.92
47	A	503	NAI	PN-O3-PA	-2.43	124.49	132.83
49	r	502	PLX	C1A-N1-C1	2.38	119.66	109.92
49	j	202	PLX	C1A-N1-C1	2.35	119.55	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	s	402	UQ	CM5-C5-C6	-2.34	120.58	124.40
46	A	502	FMN	C4A-C10-N10	2.33	119.88	116.48
53	J	401	NDP	C4A-C5A-N7A	-2.31	106.99	109.40
49	J	403	PLX	C1A-N1-C1	2.31	119.36	109.92
46	A	502	FMN	C9A-C5A-N5	-2.30	119.93	122.43
49	C	303	PLX	C1A-N1-C1	2.24	119.07	109.92
46	A	502	FMN	C10-C4A-N5	-2.22	120.14	124.86
46	A	502	FMN	C4A-C10-N1	-2.22	119.58	124.73
51	X	201	8Q1	C43-S44-C1	2.22	108.77	101.87
50	C	304	970	C15-C14-C23	2.16	112.37	110.62
49	r	503	PLX	C1A-N1-C1	2.16	118.74	109.92
51	G	201	8Q1	C38-C39-N41	2.15	120.05	116.42
51	G	201	8Q1	O4-C1-S44	-2.15	119.82	122.61
58	w	401	ADP	C4-C5-N7	-2.12	107.19	109.40
51	G	201	8Q1	C43-S44-C1	2.10	108.42	101.87
50	C	304	970	C07-C06-C12	2.08	120.78	118.74
50	C	304	970	C01-C02-C04	-2.07	111.67	116.47
50	C	304	970	O26-C20-C21	-2.06	120.57	124.12
54	J	402	UQ	C10-C9-C11	-2.03	111.85	115.27

There are no chirality outliers.

All (1097) 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'
47	A	503	NAI	C5B-O5B-PA-O3
48	B	303	PEE	C11-C10-O2-C2
48	B	303	PEE	O4-C10-O2-C2
48	C	302	PEE	C17-C18-C19-C20
48	C	302	PEE	C1-O3P-P-O1P
48	C	302	PEE	O4P-C4-C5-N
48	U	101	PEE	C1-O3P-P-O1P
48	W	201	PEE	C1-O3P-P-O2P
48	W	201	PEE	C1-O3P-P-O1P
48	W	201	PEE	C4-O4P-P-O2P
48	W	201	PEE	O4P-C4-C5-N
48	i	402	PEE	C11-C10-O2-C2
48	i	402	PEE	C1-O3P-P-O2P
48	i	402	PEE	C1-O3P-P-O1P
48	i	402	PEE	C1-O3P-P-O4P
48	i	402	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
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	j	201	PEE	C4-O4P-P-O2P
48	j	201	PEE	C4-O4P-P-O1P
48	j	201	PEE	O4P-C4-C5-N
48	l	703	PEE	O3P-C1-C2-O2
48	r	501	PEE	C1-O3P-P-O1P
48	r	501	PEE	C1-O3P-P-O4P
48	r	501	PEE	C4-O4P-P-O1P
49	C	303	PLX	O6-C4-C5-O8
49	C	303	PLX	N1-C1-C2-O1
49	J	403	PLX	O7-C6-O6-C4
49	J	403	PLX	N1-C1-C2-O1
49	a	202	PLX	O7-C6-O6-C4
49	a	202	PLX	C2-O1-P1-O2
49	a	202	PLX	C2-O1-P1-O3
49	a	202	PLX	O9-C24-O8-C5
49	g	201	PLX	O7-C6-C7-C8
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	C2-O1-P1-O4
49	g	201	PLX	C2-O1-P1-O2
49	g	201	PLX	C2-O1-P1-O3
49	g	201	PLX	O9-C24-O8-C5
49	g	201	PLX	O9-C24-C25-C26
49	j	202	PLX	O7-C6-C7-C8
49	j	202	PLX	C7-C6-O6-C4
49	j	202	PLX	C3-O4-P1-O1
49	j	202	PLX	C3-O4-P1-O2
49	j	202	PLX	C3-O4-P1-O3
49	j	202	PLX	O9-C24-O8-C5
49	r	502	PLX	O7-C6-C7-C8
49	r	502	PLX	O7-C6-O6-C4
49	r	502	PLX	C5-C4-O6-C6
49	r	502	PLX	O9-C24-C25-C26
49	r	503	PLX	C3-O4-P1-O2
49	r	503	PLX	C2-O1-P1-O4
49	r	503	PLX	O9-C24-C25-C26
50	C	304	970	C03-C02-C04-C05
50	C	304	970	C03-C02-C04-O08

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Mol	Chain	Res	Type	Atoms
51	G	201	8Q1	C28-C29-C32-C34
51	G	201	8Q1	C28-C29-C32-O33
51	G	201	8Q1	C30-C29-C32-C34
51	G	201	8Q1	C30-C29-C32-O33
51	G	201	8Q1	C31-C29-C32-C34
51	G	201	8Q1	C31-C29-C32-O33
51	G	201	8Q1	C42-C43-S44-C1
51	G	201	8Q1	C28-O27-P24-O2
51	G	201	8Q1	C28-O27-P24-O1
51	X	201	8Q1	O4-C1-S44-C43
51	X	201	8Q1	C6-C1-S44-C43
51	X	201	8Q1	C28-C29-C32-C34
51	X	201	8Q1	C28-C29-C32-O33
51	X	201	8Q1	C30-C29-C32-C34
51	X	201	8Q1	C30-C29-C32-O33
51	X	201	8Q1	C31-C29-C32-C34
51	X	201	8Q1	C31-C29-C32-O33
51	X	201	8Q1	N41-C42-C43-S44
51	X	201	8Q1	C28-O27-P24-O2
51	X	201	8Q1	C28-O27-P24-O1
52	I	201	CDL	CA2-OA2-PA1-OA3
52	I	201	CDL	CA2-OA2-PA1-OA4
52	I	201	CDL	CA2-OA2-PA1-OA5
52	I	201	CDL	CA3-OA5-PA1-OA3
52	I	201	CDL	CB2-OB2-PB2-OB3
52	I	201	CDL	CB2-OB2-PB2-OB4
52	I	201	CDL	CB2-OB2-PB2-OB5
52	I	201	CDL	CB3-OB5-PB2-OB3
52	V	201	CDL	CB2-OB2-PB2-OB3
52	V	201	CDL	CB3-OB5-PB2-OB4
52	V	202	CDL	CA2-OA2-PA1-OA3
52	V	202	CDL	CA2-OA2-PA1-OA4
52	V	202	CDL	CA2-OA2-PA1-OA5
52	V	202	CDL	CA3-OA5-PA1-OA3
52	V	202	CDL	OA6-CA4-CA6-OA8
52	V	202	CDL	CB2-OB2-PB2-OB3
52	V	202	CDL	CB3-OB5-PB2-OB2
52	V	202	CDL	CB3-OB5-PB2-OB3
52	V	202	CDL	CB3-OB5-PB2-OB4
52	a	201	CDL	O1-C1-CA2-OA2
52	a	201	CDL	CA2-OA2-PA1-OA3
52	a	201	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
52	a	201	CDL	CB2-OB2-PB2-OB3
52	a	201	CDL	CB3-OB5-PB2-OB3
52	a	201	CDL	CB3-OB5-PB2-OB4
52	a	201	CDL	OB7-CB5-OB6-CB4
52	g	202	CDL	O1-C1-CB2-OB2
52	g	202	CDL	CA3-OA5-PA1-OA3
52	g	202	CDL	CA3-OA5-PA1-OA4
52	g	202	CDL	CB3-OB5-PB2-OB2
52	g	202	CDL	CB3-OB5-PB2-OB3
52	g	202	CDL	CB3-OB5-PB2-OB4
52	i	401	CDL	CB3-OB5-PB2-OB3
52	i	403	CDL	CA3-OA5-PA1-OA2
52	i	403	CDL	CA3-OA5-PA1-OA3
52	i	403	CDL	CB3-OB5-PB2-OB3
52	i	403	CDL	CB3-OB5-PB2-OB4
52	l	701	CDL	O1-C1-CA2-OA2
52	l	701	CDL	CA2-OA2-PA1-OA3
52	l	701	CDL	CA2-OA2-PA1-OA5
52	l	701	CDL	CB2-OB2-PB2-OB3
52	l	701	CDL	CB2-OB2-PB2-OB4
52	l	701	CDL	CB3-OB5-PB2-OB3
52	l	702	CDL	O1-C1-CB2-OB2
52	l	702	CDL	CA3-OA5-PA1-OA3
52	l	702	CDL	CB2-OB2-PB2-OB4
52	l	702	CDL	C51-CB5-OB6-CB4
52	o	201	CDL	CA2-OA2-PA1-OA3
52	o	201	CDL	CA2-OA2-PA1-OA4
52	o	201	CDL	CA3-OA5-PA1-OA3
52	o	201	CDL	OA6-CA4-CA6-OA8
52	o	201	CDL	CB3-OB5-PB2-OB3
52	o	201	CDL	CB3-OB5-PB2-OB4
52	s	401	CDL	O1-C1-CA2-OA2
52	s	401	CDL	CB2-C1-CA2-OA2
52	s	401	CDL	CA2-OA2-PA1-OA3
52	s	401	CDL	CA2-OA2-PA1-OA4
52	s	401	CDL	CA3-OA5-PA1-OA2
52	s	401	CDL	CA3-OA5-PA1-OA3
52	s	401	CDL	CA3-OA5-PA1-OA4
52	s	401	CDL	CB2-OB2-PB2-OB3
52	s	401	CDL	CB2-OB2-PB2-OB4
52	s	401	CDL	C51-CB5-OB6-CB4
53	J	401	NDP	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
53	J	401	NDP	O4B-C4B-C5B-O5B
54	J	402	UQ	C7-C8-C9-C11
54	J	402	UQ	C17-C18-C19-C21
54	s	402	UQ	C7-C8-C9-C10
54	s	402	UQ	C7-C8-C9-C11
54	s	402	UQ	C22-C23-C24-C26
58	w	401	ADP	PA-O3A-PB-O2B
48	U	101	PEE	O5-C30-O3-C3
52	i	401	CDL	OA9-CA7-OA8-CA6
52	l	701	CDL	OA9-CA7-OA8-CA6
52	l	702	CDL	OB9-CB7-OB8-CB6
48	C	302	PEE	O4-C10-O2-C2
48	i	402	PEE	O4-C10-O2-C2
48	l	704	PEE	O4-C10-O2-C2
52	i	403	CDL	OB7-CB5-OB6-CB4
52	l	702	CDL	OB7-CB5-OB6-CB4
52	s	401	CDL	OB7-CB5-OB6-CB4
48	U	101	PEE	C31-C30-O3-C3
52	l	701	CDL	C31-CA7-OA8-CA6
48	C	302	PEE	C11-C10-O2-C2
48	l	704	PEE	C11-C10-O2-C2
52	a	201	CDL	C51-CB5-OB6-CB4
52	i	403	CDL	C51-CB5-OB6-CB4
54	s	402	UQ	C12-C11-C9-C10
54	s	402	UQ	C23-C24-C26-C27
52	i	401	CDL	C31-CA7-OA8-CA6
52	i	403	CDL	C71-CB7-OB8-CB6
52	l	702	CDL	C71-CB7-OB8-CB6
48	U	101	PEE	C17-C18-C19-C20
48	W	201	PEE	C17-C18-C19-C20
48	l	704	PEE	C37-C38-C39-C40
54	J	402	UQ	C22-C23-C24-C26
54	J	402	UQ	C7-C8-C9-C10
49	J	403	PLX	C27-C28-C29-C30
54	J	402	UQ	C12-C13-C14-C16
54	s	402	UQ	C17-C18-C19-C21
52	l	701	CDL	C32-C33-C34-C35
52	g	202	CDL	O1-C1-CA2-OA2
52	i	403	CDL	O1-C1-CA2-OA2
52	l	701	CDL	O1-C1-CB2-OB2
52	l	702	CDL	O1-C1-CA2-OA2
48	l	703	PEE	C11-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
52	V	201	CDL	C11-CA5-OA6-CA4
52	o	201	CDL	C51-CB5-OB6-CB4
52	V	201	CDL	C11-C12-C13-C14
52	l	701	CDL	C55-C56-C57-C58
52	l	702	CDL	C35-C36-C37-C38
49	r	502	PLX	C9-C10-C11-C12
52	V	202	CDL	C73-C74-C75-C76
52	l	702	CDL	C75-C76-C77-C78
49	C	303	PLX	C25-C26-C27-C28
58	w	401	ADP	O4'-C4'-C5'-O5'
58	w	401	ADP	C3'-C4'-C5'-O5'
52	o	201	CDL	OB7-CB5-OB6-CB4
49	J	403	PLX	C25-C26-C27-C28
52	i	403	CDL	OB9-CB7-OB8-CB6
49	g	201	PLX	C9-C10-C11-C12
49	r	502	PLX	C11-C12-C13-C14
54	J	402	UQ	C12-C11-C9-C8
49	g	201	PLX	C7-C8-C9-C10
48	W	201	PEE	C31-C30-O3-C3
52	l	702	CDL	C33-C34-C35-C36
52	s	401	CDL	C14-C15-C16-C17
49	C	303	PLX	C27-C28-C29-C30
52	I	201	CDL	C51-C52-C53-C54
52	V	202	CDL	CB2-C1-CA2-OA2
52	a	201	CDL	CB2-C1-CA2-OA2
52	g	202	CDL	CA2-C1-CB2-OB2
52	l	701	CDL	CB2-C1-CA2-OA2
52	l	701	CDL	CA2-C1-CB2-OB2
52	l	702	CDL	CB2-C1-CA2-OA2
52	l	702	CDL	CA2-C1-CB2-OB2
48	l	703	PEE	O4-C10-O2-C2
49	j	202	PLX	C13-C14-C15-C16
49	r	502	PLX	C7-C8-C9-C10
48	i	402	PEE	C31-C30-O3-C3
48	l	703	PEE	C31-C30-O3-C3
52	V	201	CDL	C31-CA7-OA8-CA6
52	a	201	CDL	C71-CB7-OB8-CB6
52	l	701	CDL	C71-CB7-OB8-CB6
52	s	401	CDL	C31-C32-C33-C34
49	j	202	PLX	O4-C3-C4-O6
52	V	201	CDL	OB5-CB3-CB4-OB6
52	V	201	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
48	l	703	PEE	O5-C30-O3-C3
49	J	403	PLX	C12-C13-C14-C15
48	j	201	PEE	C11-C10-O2-C2
48	i	402	PEE	C11-C12-C13-C14
53	J	401	NDP	C2D-C1D-N1N-C6N
52	a	201	CDL	CB7-C71-C72-C73
52	i	401	CDL	CB5-C51-C52-C53
52	i	401	CDL	CB7-C71-C72-C73
52	l	702	CDL	CB5-C51-C52-C53
48	r	501	PEE	C17-C18-C19-C20
54	s	402	UQ	C27-C28-C29-C30
54	J	402	UQ	C17-C18-C19-C20
48	i	402	PEE	O5-C30-O3-C3
48	C	302	PEE	C30-C31-C32-C33
52	I	201	CDL	CB5-C51-C52-C53
52	i	401	CDL	CA7-C31-C32-C33
52	i	403	CDL	CB7-C71-C72-C73
52	l	701	CDL	CB7-C71-C72-C73
52	l	702	CDL	CB7-C71-C72-C73
52	s	401	CDL	CA7-C31-C32-C33
52	V	201	CDL	OA7-CA5-OA6-CA4
49	g	201	PLX	C2-C1-N1-C1A
52	l	701	CDL	CB5-C51-C52-C53
52	s	401	CDL	CB7-C71-C72-C73
48	B	303	PEE	C34-C35-C36-C37
48	r	501	PEE	C11-C10-O2-C2
52	l	701	CDL	OB9-CB7-OB8-CB6
52	o	201	CDL	C36-C37-C38-C39
52	V	201	CDL	C62-C63-C64-C65
52	a	201	CDL	OB9-CB7-OB8-CB6
52	a	201	CDL	CA5-C11-C12-C13
52	V	202	CDL	O1-C1-CA2-OA2
52	a	201	CDL	O1-C1-CB2-OB2
52	i	401	CDL	O1-C1-CA2-OA2
52	o	201	CDL	O1-C1-CA2-OA2
48	W	201	PEE	O5-C30-O3-C3
52	V	201	CDL	OA9-CA7-OA8-CA6
48	l	704	PEE	C21-C22-C23-C24
48	B	303	PEE	C17-C18-C19-C20
48	i	402	PEE	C37-C38-C39-C40
48	r	501	PEE	C41-C42-C43-C44
52	l	701	CDL	C81-C82-C83-C84

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Mol	Chain	Res	Type	Atoms
52	V	201	CDL	C58-C59-C60-C61
48	C	302	PEE	C1-O3P-P-O4P
48	C	302	PEE	C4-O4P-P-O3P
48	U	101	PEE	C1-O3P-P-O4P
48	W	201	PEE	C1-O3P-P-O4P
48	W	201	PEE	C4-O4P-P-O3P
48	j	201	PEE	C1-O3P-P-O4P
48	r	501	PEE	C4-O4P-P-O3P
49	a	202	PLX	C2-O1-P1-O4
49	g	201	PLX	C3-O4-P1-O1
49	r	502	PLX	C3-O4-P1-O1
52	I	201	CDL	CB3-OB5-PB2-OB2
52	V	201	CDL	CB2-OB2-PB2-OB5
52	V	202	CDL	CA3-OA5-PA1-OA2
52	a	201	CDL	CA2-OA2-PA1-OA5
52	a	201	CDL	CA3-OA5-PA1-OA2
52	a	201	CDL	CB2-OB2-PB2-OB5
52	a	201	CDL	CB3-OB5-PB2-OB2
52	g	202	CDL	CA3-OA5-PA1-OA2
52	g	202	CDL	CB2-OB2-PB2-OB5
52	i	401	CDL	CA2-OA2-PA1-OA5
52	i	401	CDL	CA3-OA5-PA1-OA2
52	i	401	CDL	CB3-OB5-PB2-OB2
52	i	403	CDL	CB2-OB2-PB2-OB5
52	i	403	CDL	CB3-OB5-PB2-OB2
52	l	701	CDL	CB2-OB2-PB2-OB5
52	o	201	CDL	CB3-OB5-PB2-OB2
52	s	401	CDL	CA2-OA2-PA1-OA5
52	s	401	CDL	CB2-OB2-PB2-OB5
52	a	201	CDL	C31-CA7-OA8-CA6
52	I	201	CDL	C11-C12-C13-C14
52	g	202	CDL	CB2-C1-CA2-OA2
52	i	403	CDL	CB2-C1-CA2-OA2
52	o	201	CDL	CB2-C1-CA2-OA2
48	j	201	PEE	O4-C10-O2-C2
48	r	501	PEE	O4-C10-O2-C2
49	g	201	PLX	C2-C1-N1-C1B
49	a	202	PLX	O6-C6-C7-C8
49	r	502	PLX	O6-C6-C7-C8
49	j	202	PLX	C16-C17-C18-C19
49	r	502	PLX	C27-C28-C29-C30
52	V	202	CDL	C76-C77-C78-C79

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Mol	Chain	Res	Type	Atoms
48	i	402	PEE	C21-C22-C23-C24
48	r	501	PEE	C21-C22-C23-C24
49	C	303	PLX	C10-C11-C12-C13
49	C	303	PLX	C35-C36-C37-C38
49	a	202	PLX	C17-C18-C19-C20
49	g	201	PLX	C28-C29-C30-C31
49	j	202	PLX	C27-C28-C29-C30
52	V	201	CDL	C31-C32-C33-C34
52	i	401	CDL	C59-C60-C61-C62
52	l	701	CDL	C11-C12-C13-C14
52	l	701	CDL	C59-C60-C61-C62
52	l	702	CDL	C55-C56-C57-C58
52	o	201	CDL	C17-C18-C19-C20
52	o	201	CDL	C54-C55-C56-C57
52	o	201	CDL	C60-C61-C62-C63
52	s	401	CDL	C73-C74-C75-C76
49	J	403	PLX	C33-C34-C35-C36
49	r	502	PLX	C11-C10-C9-C8
49	r	503	PLX	C25-C26-C27-C28
52	V	201	CDL	C35-C36-C37-C38
52	V	201	CDL	C71-C72-C73-C74
52	V	201	CDL	C78-C79-C80-C81
52	g	202	CDL	C75-C76-C77-C78
52	o	201	CDL	C14-C15-C16-C17
52	o	201	CDL	C82-C83-C84-C85
48	W	201	PEE	C12-C13-C14-C15
49	a	202	PLX	C10-C11-C12-C13
49	a	202	PLX	C9-C10-C11-C12
49	j	202	PLX	C14-C15-C16-C17
52	g	202	CDL	C55-C56-C57-C58
52	l	702	CDL	C37-C38-C39-C40
48	j	201	PEE	C23-C24-C25-C26
48	j	201	PEE	C13-C14-C15-C16
49	C	303	PLX	C9-C10-C11-C12
49	J	403	PLX	C30-C31-C32-C33
49	r	502	PLX	C12-C13-C14-C15
52	V	202	CDL	C71-C72-C73-C74
52	i	401	CDL	C18-C19-C20-C21
52	i	403	CDL	C32-C33-C34-C35
52	l	701	CDL	C52-C53-C54-C55
48	r	501	PEE	C20-C21-C22-C23
49	C	303	PLX	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
49	j	202	PLX	C33-C34-C35-C36
49	r	503	PLX	C10-C11-C12-C13
52	g	202	CDL	C73-C74-C75-C76
52	i	401	CDL	C55-C56-C57-C58
52	o	201	CDL	C37-C38-C39-C40
52	I	201	CDL	CA7-C31-C32-C33
52	l	702	CDL	C31-CA7-OA8-CA6
48	W	201	PEE	C21-C22-C23-C24
49	g	201	PLX	C13-C14-C15-C16
49	g	201	PLX	C30-C31-C32-C33
49	j	202	PLX	C11-C12-C13-C14
49	j	202	PLX	C25-C26-C27-C28
52	V	202	CDL	C75-C76-C77-C78
52	a	201	CDL	C37-C38-C39-C40
52	i	401	CDL	C76-C77-C78-C79
52	l	701	CDL	C37-C38-C39-C40
52	l	701	CDL	C75-C76-C77-C78
52	l	702	CDL	C11-C12-C13-C14
52	l	702	CDL	C32-C33-C34-C35
52	s	401	CDL	C59-C60-C61-C62
52	s	401	CDL	C71-C72-C73-C74
52	a	201	CDL	OA9-CA7-OA8-CA6
49	C	303	PLX	C15-C16-C17-C18
49	j	202	PLX	C10-C11-C12-C13
52	a	201	CDL	C17-C18-C19-C20
52	l	702	CDL	C82-C83-C84-C85
52	o	201	CDL	C12-C13-C14-C15
48	j	201	PEE	C12-C13-C14-C15
49	J	403	PLX	C9-C10-C11-C12
49	g	201	PLX	C14-C15-C16-C17
49	r	502	PLX	C33-C34-C35-C36
52	V	201	CDL	C75-C76-C77-C78
52	g	202	CDL	C52-C53-C54-C55
52	i	403	CDL	C31-C32-C33-C34
52	i	403	CDL	C80-C81-C82-C83
52	l	701	CDL	C71-C72-C73-C74
52	l	701	CDL	C73-C74-C75-C76
52	l	701	CDL	C82-C83-C84-C85
52	l	702	CDL	C62-C63-C64-C65
52	l	702	CDL	C71-C72-C73-C74
52	o	201	CDL	C83-C84-C85-C86
48	r	501	PEE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
49	g	201	PLX	C32-C33-C34-C35
49	r	503	PLX	C16-C17-C18-C19
52	V	201	CDL	C15-C16-C17-C18
52	i	401	CDL	C38-C39-C40-C41
52	l	701	CDL	C62-C63-C64-C65
49	J	403	PLX	C7-C8-C9-C10
52	a	201	CDL	C62-C63-C64-C65
52	i	401	CDL	C82-C83-C84-C85
52	l	702	CDL	C80-C81-C82-C83
52	s	401	CDL	C35-C36-C37-C38
48	B	303	PEE	C35-C36-C37-C38
48	r	501	PEE	C15-C16-C17-C18
48	W	201	PEE	C13-C14-C15-C16
49	a	202	PLX	C27-C28-C29-C30
49	g	201	PLX	C10-C11-C12-C13
52	V	201	CDL	C17-C18-C19-C20
52	V	201	CDL	C56-C57-C58-C59
52	a	201	CDL	C73-C74-C75-C76
52	s	401	CDL	C36-C37-C38-C39
48	l	703	PEE	C11-C12-C13-C14
51	X	201	8Q1	C6-C7-C8-C9
52	V	201	CDL	C40-C41-C42-C43
52	V	201	CDL	C55-C56-C57-C58
52	V	202	CDL	C11-C12-C13-C14
52	V	202	CDL	C17-C18-C19-C20
52	a	201	CDL	C52-C53-C54-C55
52	a	201	CDL	C82-C83-C84-C85
52	i	403	CDL	C19-C20-C21-C22
52	s	401	CDL	C52-C53-C54-C55
49	C	303	PLX	C30-C31-C32-C33
49	J	403	PLX	C28-C29-C30-C31
49	r	502	PLX	C28-C29-C30-C31
52	V	201	CDL	C72-C73-C74-C75
52	a	201	CDL	C60-C61-C62-C63
52	s	401	CDL	C17-C18-C19-C20
49	g	201	PLX	C11-C10-C9-C8
49	r	503	PLX	C28-C29-C30-C31
52	a	201	CDL	C75-C76-C77-C78
52	i	403	CDL	C52-C53-C54-C55
48	r	501	PEE	C12-C13-C14-C15
49	g	201	PLX	C33-C34-C35-C36
52	V	201	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
52	i	401	CDL	C75-C76-C77-C78
52	l	701	CDL	C33-C34-C35-C36
48	l	704	PEE	C34-C35-C36-C37
49	C	303	PLX	C14-C15-C16-C17
49	C	303	PLX	C33-C34-C35-C36
49	g	201	PLX	C27-C28-C29-C30
52	V	201	CDL	C59-C60-C61-C62
49	J	403	PLX	C14-C15-C16-C17
52	l	701	CDL	C14-C15-C16-C17
49	J	403	PLX	C31-C32-C33-C34
52	i	403	CDL	C59-C60-C61-C62
52	o	201	CDL	C32-C33-C34-C35
52	I	201	CDL	C51-CB5-OB6-CB4
52	V	201	CDL	C51-CB5-OB6-CB4
49	a	202	PLX	C34-C35-C36-C37
52	V	202	CDL	C81-C82-C83-C84
52	i	403	CDL	C55-C56-C57-C58
54	s	402	UQ	C27-C28-C29-C31
49	C	303	PLX	O9-C24-C25-C26
49	a	202	PLX	O9-C24-C25-C26
48	l	704	PEE	C11-C12-C13-C14
49	r	502	PLX	C25-C26-C27-C28
49	r	502	PLX	C30-C31-C32-C33
52	V	201	CDL	C57-C58-C59-C60
52	l	701	CDL	C36-C37-C38-C39
52	o	201	CDL	C59-C60-C61-C62
48	U	101	PEE	C35-C36-C37-C38
48	W	201	PEE	C19-C20-C21-C22
48	i	402	PEE	C19-C20-C21-C22
49	a	202	PLX	C33-C34-C35-C36
49	g	201	PLX	C25-C26-C27-C28
52	g	202	CDL	CB7-C71-C72-C73
52	a	201	CDL	CA2-C1-CB2-OB2
52	I	201	CDL	OB7-CB5-OB6-CB4
52	V	201	CDL	OB7-CB5-OB6-CB4
49	J	403	PLX	C26-C27-C28-C29
52	V	201	CDL	C52-C53-C54-C55
52	l	701	CDL	C34-C35-C36-C37
52	s	401	CDL	C75-C76-C77-C78
48	j	201	PEE	C11-C12-C13-C14
52	i	403	CDL	C43-C44-C45-C46
52	i	403	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
52	s	401	CDL	C32-C33-C34-C35
49	a	202	PLX	C7-C8-C9-C10
52	o	201	CDL	C57-C58-C59-C60
52	V	201	CDL	C71-CB7-OB8-CB6
48	B	303	PEE	C40-C41-C42-C43
52	o	201	CDL	C74-C75-C76-C77
49	a	202	PLX	C13-C14-C15-C16
52	V	201	CDL	OB9-CB7-OB8-CB6
52	l	702	CDL	OA9-CA7-OA8-CA6
52	i	401	CDL	C14-C15-C16-C17
48	j	201	PEE	C19-C20-C21-C22
52	l	702	CDL	OA7-CA5-OA6-CA4
52	l	701	CDL	CA7-C31-C32-C33
52	i	401	CDL	C71-CB7-OB8-CB6
52	a	201	CDL	C36-C37-C38-C39
52	i	401	CDL	C77-C78-C79-C80
52	o	201	CDL	C35-C36-C37-C38
52	l	702	CDL	CA7-C31-C32-C33
49	g	201	PLX	C16-C17-C18-C19
52	i	403	CDL	C41-C42-C43-C44
52	s	401	CDL	C78-C79-C80-C81
52	l	702	CDL	C81-C82-C83-C84
52	o	201	CDL	C55-C56-C57-C58
52	a	201	CDL	C11-C12-C13-C14
52	i	401	CDL	C73-C74-C75-C76
52	i	403	CDL	C51-C52-C53-C54
52	l	701	CDL	C51-CB5-OB6-CB4
52	l	702	CDL	C11-CA5-OA6-CA4
52	I	201	CDL	OA5-CA3-CA4-OA6
52	V	202	CDL	OA5-CA3-CA4-OA6
52	i	401	CDL	OA5-CA3-CA4-OA6
52	o	201	CDL	OB5-CB3-CB4-OB6
48	r	501	PEE	C31-C32-C33-C34
52	l	702	CDL	C39-C40-C41-C42
52	V	202	CDL	OB6-CB4-CB6-OB8
52	i	403	CDL	OB6-CB4-CB6-OB8
48	B	303	PEE	C12-C13-C14-C15
49	a	202	PLX	C30-C31-C32-C33
52	g	202	CDL	C54-C55-C56-C57
49	g	201	PLX	C2-C1-N1-C1C
49	J	403	PLX	C16-C17-C18-C19
52	a	201	CDL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
48	l	703	PEE	C23-C24-C25-C26
49	r	503	PLX	C11-C12-C13-C14
52	s	401	CDL	C11-C12-C13-C14
48	l	703	PEE	C31-C32-C33-C34
52	I	201	CDL	C71-C72-C73-C74
49	j	202	PLX	C7-C8-C9-C10
49	r	502	PLX	C16-C17-C18-C19
49	r	503	PLX	C7-C8-C9-C10
52	i	401	CDL	OB9-CB7-OB8-CB6
52	l	701	CDL	OB7-CB5-OB6-CB4
49	g	201	PLX	C12-C13-C14-C15
49	r	503	PLX	C14-C15-C16-C17
49	r	503	PLX	C30-C31-C32-C33
52	V	201	CDL	C14-C15-C16-C17
52	l	702	CDL	C59-C60-C61-C62
48	U	101	PEE	C36-C37-C38-C39
46	A	502	FMN	O2'-C2'-C3'-C4'
48	j	201	PEE	C4-O4P-P-O3P
49	a	202	PLX	C3-O4-P1-O1
49	r	503	PLX	C3-O4-P1-O1
52	V	201	CDL	CB3-OB5-PB2-OB2
52	V	202	CDL	CB2-OB2-PB2-OB5
52	l	701	CDL	CB3-OB5-PB2-OB2
52	l	702	CDL	CA3-OA5-PA1-OA2
52	l	702	CDL	CB2-OB2-PB2-OB5
52	o	201	CDL	CA2-OA2-PA1-OA5
52	i	403	CDL	C72-C73-C74-C75
46	A	502	FMN	C3'-C4'-C5'-O5'
48	l	703	PEE	O3P-C1-C2-C3
52	V	201	CDL	OB5-CB3-CB4-CB6
52	i	401	CDL	OA5-CA3-CA4-CA6
52	i	401	CDL	OB5-CB3-CB4-CB6
52	a	201	CDL	C39-C40-C41-C42
48	U	101	PEE	C12-C13-C14-C15
49	r	502	PLX	C34-C35-C36-C37
52	V	201	CDL	C37-C38-C39-C40
52	i	403	CDL	C11-C12-C13-C14
52	i	403	CDL	C62-C63-C64-C65
48	l	703	PEE	C19-C20-C21-C22
52	o	201	CDL	CA7-C31-C32-C33
52	i	403	CDL	C21-C22-C23-C24
52	s	401	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
52	l	701	CDL	C74-C75-C76-C77
48	U	101	PEE	C11-C12-C13-C14
48	W	201	PEE	C24-C25-C26-C27
52	a	201	CDL	C35-C36-C37-C38
52	i	403	CDL	CA5-C11-C12-C13
48	l	703	PEE	C40-C41-C42-C43
52	V	202	CDL	C14-C15-C16-C17
52	i	403	CDL	C17-C18-C19-C20
52	i	403	CDL	C76-C77-C78-C79
48	C	302	PEE	C1-C2-C3-O3
48	W	201	PEE	C1-C2-C3-O3
48	i	402	PEE	C1-C2-C3-O3
48	j	201	PEE	C1-C2-C3-O3
48	j	201	PEE	C32-C33-C34-C35
49	C	303	PLX	C3-C4-C5-O8
49	J	403	PLX	C3-C4-C5-O8
49	r	503	PLX	C13-C14-C15-C16
52	V	201	CDL	CA3-CA4-CA6-OA8
52	V	201	CDL	CB3-CB4-CB6-OB8
52	V	202	CDL	CA3-CA4-CA6-OA8
52	V	202	CDL	C32-C33-C34-C35
52	i	403	CDL	CA3-CA4-CA6-OA8
52	o	201	CDL	CA3-CA4-CA6-OA8
52	o	201	CDL	CB3-CB4-CB6-OB8
48	l	704	PEE	C13-C14-C15-C16
49	C	303	PLX	C19-C20-C21-C22
49	C	303	PLX	C28-C29-C30-C31
49	J	403	PLX	C4-C5-O8-C24
48	B	303	PEE	C23-C24-C25-C26
49	r	503	PLX	C36-C37-C38-C39
52	s	401	CDL	C12-C11-CA5-OA6
52	i	403	CDL	C42-C43-C44-C45
52	l	702	CDL	C17-C18-C19-C20
49	J	403	PLX	O8-C24-C25-C26
49	j	202	PLX	O6-C6-C7-C8
49	j	202	PLX	O8-C24-C25-C26
49	r	502	PLX	O8-C24-C25-C26
49	r	503	PLX	C29-C30-C31-C32
52	g	202	CDL	C74-C75-C76-C77
48	B	303	PEE	C38-C39-C40-C41
48	W	201	PEE	C15-C16-C17-C18
52	a	201	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
47	A	503	NAI	C3D-C4D-C5D-O5D
52	i	403	CDL	C15-C16-C17-C18
52	s	401	CDL	C33-C34-C35-C36
52	V	201	CDL	C32-C33-C34-C35
52	i	401	CDL	C40-C41-C42-C43
48	C	302	PEE	C42-C43-C44-C45
49	a	202	PLX	C11-C12-C13-C14
52	I	201	CDL	C12-C13-C14-C15
52	l	702	CDL	C44-C45-C46-C47
48	r	501	PEE	C44-C45-C46-C47
51	G	201	8Q1	C28-O27-P24-O3
51	X	201	8Q1	C28-O27-P24-O3
49	C	303	PLX	C17-C18-C19-C20
52	i	403	CDL	C22-C23-C24-C25
48	B	303	PEE	C31-C30-O3-C3
48	l	704	PEE	C31-C30-O3-C3
49	J	403	PLX	O4-C3-C4-O6
49	g	201	PLX	O4-C3-C4-O6
52	V	202	CDL	OB5-CB3-CB4-OB6
52	l	701	CDL	OB5-CB3-CB4-OB6
52	i	401	CDL	C35-C36-C37-C38
49	j	202	PLX	C19-C20-C21-C22
48	l	703	PEE	C15-C16-C17-C18
52	l	702	CDL	C16-C17-C18-C19
48	l	703	PEE	O2-C2-C3-O3
49	j	202	PLX	O6-C4-C5-O8
52	i	401	CDL	OB6-CB4-CB6-OB8
52	i	403	CDL	OA6-CA4-CA6-OA8
52	o	201	CDL	OB6-CB4-CB6-OB8
52	o	201	CDL	C72-C73-C74-C75
52	a	201	CDL	C64-C65-C66-C67
52	l	701	CDL	C35-C36-C37-C38
48	l	704	PEE	C10-C11-C12-C13
49	j	202	PLX	C18-C19-C20-C21
52	V	202	CDL	C12-C13-C14-C15
48	C	302	PEE	C12-C13-C14-C15
52	i	401	CDL	C31-C32-C33-C34
52	i	401	CDL	C71-C72-C73-C74
53	J	401	NDP	PN-O3-PA-O1A
48	j	201	PEE	C22-C23-C24-C25
49	j	202	PLX	C15-C16-C17-C18
48	r	501	PEE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
48	r	501	PEE	C38-C39-C40-C41
48	i	402	PEE	O3P-C1-C2-C3
49	J	403	PLX	O4-C3-C4-C5
49	j	202	PLX	O4-C3-C4-C5
52	I	201	CDL	OA5-CA3-CA4-CA6
52	I	201	CDL	OB5-CB3-CB4-CB6
52	V	202	CDL	OA5-CA3-CA4-CA6
48	l	703	PEE	C30-C31-C32-C33
49	a	202	PLX	C25-C26-C27-C28
52	i	403	CDL	C14-C15-C16-C17
52	V	202	CDL	C31-CA7-OA8-CA6
52	i	403	CDL	C31-CA7-OA8-CA6
49	r	503	PLX	C17-C18-C19-C20
49	r	503	PLX	C27-C28-C29-C30
48	j	201	PEE	C31-C30-O3-C3
52	i	403	CDL	CB5-C51-C52-C53
48	r	501	PEE	C43-C44-C45-C46
52	i	401	CDL	C16-C17-C18-C19
52	i	403	CDL	C36-C37-C38-C39
48	i	402	PEE	C2-C1-O3P-P
48	l	704	PEE	C18-C19-C20-C21
48	C	302	PEE	C11-C12-C13-C14
49	r	502	PLX	C31-C32-C33-C34
52	a	201	CDL	C34-C35-C36-C37
52	a	201	CDL	C20-C21-C22-C23
48	B	303	PEE	C13-C14-C15-C16
52	V	202	CDL	C19-C20-C21-C22
52	s	401	CDL	C15-C16-C17-C18
48	l	704	PEE	C1-C2-C3-O3
49	r	503	PLX	C3-C4-C5-O8
52	V	202	CDL	CB3-CB4-CB6-OB8
52	i	403	CDL	CB3-CB4-CB6-OB8
49	r	502	PLX	C14-C15-C16-C17
52	V	202	CDL	C52-C53-C54-C55
52	a	201	CDL	C74-C75-C76-C77
52	i	401	CDL	C11-C12-C13-C14
48	l	704	PEE	O5-C30-O3-C3
52	V	201	CDL	C54-C55-C56-C57
49	J	403	PLX	C5-C4-O6-C6
49	a	202	PLX	C5-C4-O6-C6
49	r	502	PLX	C3-C4-O6-C6
49	r	503	PLX	C5-C4-O6-C6

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Mol	Chain	Res	Type	Atoms
48	i	402	PEE	C10-C11-C12-C13
49	J	403	PLX	C34-C35-C36-C37
52	I	201	CDL	C52-C53-C54-C55
52	V	201	CDL	OA5-CA3-CA4-OA6
52	l	702	CDL	OB5-CB3-CB4-OB6
52	V	202	CDL	C71-CB7-OB8-CB6
48	B	303	PEE	O5-C30-O3-C3
48	r	501	PEE	C10-C11-C12-C13
52	i	403	CDL	C82-C83-C84-C85
49	g	201	PLX	C19-C20-C21-C22
52	a	201	CDL	C21-C22-C23-C24
48	i	402	PEE	O2-C2-C3-O3
48	j	201	PEE	O2-C2-C3-O3
48	l	704	PEE	O2-C2-C3-O3
49	J	403	PLX	O6-C4-C5-O8
52	s	401	CDL	OB6-CB4-CB6-OB8
48	C	302	PEE	C44-C45-C46-C47
48	r	501	PEE	C33-C34-C35-C36
52	o	201	CDL	C11-C12-C13-C14
48	C	302	PEE	C13-C14-C15-C16
51	X	201	8Q1	C11-C10-C9-C8
52	o	201	CDL	CA2-C1-CB2-OB2
52	s	401	CDL	C55-C56-C57-C58
52	i	401	CDL	CA5-C11-C12-C13
49	J	403	PLX	C15-C16-C17-C18
49	r	502	PLX	C13-C14-C15-C16
52	i	401	CDL	C44-C45-C46-C47
48	C	302	PEE	C34-C35-C36-C37
52	s	401	CDL	C40-C41-C42-C43
49	g	201	PLX	C36-C37-C38-C39
48	r	501	PEE	C30-C31-C32-C33
52	V	202	CDL	C84-C85-C86-C87
49	a	202	PLX	C12-C13-C14-C15
49	r	503	PLX	C12-C13-C14-C15
52	l	702	CDL	C12-C13-C14-C15
49	r	503	PLX	O8-C24-C25-C26
52	V	202	CDL	C82-C83-C84-C85
48	C	302	PEE	O3P-C1-C2-C3
49	g	201	PLX	O4-C3-C4-C5
52	V	201	CDL	OA5-CA3-CA4-CA6
52	l	701	CDL	OB5-CB3-CB4-CB6
52	l	702	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
52	o	201	CDL	OB5-CB3-CB4-CB6
48	B	303	PEE	C11-C12-C13-C14
48	r	501	PEE	C34-C35-C36-C37
52	a	201	CDL	C14-C15-C16-C17
48	U	101	PEE	C15-C16-C17-C18
49	J	403	PLX	C13-C14-C15-C16
52	V	202	CDL	CA5-C11-C12-C13
49	j	202	PLX	C11-C10-C9-C8
52	o	201	CDL	C75-C76-C77-C78
52	o	201	CDL	C73-C74-C75-C76
52	V	201	CDL	CA6-CA4-OA6-CA5
48	i	402	PEE	C24-C25-C26-C27
52	V	202	CDL	C53-C54-C55-C56
52	I	201	CDL	C71-CB7-OB8-CB6
52	o	201	CDL	OA5-CA3-CA4-OA6
52	i	401	CDL	C64-C65-C66-C67
52	o	201	CDL	C53-C54-C55-C56
47	A	503	NAI	C2D-C1D-N1N-C2N
48	j	201	PEE	O5-C30-O3-C3
52	V	202	CDL	OA9-CA7-OA8-CA6
52	i	403	CDL	OA9-CA7-OA8-CA6
49	r	503	PLX	C35-C36-C37-C38
52	g	202	CDL	C56-C57-C58-C59
48	W	201	PEE	O2-C2-C3-O3
49	r	503	PLX	O6-C4-C5-O8
52	g	202	CDL	C71-C72-C73-C74
53	J	401	NDP	C5B-O5B-PA-O3
52	V	202	CDL	OB9-CB7-OB8-CB6
52	i	403	CDL	C71-C72-C73-C74
52	I	201	CDL	OB9-CB7-OB8-CB6
51	G	201	8Q1	C12-C13-C14-C15
52	i	403	CDL	C83-C84-C85-C86
52	s	401	CDL	C56-C57-C58-C59
49	a	202	PLX	C24-C25-C26-C27
48	l	704	PEE	C4-O4P-P-O3P
49	J	403	PLX	C2-O1-P1-O4
49	r	502	PLX	C2-O1-P1-O4
52	V	201	CDL	CA3-OA5-PA1-OA2
52	i	403	CDL	CA2-OA2-PA1-OA5
52	i	401	CDL	C39-C40-C41-C42
52	i	401	CDL	O1-C1-CB2-OB2
54	J	402	UQ	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
48	l	704	PEE	C2-C1-O3P-P
52	i	401	CDL	C1-CB2-OB2-PB2
52	i	403	CDL	C1-CB2-OB2-PB2
52	o	201	CDL	C1-CB2-OB2-PB2
47	A	503	NAI	C5B-O5B-PA-O1A
48	C	302	PEE	C1-O3P-P-O2P
48	C	302	PEE	C4-O4P-P-O2P
48	C	302	PEE	C4-O4P-P-O1P
48	W	201	PEE	C4-O4P-P-O1P
48	j	201	PEE	C1-O3P-P-O1P
48	r	501	PEE	C1-O3P-P-O2P
48	r	501	PEE	C4-O4P-P-O2P
49	C	303	PLX	C2-O1-P1-O3
49	J	403	PLX	C2-O1-P1-O2
49	J	403	PLX	C2-O1-P1-O3
49	a	202	PLX	C3-O4-P1-O3
49	r	502	PLX	C3-O4-P1-O2
49	r	502	PLX	C3-O4-P1-O3
49	r	502	PLX	C2-O1-P1-O3
49	r	503	PLX	C2-O1-P1-O3
52	I	201	CDL	CB3-OB5-PB2-OB4
52	V	201	CDL	CA3-OA5-PA1-OA3
52	V	201	CDL	CB2-OB2-PB2-OB4
52	V	201	CDL	CB3-OB5-PB2-OB3
52	V	202	CDL	CA3-OA5-PA1-OA4
52	V	202	CDL	CB2-OB2-PB2-OB4
52	a	201	CDL	CA3-OA5-PA1-OA3
52	a	201	CDL	CA3-OA5-PA1-OA4
52	a	201	CDL	CB2-OB2-PB2-OB4
52	g	202	CDL	CB2-OB2-PB2-OB3
52	i	401	CDL	CA2-OA2-PA1-OA4
52	i	401	CDL	CA3-OA5-PA1-OA3
52	i	401	CDL	CA3-OA5-PA1-OA4
52	i	401	CDL	CB3-OB5-PB2-OB4
52	i	403	CDL	CA2-OA2-PA1-OA4
52	i	403	CDL	CB2-OB2-PB2-OB3
52	i	403	CDL	CB2-OB2-PB2-OB4
52	l	701	CDL	CB3-OB5-PB2-OB4
52	l	702	CDL	CA3-OA5-PA1-OA4
52	l	702	CDL	CB2-OB2-PB2-OB3
52	o	201	CDL	CB2-OB2-PB2-OB4
52	g	202	CDL	C53-C54-C55-C56

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Mol	Chain	Res	Type	Atoms
52	o	201	CDL	C64-C65-C66-C67
48	B	303	PEE	O3P-C1-C2-C3
52	o	201	CDL	OA5-CA3-CA4-CA6
52	s	401	CDL	OA5-CA3-CA4-CA6
52	s	401	CDL	CB5-C51-C52-C53
52	g	202	CDL	C57-C58-C59-C60
52	l	702	CDL	C73-C74-C75-C76
52	V	201	CDL	C12-C13-C14-C15
52	i	401	CDL	C74-C75-C76-C77
52	i	403	CDL	C39-C40-C41-C42
52	s	401	CDL	C39-C40-C41-C42
46	A	502	FMN	C1'-C2'-C3'-O3'
49	C	303	PLX	C25-C24-O8-C5
49	J	403	PLX	C1-C2-O1-P1
49	J	403	PLX	C25-C24-O8-C5
49	a	202	PLX	C25-C24-O8-C5
49	j	202	PLX	C25-C24-O8-C5
48	l	704	PEE	C15-C16-C17-C18
48	B	303	PEE	O3P-C1-C2-O2
48	C	302	PEE	O3P-C1-C2-O2
48	i	402	PEE	O3P-C1-C2-O2
52	I	201	CDL	OB5-CB3-CB4-OB6
52	s	401	CDL	OA5-CA3-CA4-OA6
48	C	302	PEE	C41-C42-C43-C44
48	U	101	PEE	C22-C23-C24-C25
52	i	403	CDL	C74-C75-C76-C77
52	l	701	CDL	C38-C39-C40-C41
48	l	704	PEE	C33-C34-C35-C36
52	i	403	CDL	C44-C45-C46-C47
52	o	201	CDL	O1-C1-CB2-OB2
48	B	303	PEE	C20-C21-C22-C23
48	l	703	PEE	C1-C2-C3-O3
48	r	501	PEE	C1-C2-C3-O3
51	G	201	8Q1	O27-C28-C29-C32
48	C	302	PEE	O2-C2-C3-O3
48	r	501	PEE	O2-C2-C3-O3
49	r	502	PLX	O6-C4-C5-O8
52	V	201	CDL	OA6-CA4-CA6-OA8
48	U	101	PEE	C24-C25-C26-C27
52	V	201	CDL	C64-C65-C66-C67
48	r	501	PEE	C31-C30-O3-C3
52	l	702	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
52	o	201	CDL	C32-C31-CA7-OA8
52	a	201	CDL	C71-C72-C73-C74
48	l	703	PEE	C10-C11-C12-C13
49	r	503	PLX	C31-C32-C33-C34
49	g	201	PLX	O8-C24-C25-C26
52	o	201	CDL	C84-C85-C86-C87
52	V	201	CDL	CA7-C31-C32-C33
48	l	703	PEE	C37-C38-C39-C40
52	s	401	CDL	C16-C17-C18-C19
49	j	202	PLX	C12-C13-C14-C15
49	r	503	PLX	C33-C34-C35-C36
51	G	201	8Q1	O27-C28-C29-C30
48	r	501	PEE	O5-C30-O3-C3
48	l	703	PEE	C3-C2-O2-C10
52	V	202	CDL	OB5-CB3-CB4-CB6
52	i	401	CDL	CB2-C1-CA2-OA2
52	o	201	CDL	C62-C63-C64-C65
48	i	402	PEE	C14-C15-C16-C17
52	i	401	CDL	OB5-CB3-CB4-OB6
49	j	202	PLX	C30-C31-C32-C33
52	i	401	CDL	C15-C16-C17-C18
52	s	401	CDL	C37-C38-C39-C40
49	a	202	PLX	C2-C1-N1-C1A
47	A	503	NAI	O4D-C1D-N1N-C2N
48	l	703	PEE	C32-C33-C34-C35
52	o	201	CDL	C81-C82-C83-C84
52	g	202	CDL	C51-CB5-OB6-CB4
52	i	403	CDL	C33-C34-C35-C36
48	U	101	PEE	C4-O4P-P-O3P
49	C	303	PLX	C3-O4-P1-O1
52	I	201	CDL	CA3-OA5-PA1-OA2
52	V	201	CDL	CA2-OA2-PA1-OA5
52	l	702	CDL	CA2-OA2-PA1-OA5
52	s	401	CDL	CB3-OB5-PB2-OB2
48	B	303	PEE	C44-C45-C46-C47
52	o	201	CDL	C77-C78-C79-C80
49	j	202	PLX	C3-C4-C5-O8
52	i	401	CDL	CB3-CB4-CB6-OB8
52	a	201	CDL	C56-C57-C58-C59
52	g	202	CDL	C32-C31-CA7-OA8
48	U	101	PEE	C31-C32-C33-C34
48	r	501	PEE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
52	l	702	CDL	C38-C39-C40-C41
48	C	302	PEE	C31-C32-C33-C34
52	a	201	CDL	C84-C85-C86-C87
52	g	202	CDL	C1-CB2-OB2-PB2
52	a	201	CDL	C12-C13-C14-C15
52	s	401	CDL	C13-C14-C15-C16
52	i	403	CDL	C79-C80-C81-C82
52	s	401	CDL	C60-C61-C62-C63
49	a	202	PLX	C6-C7-C8-C9
52	a	201	CDL	CA7-C31-C32-C33
52	g	202	CDL	C31-CA7-OA8-CA6
46	A	502	FMN	O2'-C2'-C3'-O3'
52	g	202	CDL	OA9-CA7-OA8-CA6
52	i	401	CDL	C61-C62-C63-C64
52	l	702	CDL	C31-C32-C33-C34
52	a	201	CDL	C38-C39-C40-C41
48	C	302	PEE	C16-C17-C18-C19
48	i	402	PEE	C18-C19-C20-C21
54	J	402	UQ	C9-C11-C12-C13
52	i	401	CDL	C33-C34-C35-C36
52	V	201	CDL	C51-C52-C53-C54
52	o	201	CDL	C44-C45-C46-C47
48	C	302	PEE	C38-C39-C40-C41
48	l	703	PEE	C16-C17-C18-C19
52	g	202	CDL	OB7-CB5-OB6-CB4
52	l	701	CDL	C16-C17-C18-C19
52	l	702	CDL	C56-C57-C58-C59
52	s	401	CDL	C76-C77-C78-C79
49	g	201	PLX	O6-C6-C7-C8
52	g	202	CDL	C32-C31-CA7-OA9
52	l	701	CDL	OB6-CB4-CB6-OB8
48	l	703	PEE	C33-C34-C35-C36
48	j	201	PEE	C31-C32-C33-C34
48	l	704	PEE	C23-C24-C25-C26
49	j	202	PLX	C29-C30-C31-C32
49	C	303	PLX	C11-C10-C9-C8
49	r	503	PLX	C24-C25-C26-C27
52	l	701	CDL	C17-C18-C19-C20
52	i	401	CDL	C37-C38-C39-C40
52	s	401	CDL	CB3-CB4-CB6-OB8
52	s	401	CDL	C12-C11-CA5-OA7
51	G	201	8Q1	O27-C28-C29-C31

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Mol	Chain	Res	Type	Atoms
48	U	101	PEE	C20-C21-C22-C23
52	i	403	CDL	C13-C14-C15-C16
52	o	201	CDL	CB2-OB2-PB2-OB5
49	a	202	PLX	C14-C15-C16-C17
47	A	503	NAI	C2D-C1D-N1N-C6N
52	V	201	CDL	C36-C37-C38-C39
48	r	501	PEE	O3P-C1-C2-O2
48	B	303	PEE	C18-C19-C20-C21
49	r	502	PLX	C18-C19-C20-C21
52	i	401	CDL	C62-C63-C64-C65
52	i	401	CDL	C32-C33-C34-C35
48	i	402	PEE	C32-C33-C34-C35
51	G	201	8Q1	C13-C14-C15-C16
49	g	201	PLX	C17-C18-C19-C20
52	g	202	CDL	C72-C73-C74-C75
52	l	702	CDL	C53-C54-C55-C56
48	C	302	PEE	C35-C36-C37-C38
48	l	704	PEE	C35-C36-C37-C38
53	J	401	NDP	O4D-C1D-N1N-C6N
48	B	303	PEE	C37-C38-C39-C40
54	s	402	UQ	C24-C26-C27-C28
48	W	201	PEE	C16-C17-C18-C19
52	o	201	CDL	C16-C17-C18-C19
48	B	303	PEE	C24-C25-C26-C27
49	r	503	PLX	C26-C27-C28-C29
49	r	503	PLX	C2-C1-N1-C1C
49	g	201	PLX	C11-C12-C13-C14
48	U	101	PEE	C38-C39-C40-C41
48	l	703	PEE	C42-C43-C44-C45
49	a	202	PLX	C3-C4-C5-O8
49	r	502	PLX	C3-C4-C5-O8
54	J	402	UQ	C20-C19-C21-C22
52	i	403	CDL	C12-C13-C14-C15
48	U	101	PEE	C43-C44-C45-C46
52	a	201	CDL	C43-C44-C45-C46
52	a	201	CDL	C61-C62-C63-C64
48	C	302	PEE	C18-C19-C20-C21
48	W	201	PEE	C18-C19-C20-C21
52	a	201	CDL	OB5-CB3-CB4-OB6
52	a	201	CDL	C15-C16-C17-C18
49	j	202	PLX	C34-C35-C36-C37
49	g	201	PLX	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
52	a	201	CDL	OB5-CB3-CB4-CB6
48	l	703	PEE	C13-C14-C15-C16
49	r	502	PLX	C4-C3-O4-P1
49	r	503	PLX	C19-C20-C21-C22
47	A	503	NAI	O4D-C4D-C5D-O5D
53	J	401	NDP	O4D-C4D-C5D-O5D
49	a	202	PLX	C16-C17-C18-C19
53	J	401	NDP	C2B-O2B-P2B-O1X
52	l	701	CDL	C63-C64-C65-C66
52	o	201	CDL	CA3-OA5-PA1-OA2
49	r	502	PLX	C19-C20-C21-C22
52	V	202	CDL	C16-C17-C18-C19
52	I	201	CDL	C12-C11-CA5-OA6
52	V	202	CDL	C12-C11-CA5-OA6
52	I	201	CDL	C52-C51-CB5-OB6
52	V	201	CDL	C32-C31-CA7-OA8
52	l	702	CDL	C12-C11-CA5-OA6
48	U	101	PEE	C16-C17-C18-C19
48	i	402	PEE	C38-C39-C40-C41
48	j	201	PEE	C18-C19-C20-C21
48	l	704	PEE	C38-C39-C40-C41
52	V	202	CDL	CA6-CA4-OA6-CA5
49	g	201	PLX	C26-C27-C28-C29
52	a	201	CDL	OA7-CA5-OA6-CA4
47	A	503	NAI	O4D-C1D-N1N-C6N
52	a	201	CDL	C12-C11-CA5-OA6
48	B	303	PEE	O2-C10-C11-C12
48	C	302	PEE	O3-C30-C31-C32
48	U	101	PEE	O3-C30-C31-C32
52	l	702	CDL	C32-C31-CA7-OA8
48	B	303	PEE	C41-C42-C43-C44
52	l	701	CDL	C72-C71-CB7-OB8
49	a	202	PLX	C2-C1-N1-C1C
52	l	701	CDL	C21-C22-C23-C24
51	X	201	8Q1	C13-C14-C15-C16
48	B	303	PEE	C16-C17-C18-C19
48	i	402	PEE	C16-C17-C18-C19
48	i	402	PEE	C36-C37-C38-C39
48	i	402	PEE	C13-C14-C15-C16
49	r	503	PLX	C2-C1-N1-C1B
49	r	503	PLX	C2-C1-N1-C1A
49	C	303	PLX	O7-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
53	J	401	NDP	C2B-O2B-P2B-O2X
48	j	201	PEE	C24-C25-C26-C27
52	a	201	CDL	C11-CA5-OA6-CA4
52	l	702	CDL	C72-C71-CB7-OB8
52	i	403	CDL	C64-C65-C66-C67
49	r	503	PLX	C11-C10-C9-C8
48	j	201	PEE	C16-C17-C18-C19
52	i	401	CDL	C12-C11-CA5-OA6
48	B	303	PEE	C22-C23-C24-C25
52	I	201	CDL	C72-C71-CB7-OB8
48	C	302	PEE	O5-C30-C31-C32
52	g	202	CDL	C52-C51-CB5-OB6
48	l	703	PEE	C38-C39-C40-C41
48	U	101	PEE	C34-C35-C36-C37
52	V	202	CDL	C77-C78-C79-C80
52	a	201	CDL	C53-C54-C55-C56
52	I	201	CDL	C12-C11-CA5-OA7
52	V	202	CDL	C12-C11-CA5-OA7
52	s	401	CDL	C31-CA7-OA8-CA6
52	a	201	CDL	C76-C77-C78-C79
52	I	201	CDL	C72-C71-CB7-OB9
52	l	702	CDL	C32-C31-CA7-OA9
52	V	202	CDL	CA7-C31-C32-C33
48	B	303	PEE	O4-C10-C11-C12
49	C	303	PLX	C2-O1-P1-O4
48	U	101	PEE	C21-C22-C23-C24
48	r	501	PEE	C40-C41-C42-C43
52	a	201	CDL	C12-C11-CA5-OA7
52	i	401	CDL	C12-C11-CA5-OA7
52	l	701	CDL	OA7-CA5-OA6-CA4
48	l	703	PEE	C36-C37-C38-C39
47	A	503	NAI	C5B-O5B-PA-O2A
47	A	503	NAI	C2N-C3N-C7N-N7N
48	B	303	PEE	C1-O3P-P-O1P
48	l	703	PEE	C1-O3P-P-O1P
49	a	202	PLX	C3-O4-P1-O2
49	a	202	PLX	C2-C1-N1-C1B
49	j	202	PLX	C2-O1-P1-O2
54	s	402	UQ	C6-C7-C8-C9
52	l	701	CDL	C24-C25-C26-C27
48	U	101	PEE	O5-C30-C31-C32
52	i	403	CDL	OB5-CB3-CB4-CB6

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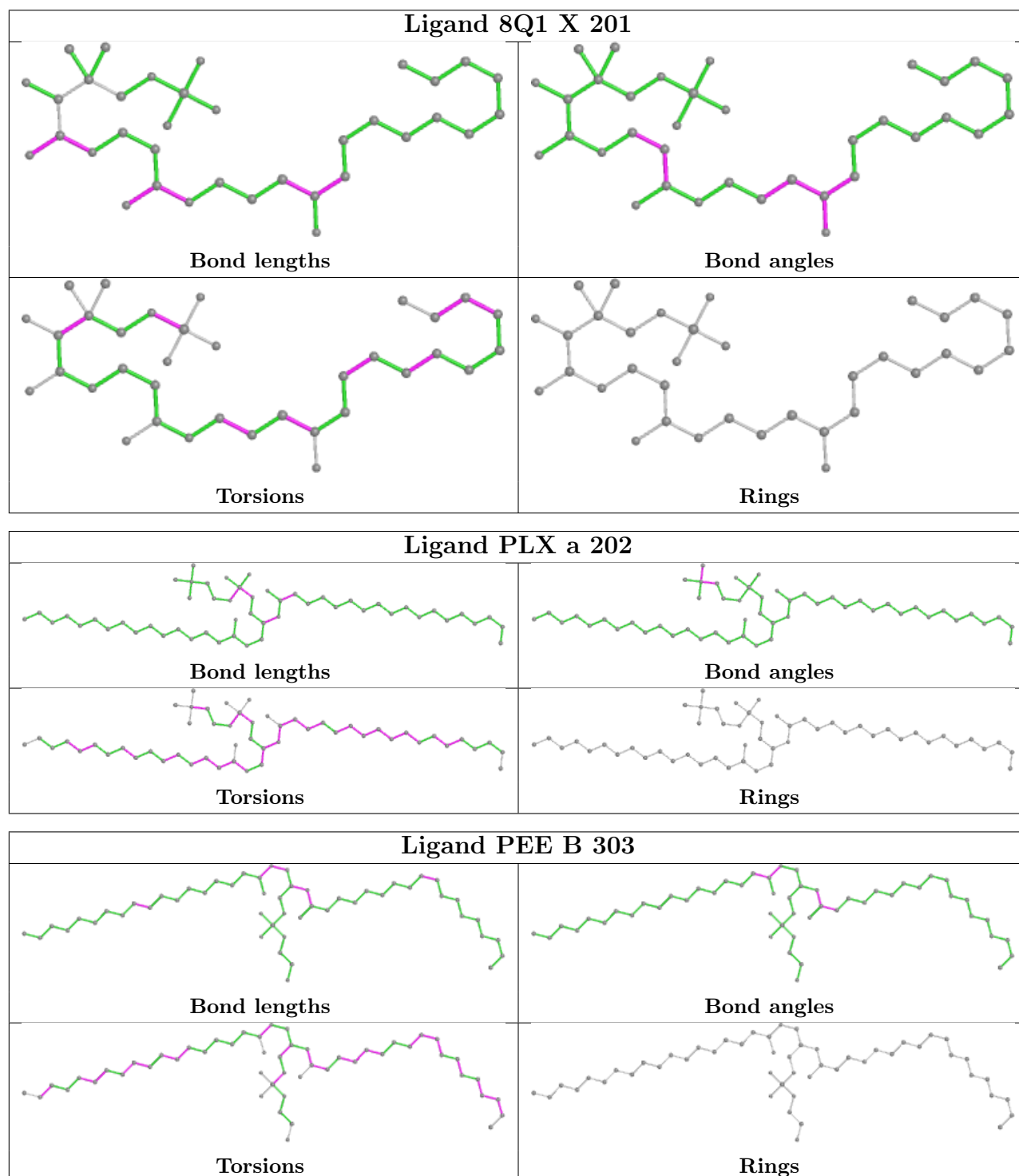
Mol	Chain	Res	Type	Atoms
52	a	201	CDL	C44-C45-C46-C47
52	l	702	CDL	C60-C61-C62-C63
52	i	403	CDL	C57-C58-C59-C60
52	I	201	CDL	C52-C51-CB5-OB7
52	l	701	CDL	C72-C71-CB7-OB9
54	s	402	UQ	C12-C13-C14-C16
52	a	201	CDL	C72-C73-C74-C75
52	g	202	CDL	C52-C51-CB5-OB7
54	s	402	UQ	C1-C2-O2-CM2
48	l	703	PEE	C1-C2-O2-C10
48	r	501	PEE	C5-C4-O4P-P
52	V	202	CDL	CA3-CA4-OA6-CA5
52	s	401	CDL	OA9-CA7-OA8-CA6
51	X	201	8Q1	C12-C13-C14-C15
52	g	202	CDL	C12-C11-CA5-OA6
48	i	402	PEE	C39-C40-C41-C42
52	V	202	CDL	C32-C31-CA7-OA8
52	V	201	CDL	C1-CB2-OB2-PB2
52	l	701	CDL	C20-C21-C22-C23
52	l	702	CDL	C72-C71-CB7-OB9
52	i	401	CDL	C32-C31-CA7-OA8
52	o	201	CDL	C52-C51-CB5-OB6
52	o	201	CDL	C52-C51-CB5-OB7
49	r	503	PLX	C9-C10-C11-C12
52	a	201	CDL	C33-C34-C35-C36
52	i	403	CDL	C72-C71-CB7-OB8
52	V	202	CDL	C32-C31-CA7-OA9
51	G	201	8Q1	C11-C10-C9-C8
52	i	401	CDL	C32-C31-CA7-OA9

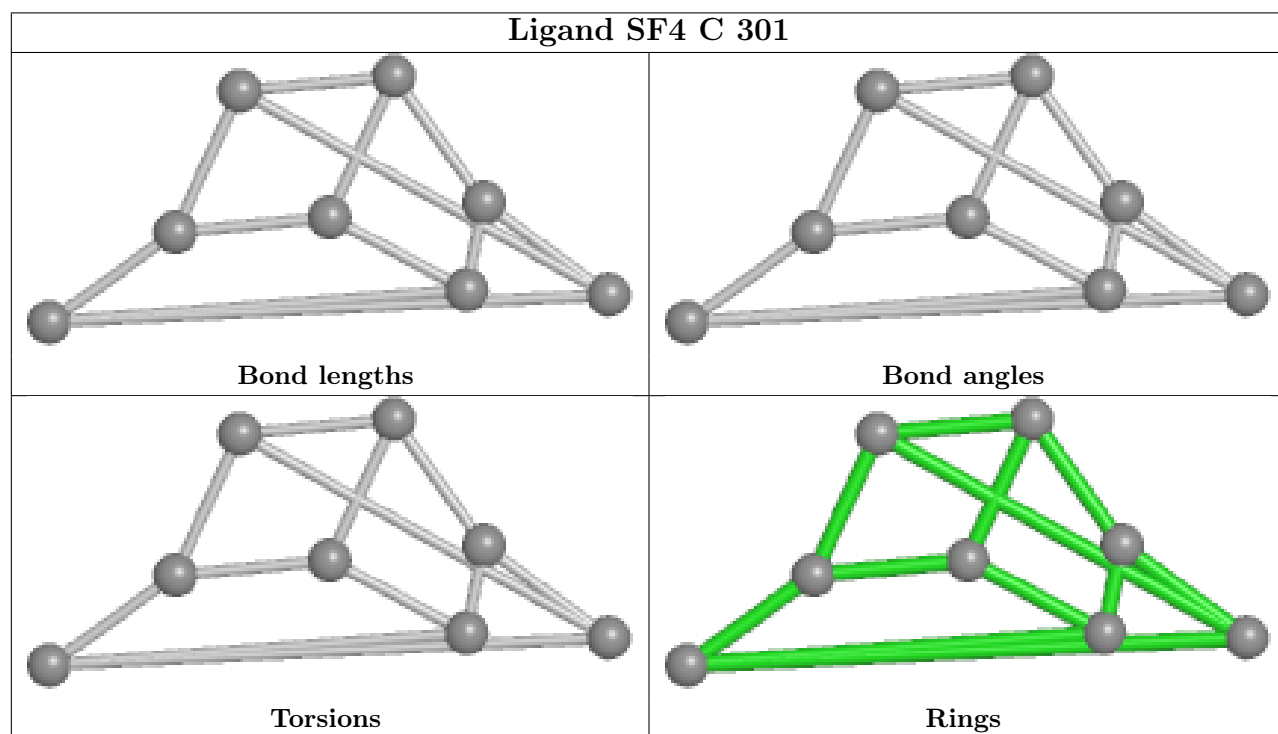
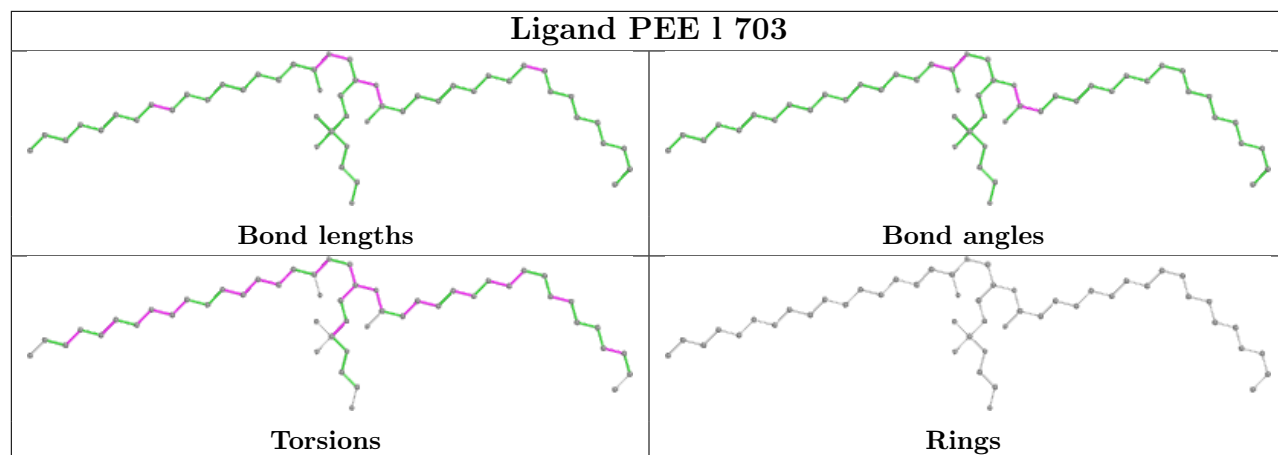
There are no ring outliers.

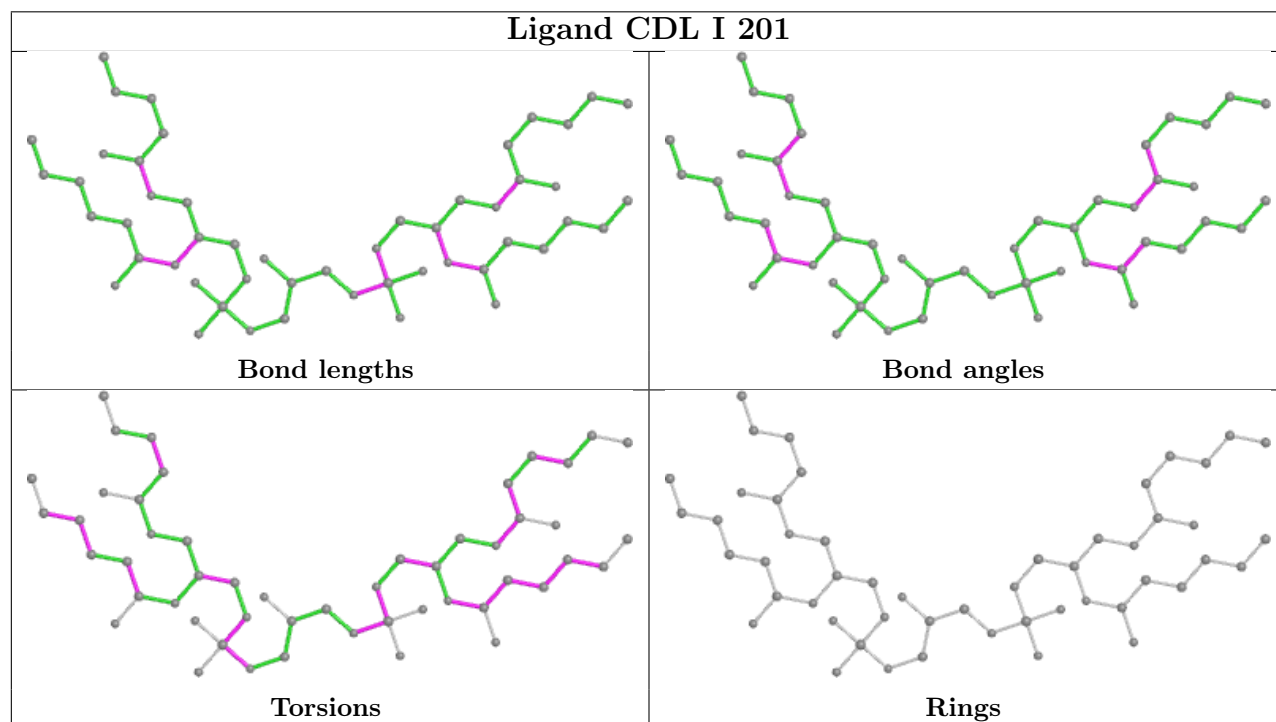
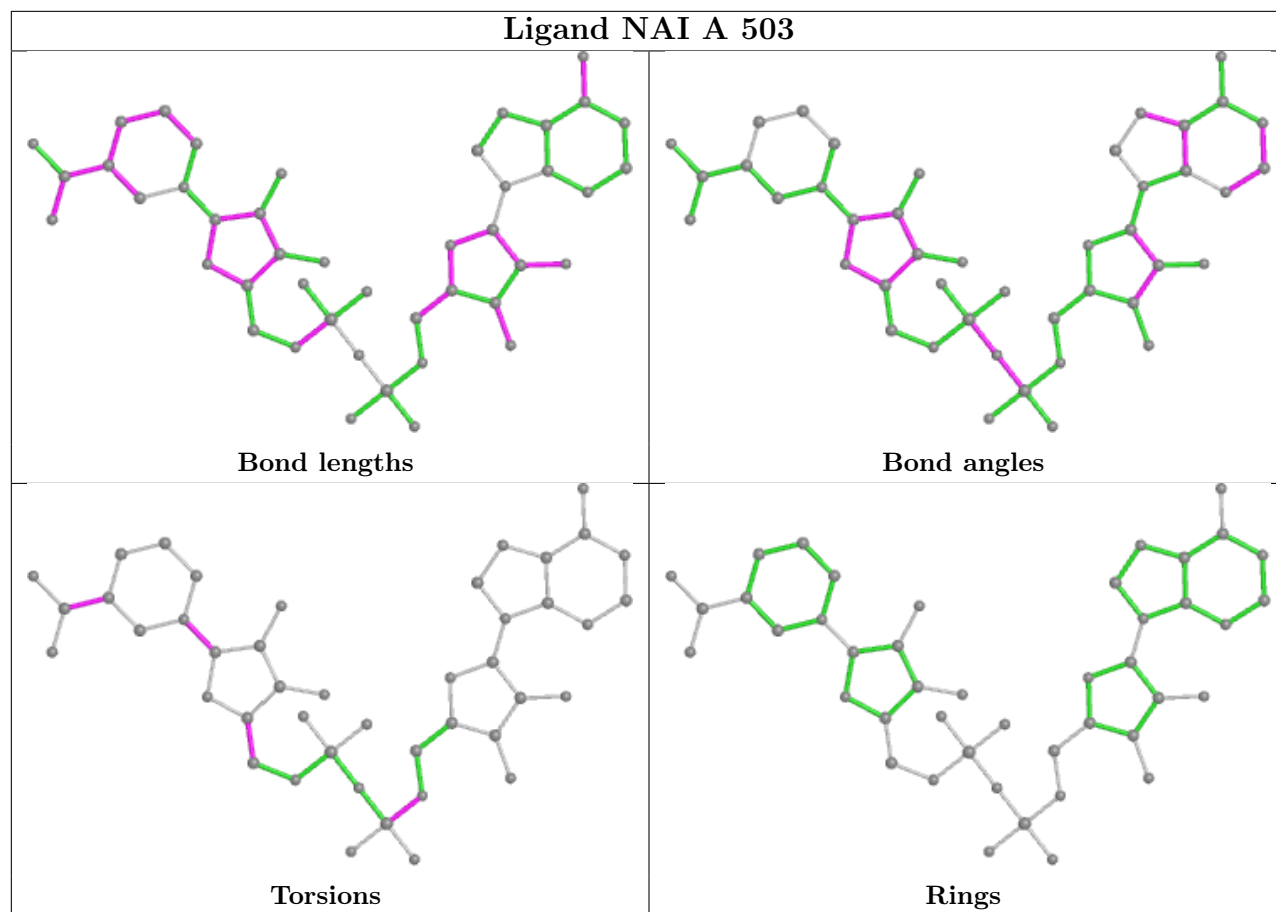
No monomer is involved in short contacts.

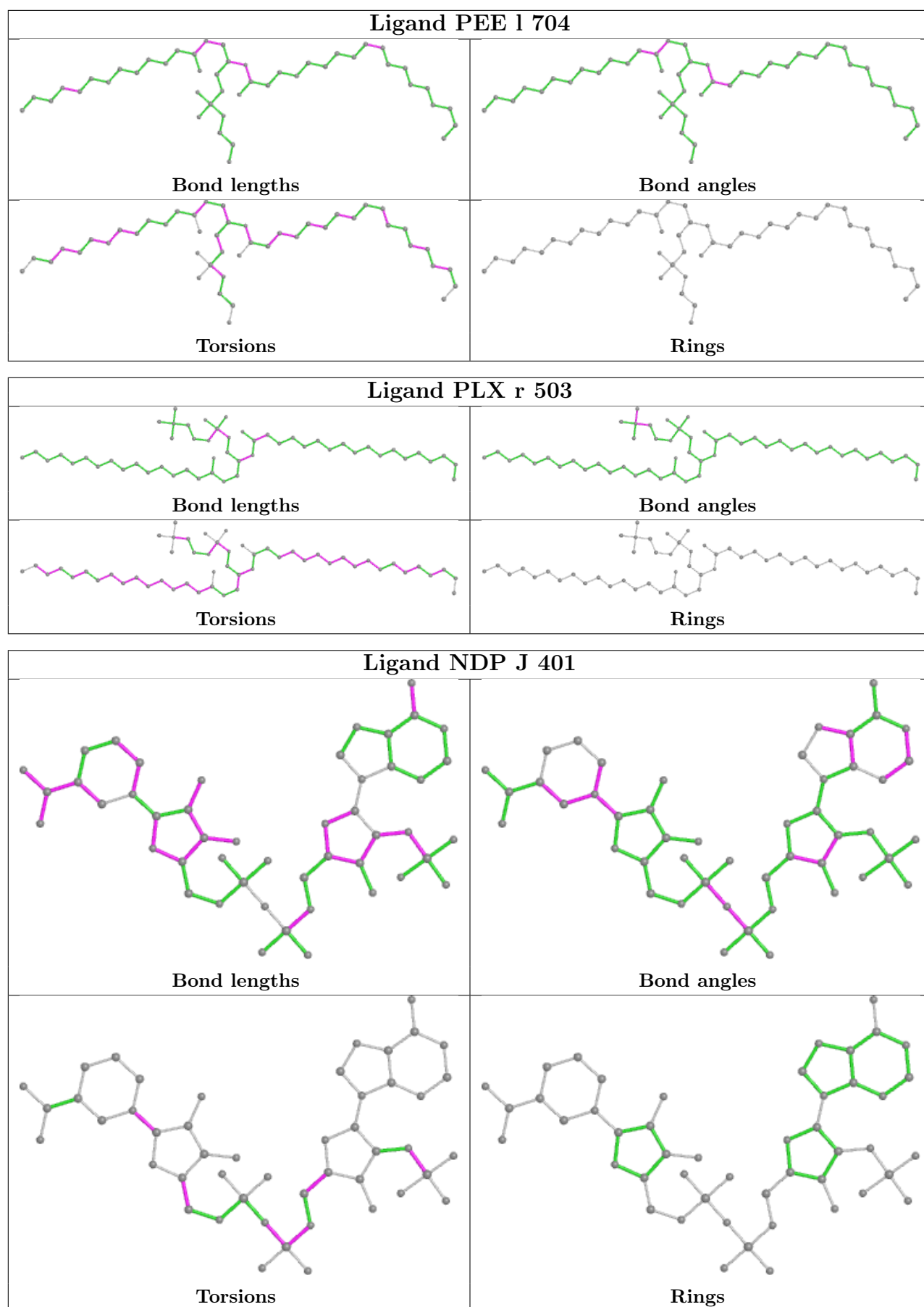
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

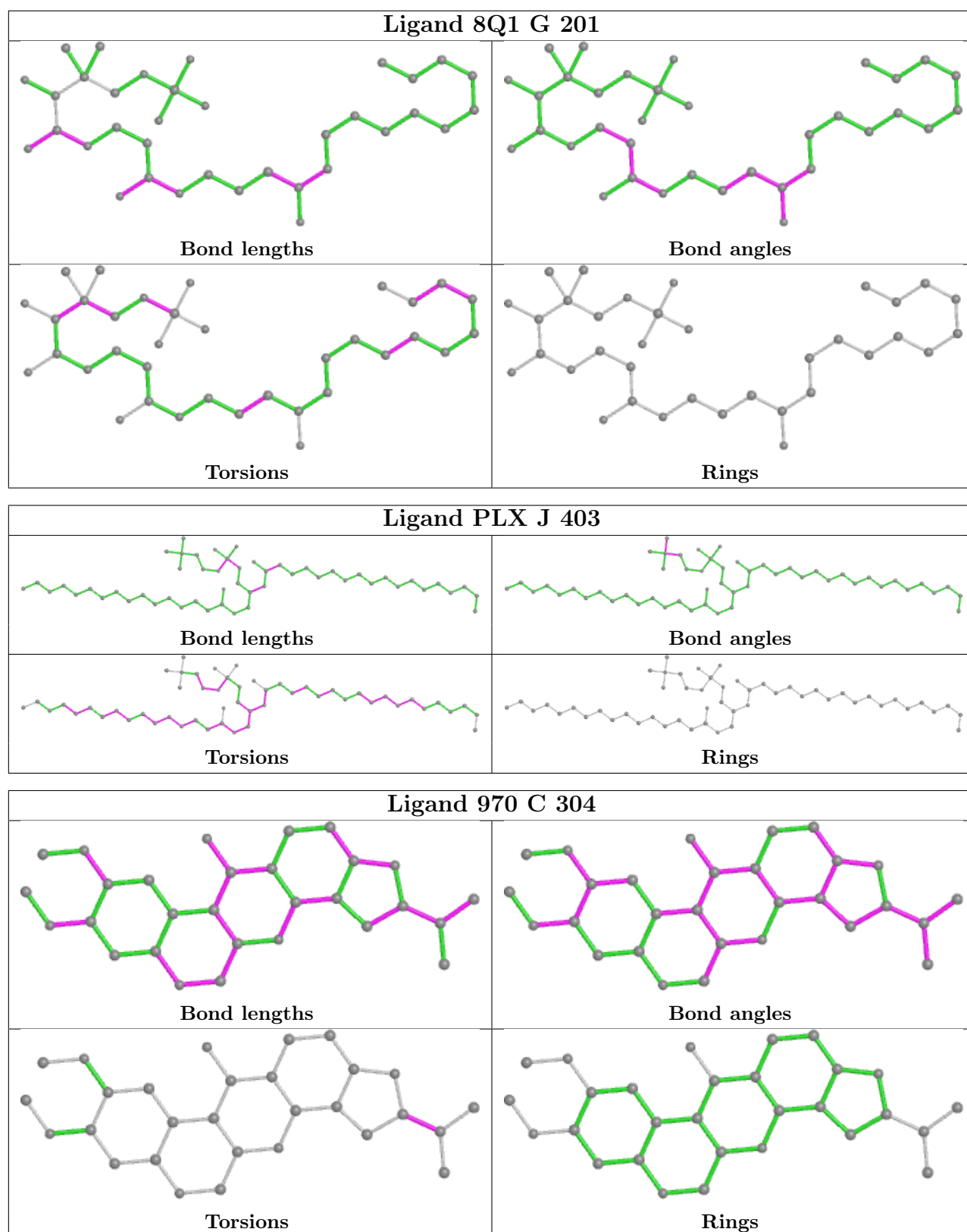
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

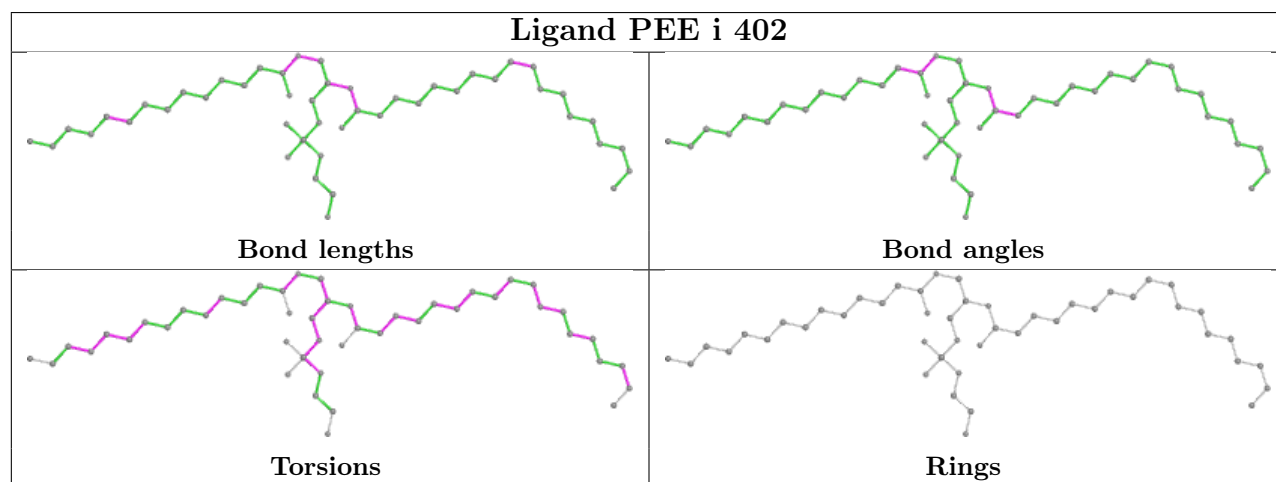
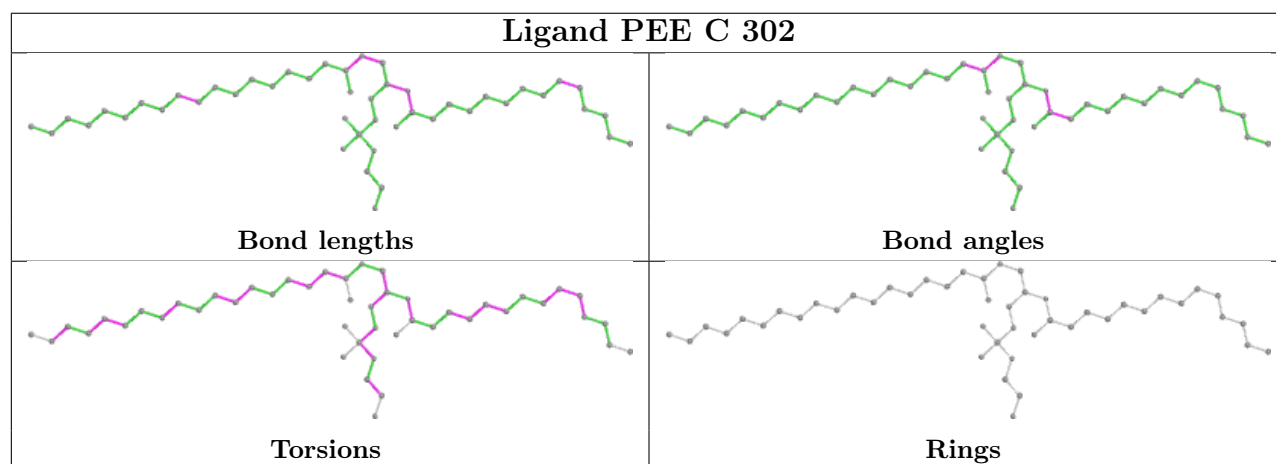
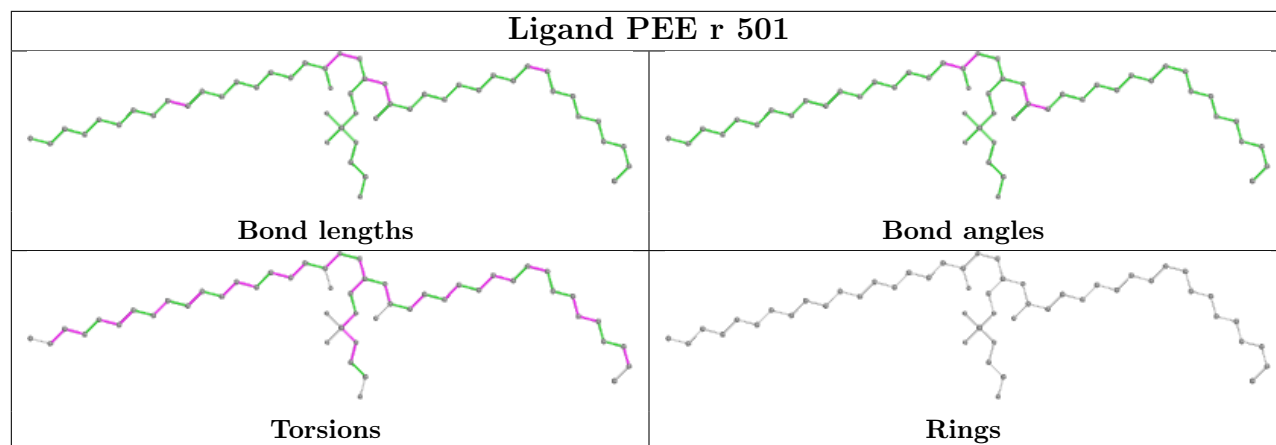


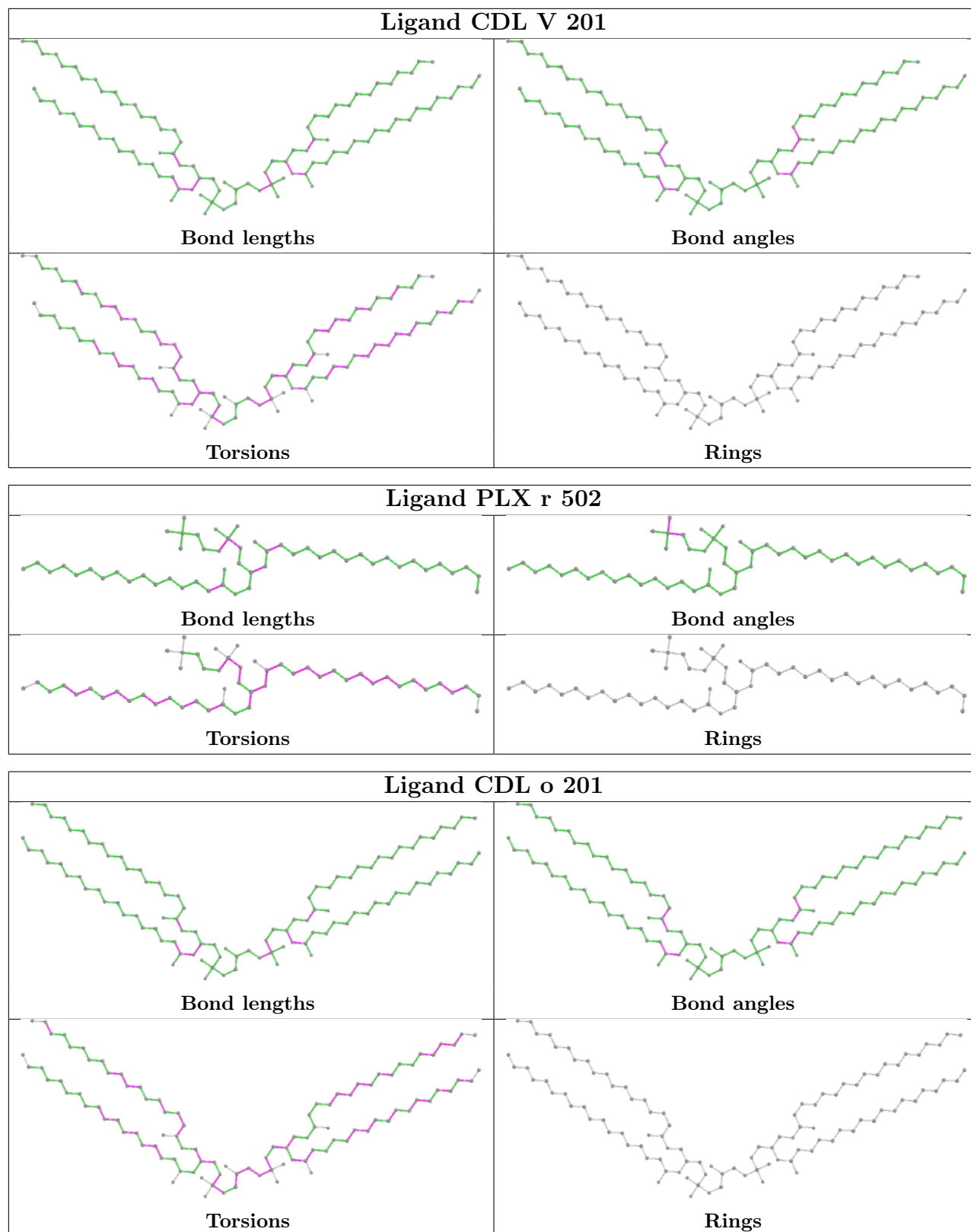


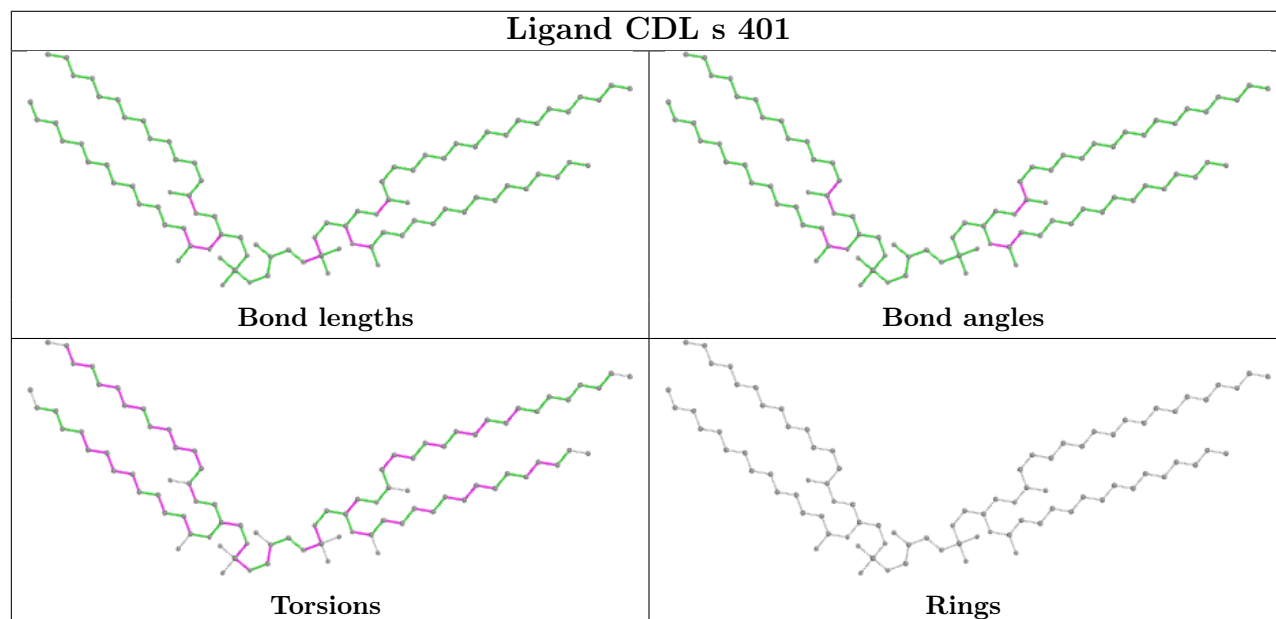
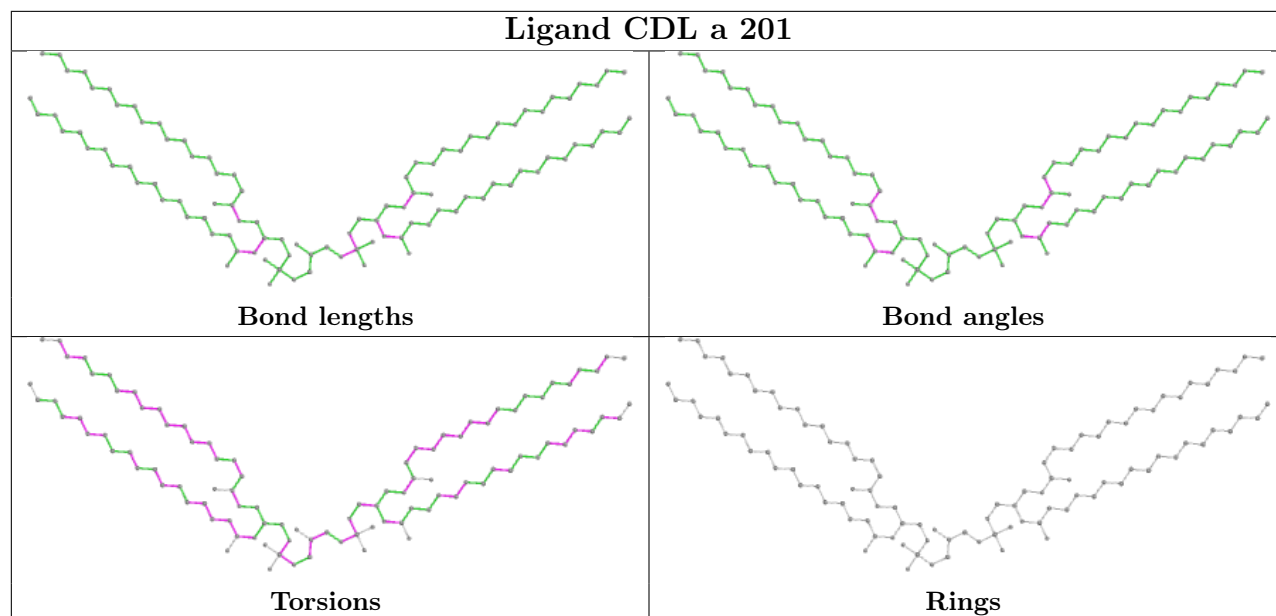


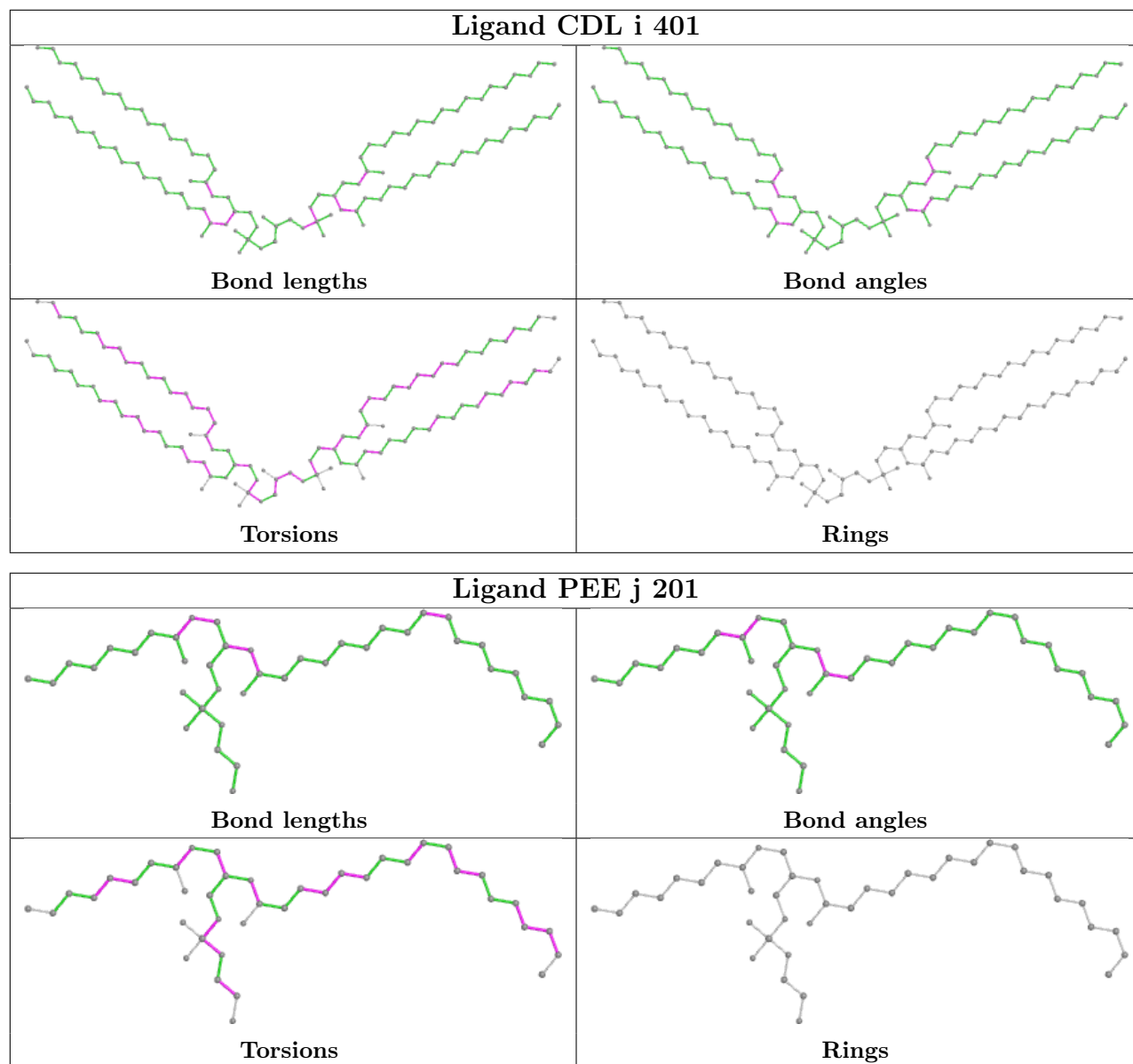


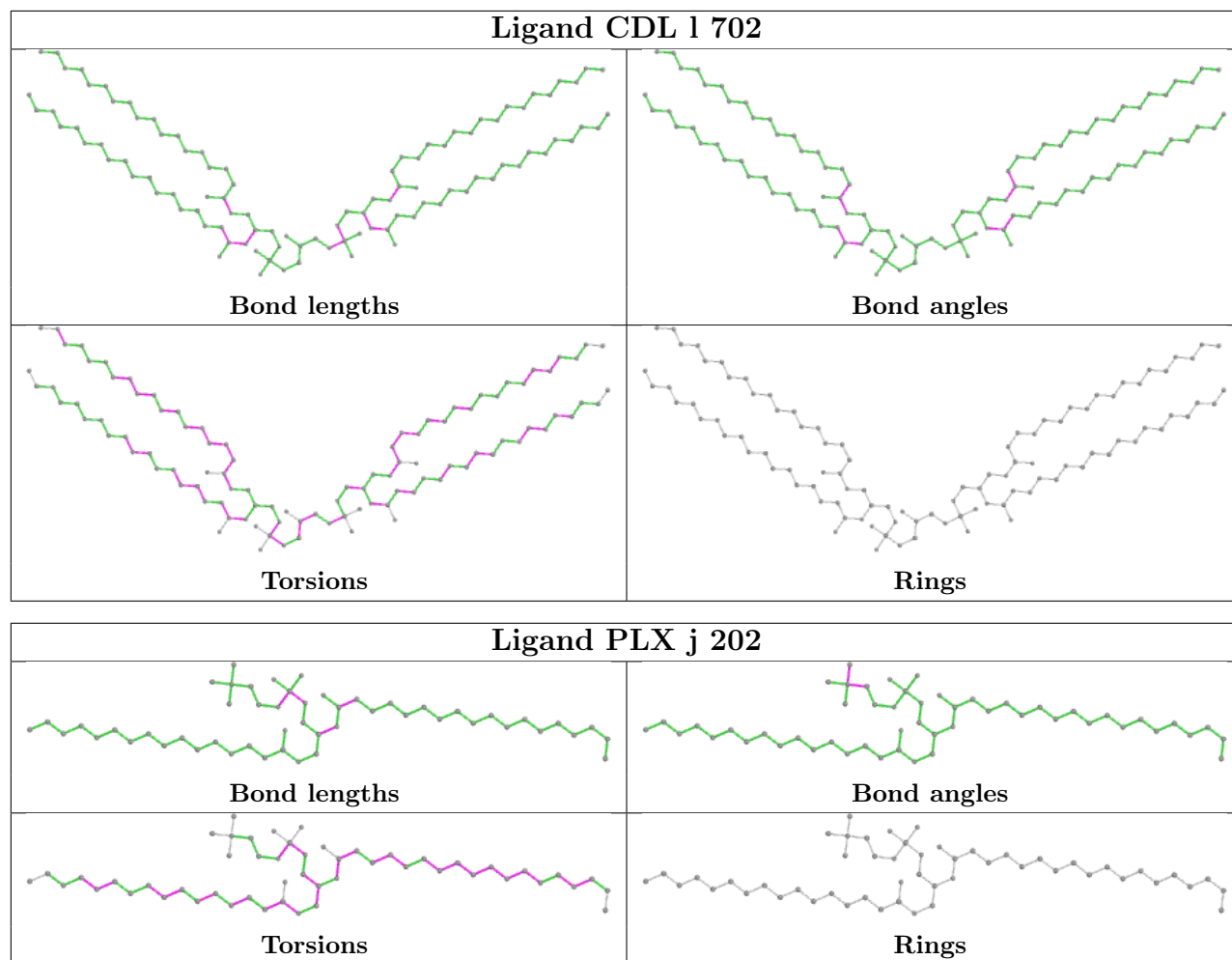


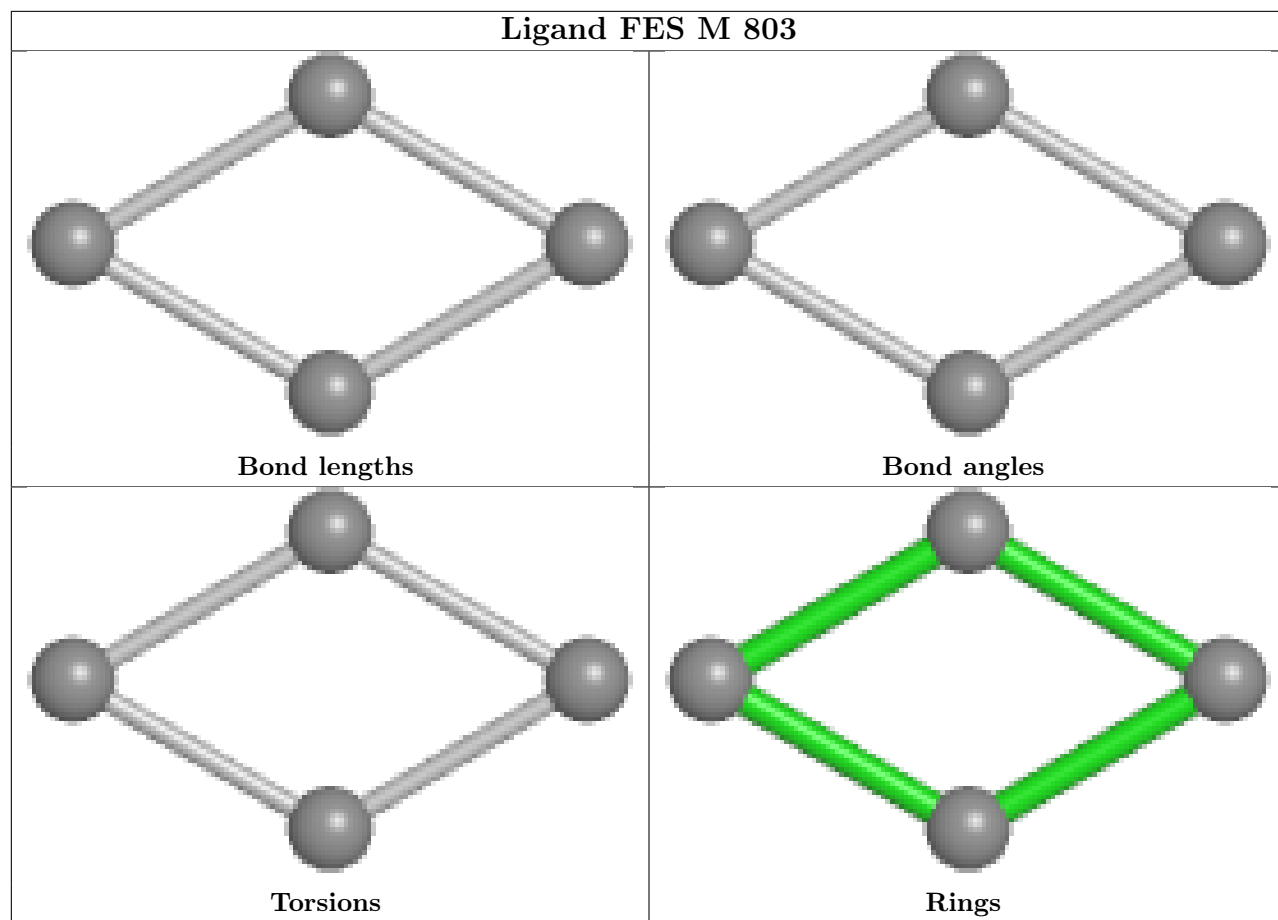


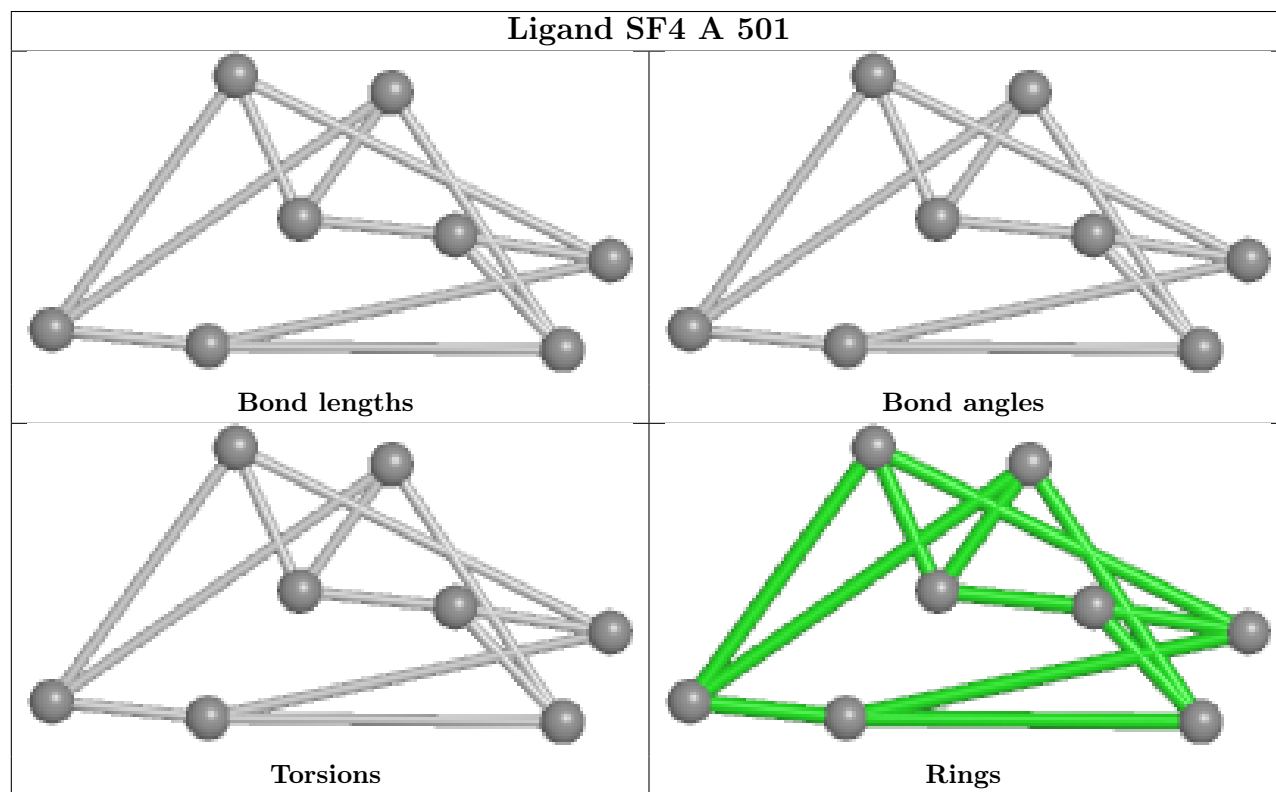
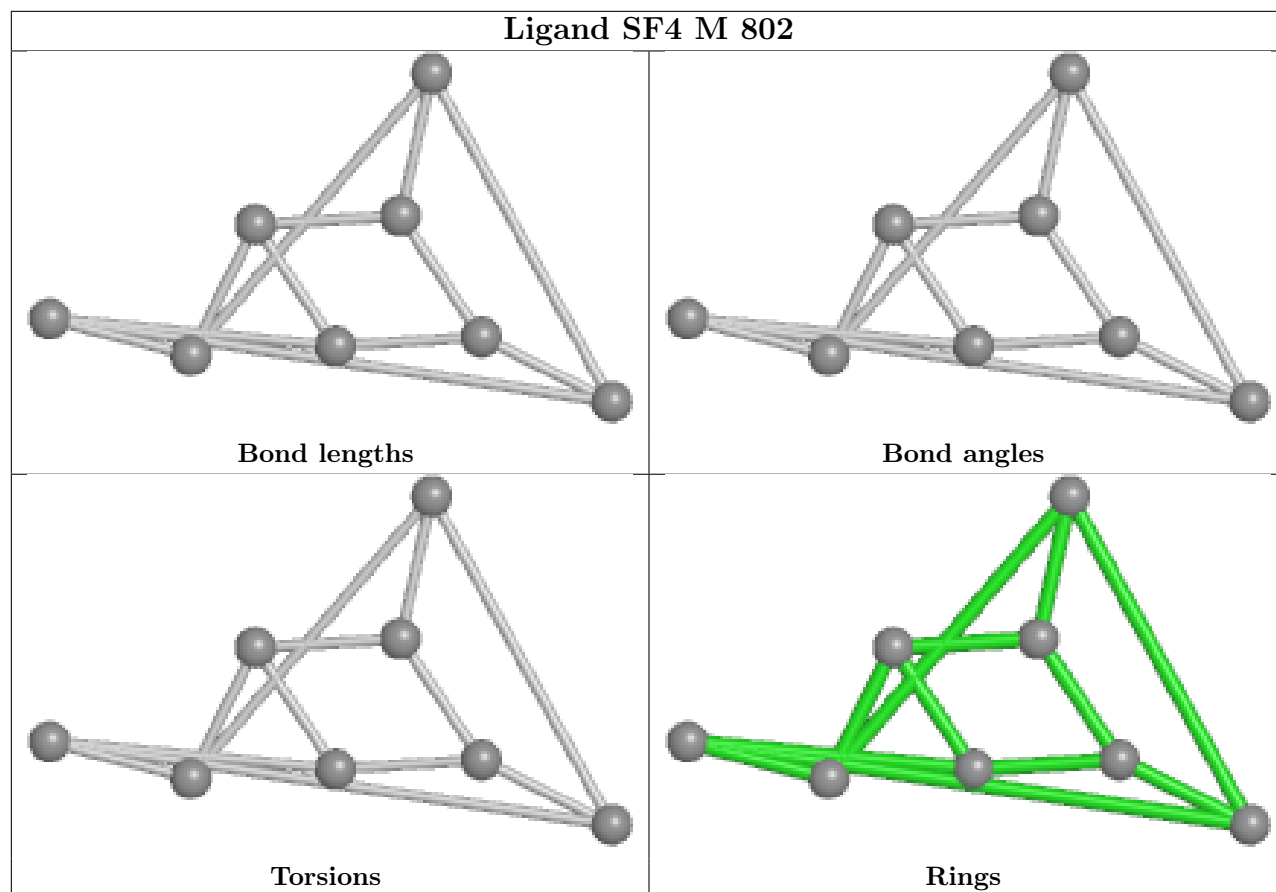


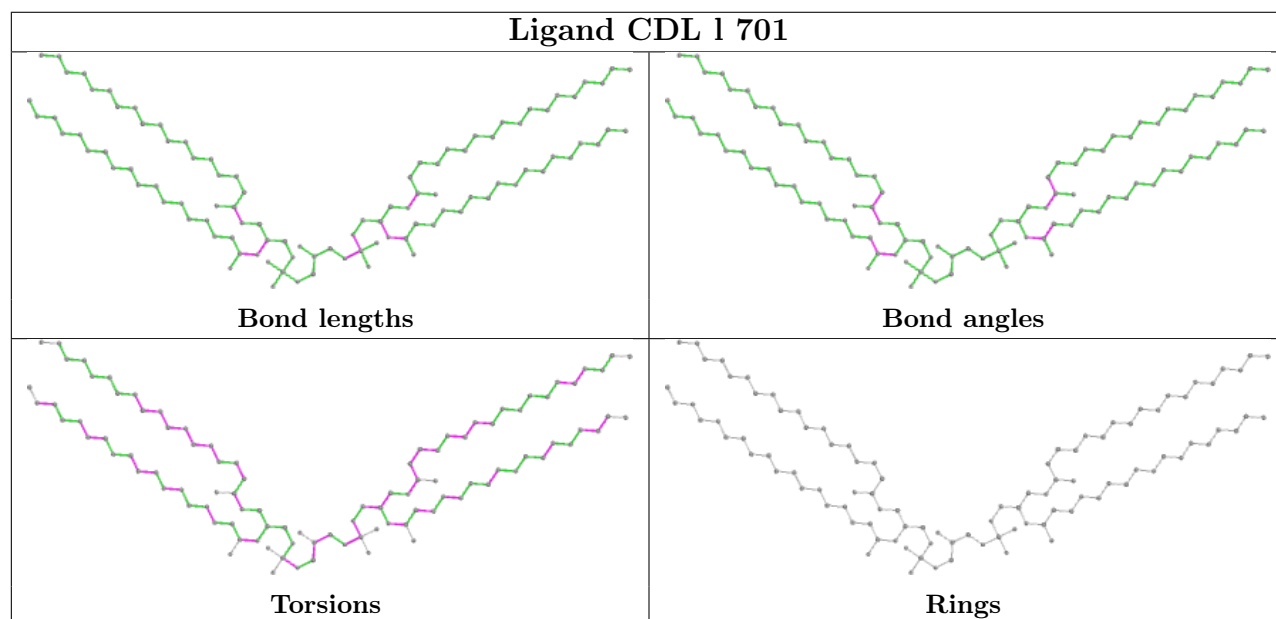
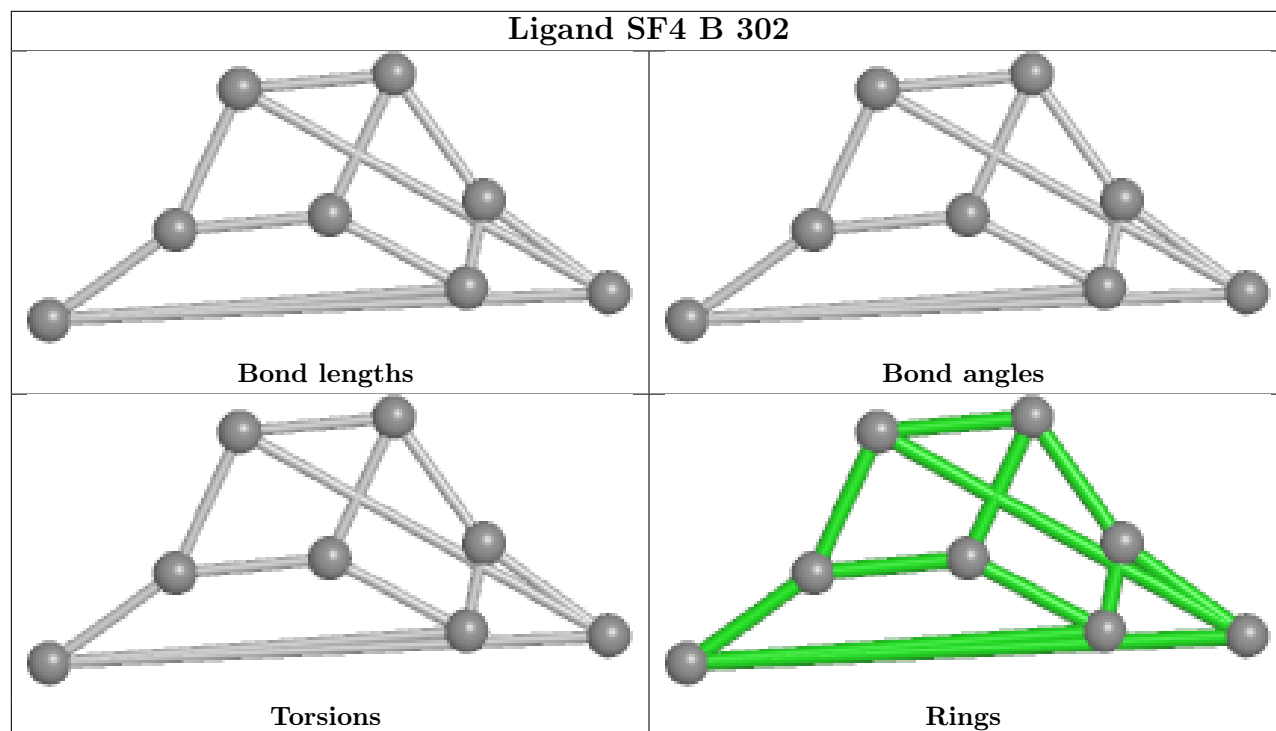


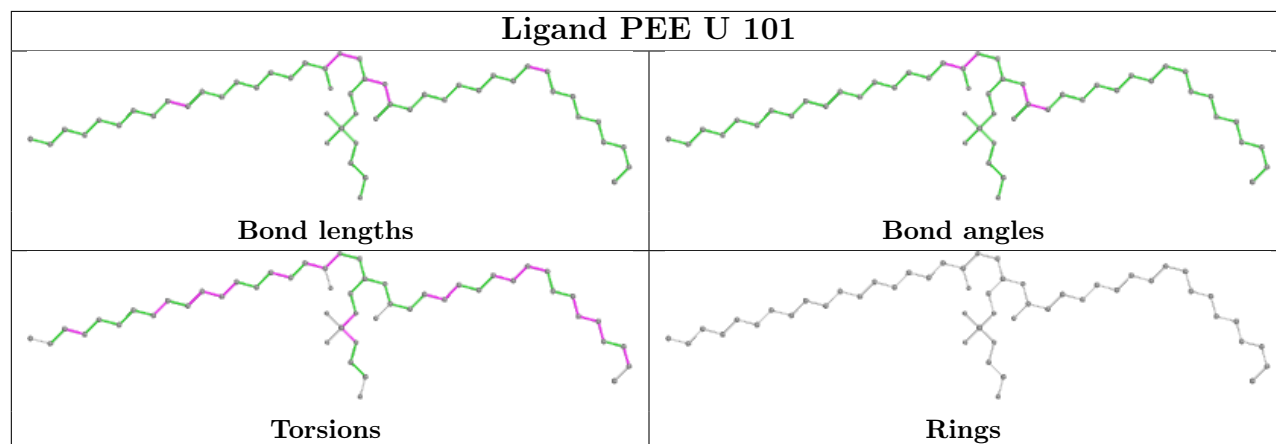
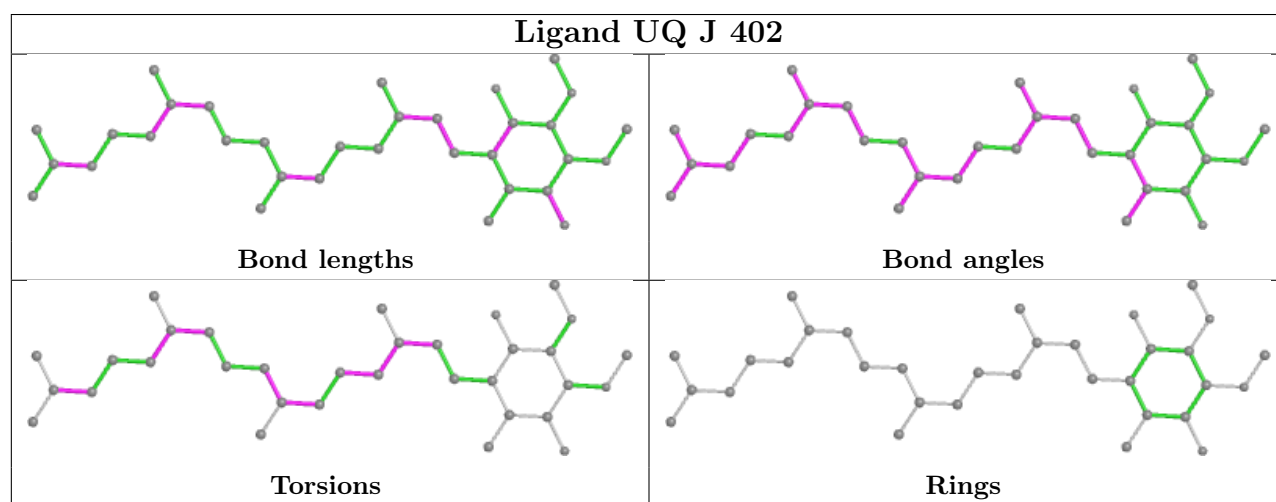
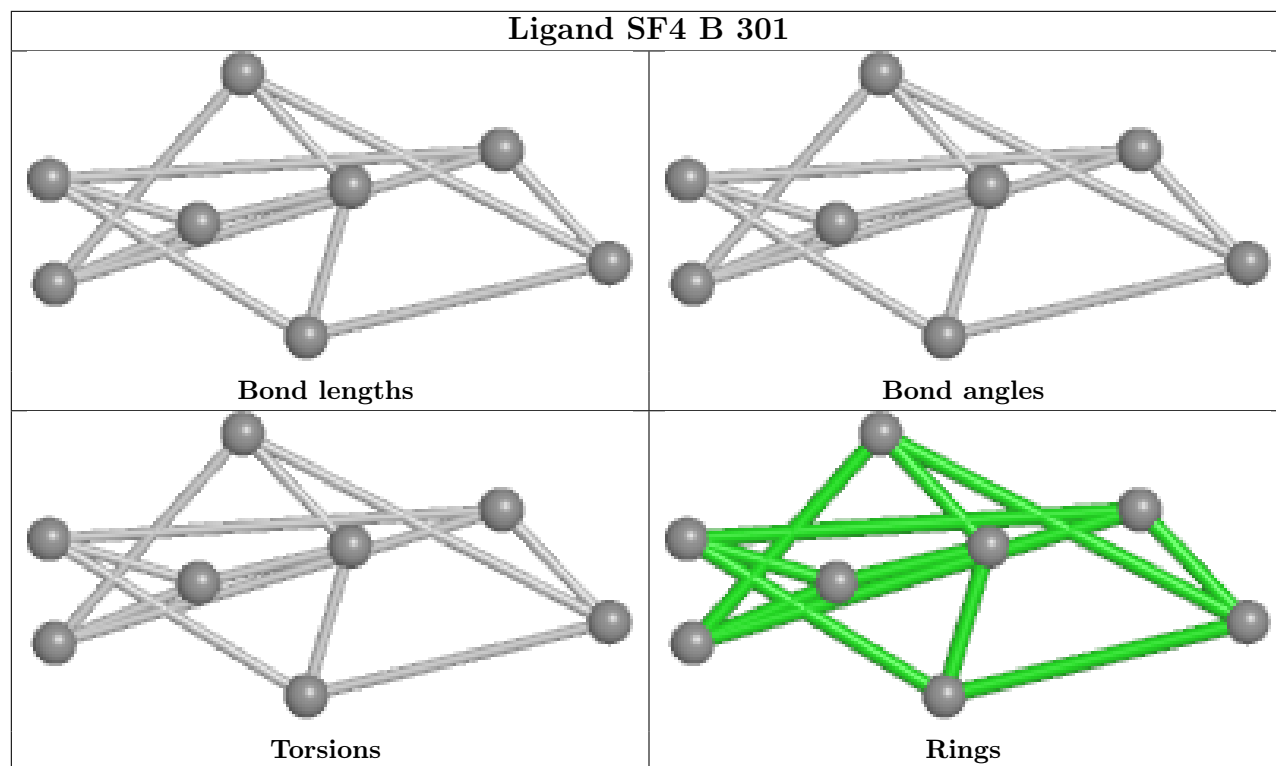


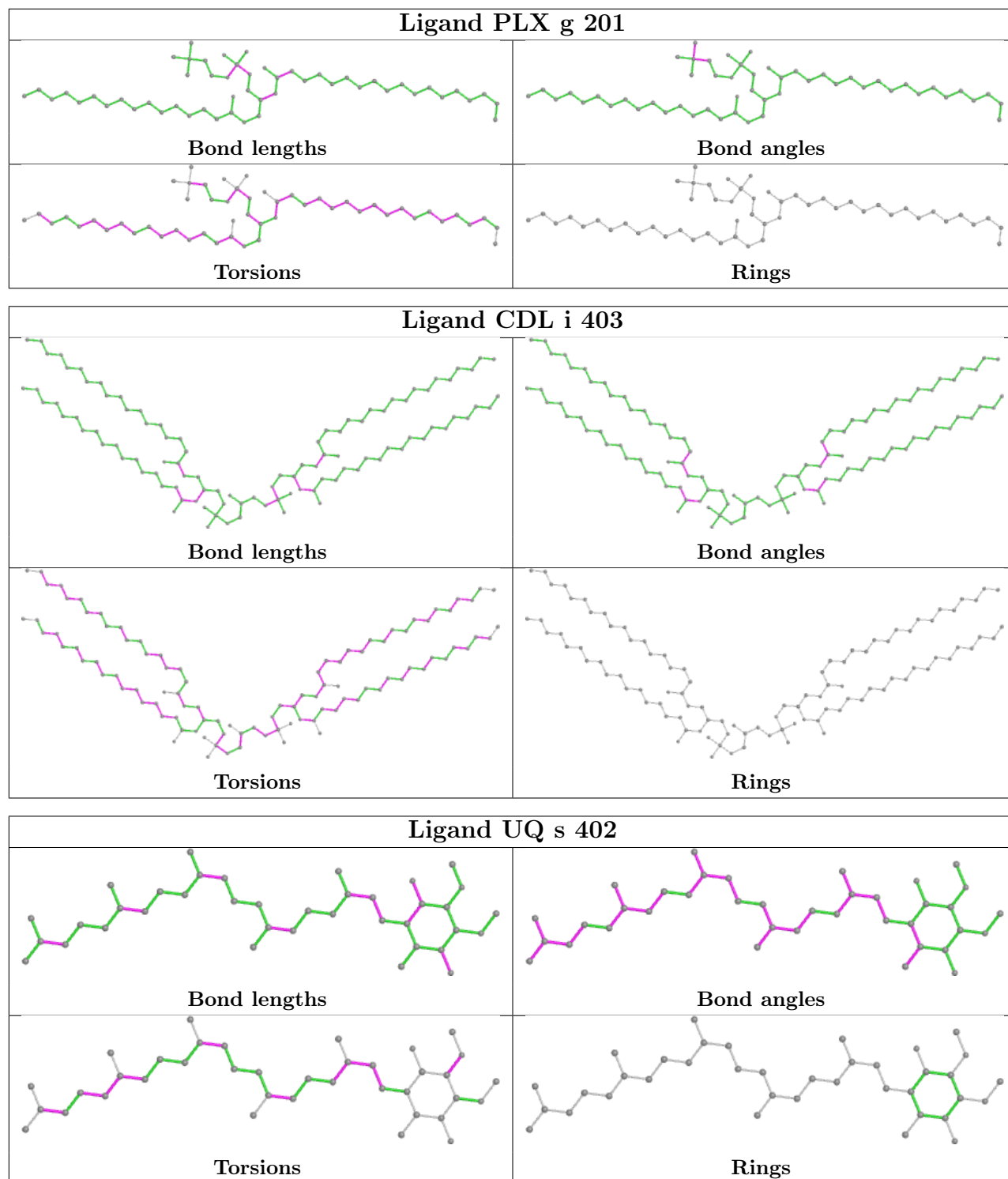


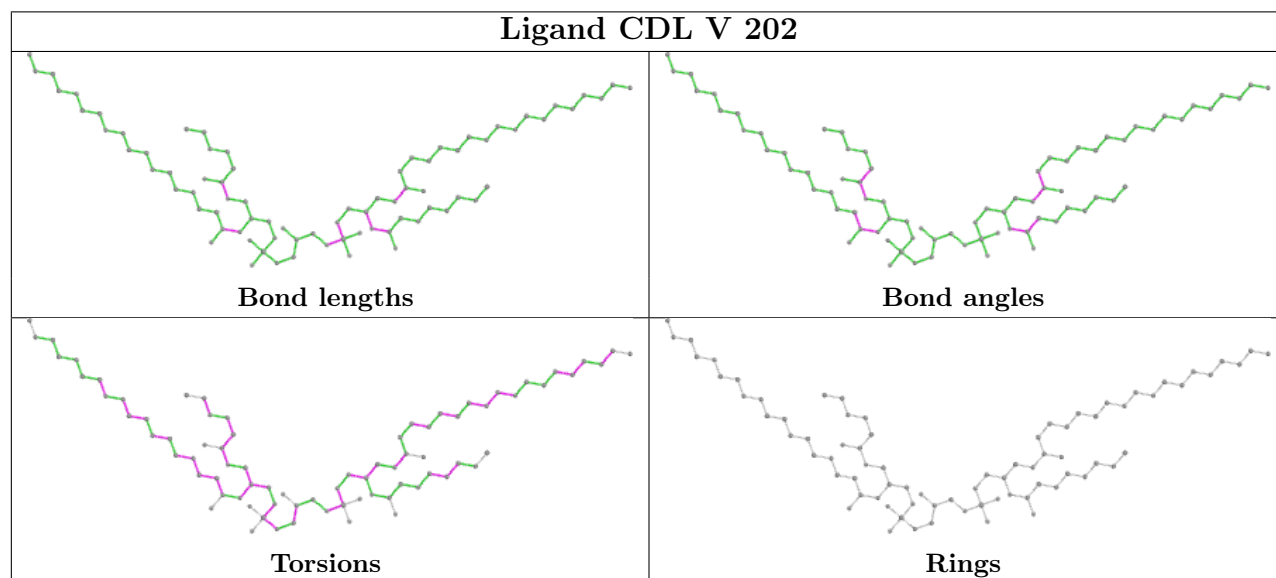
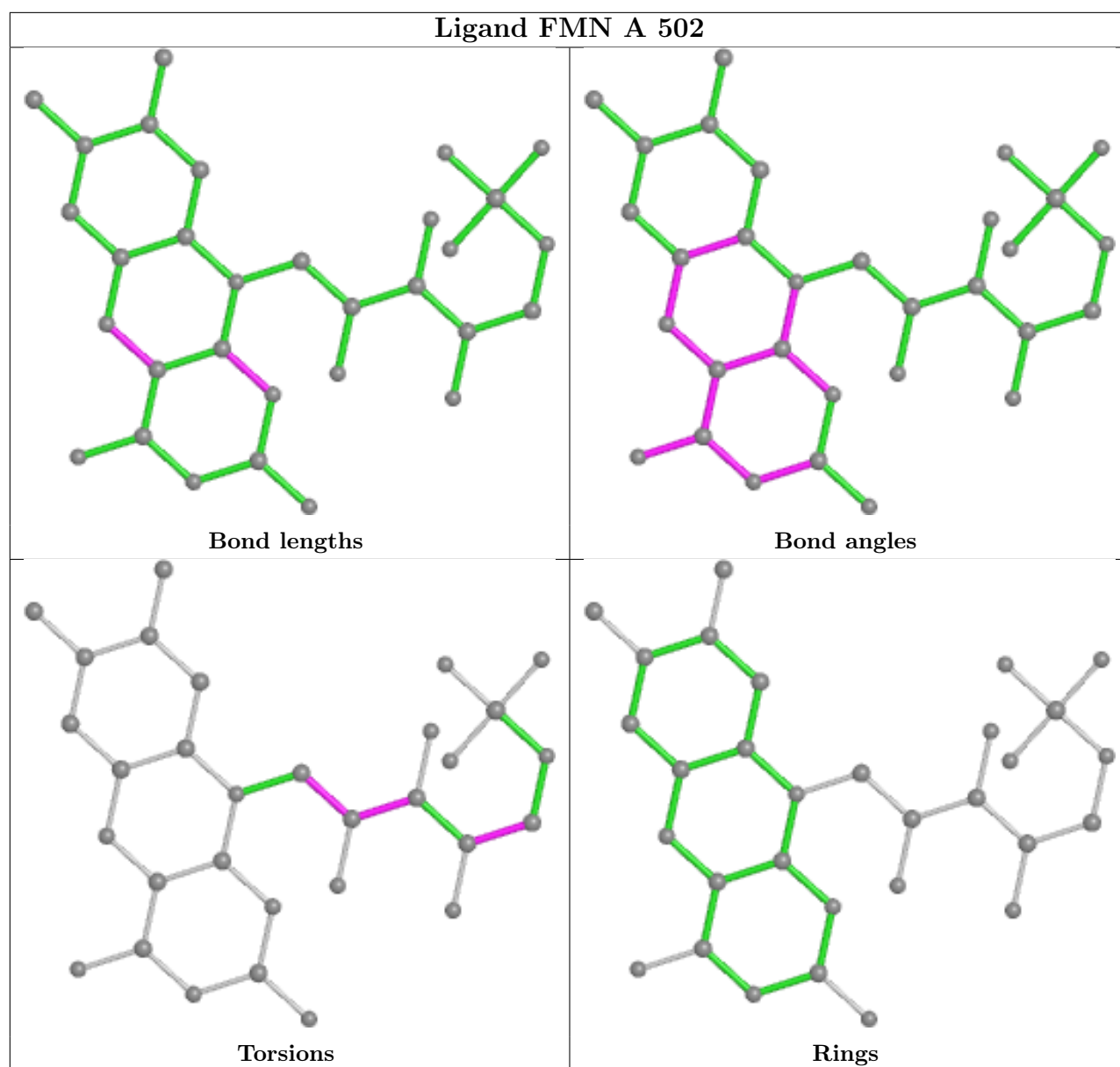


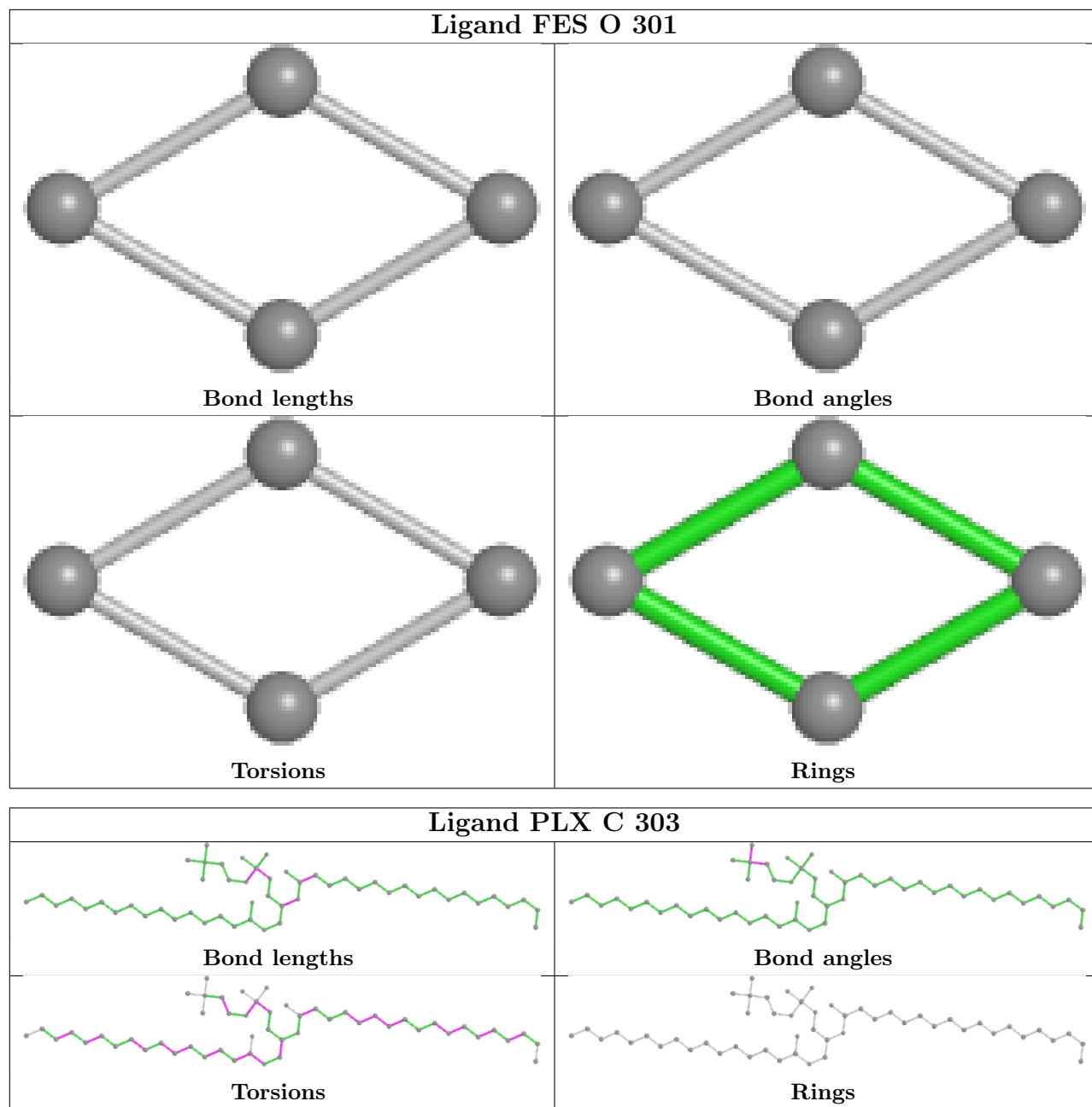


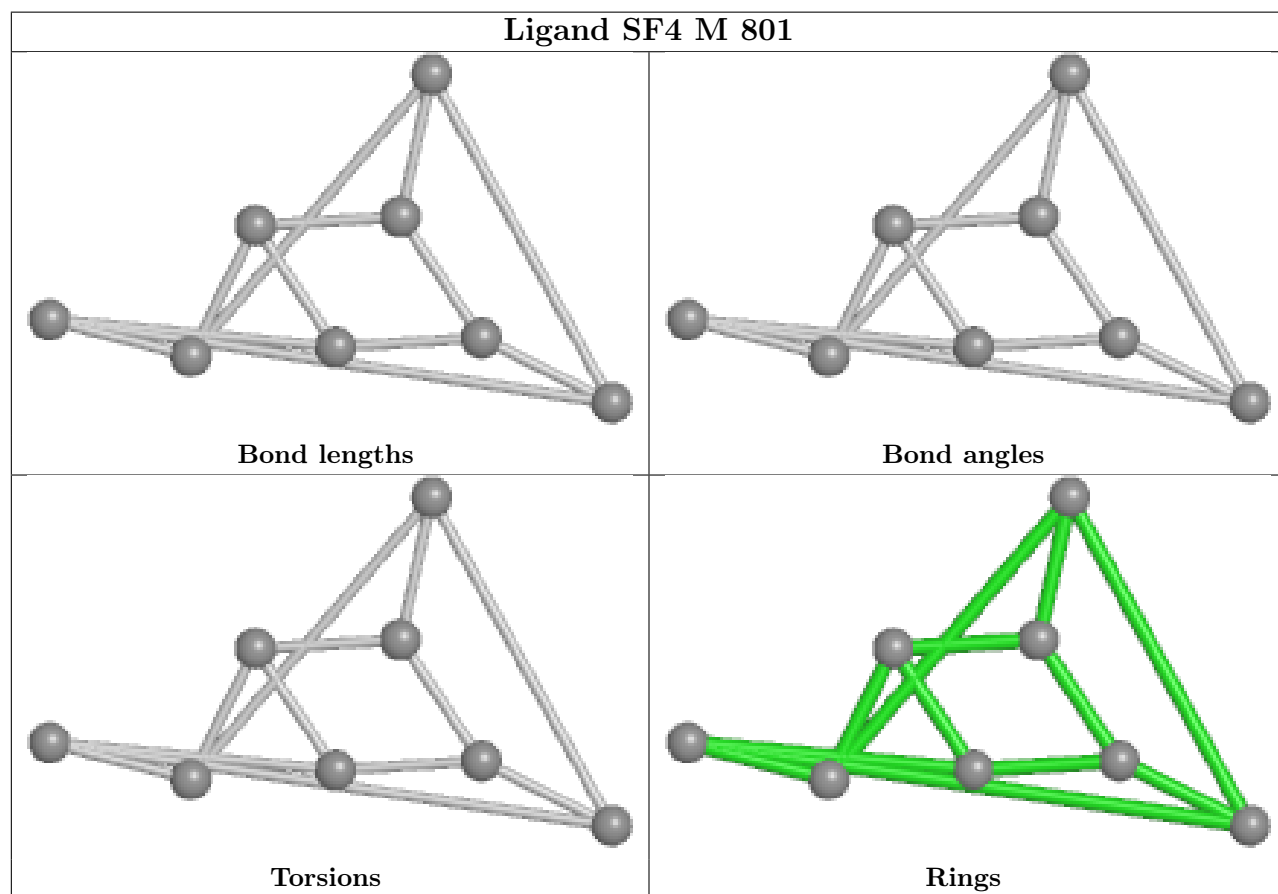
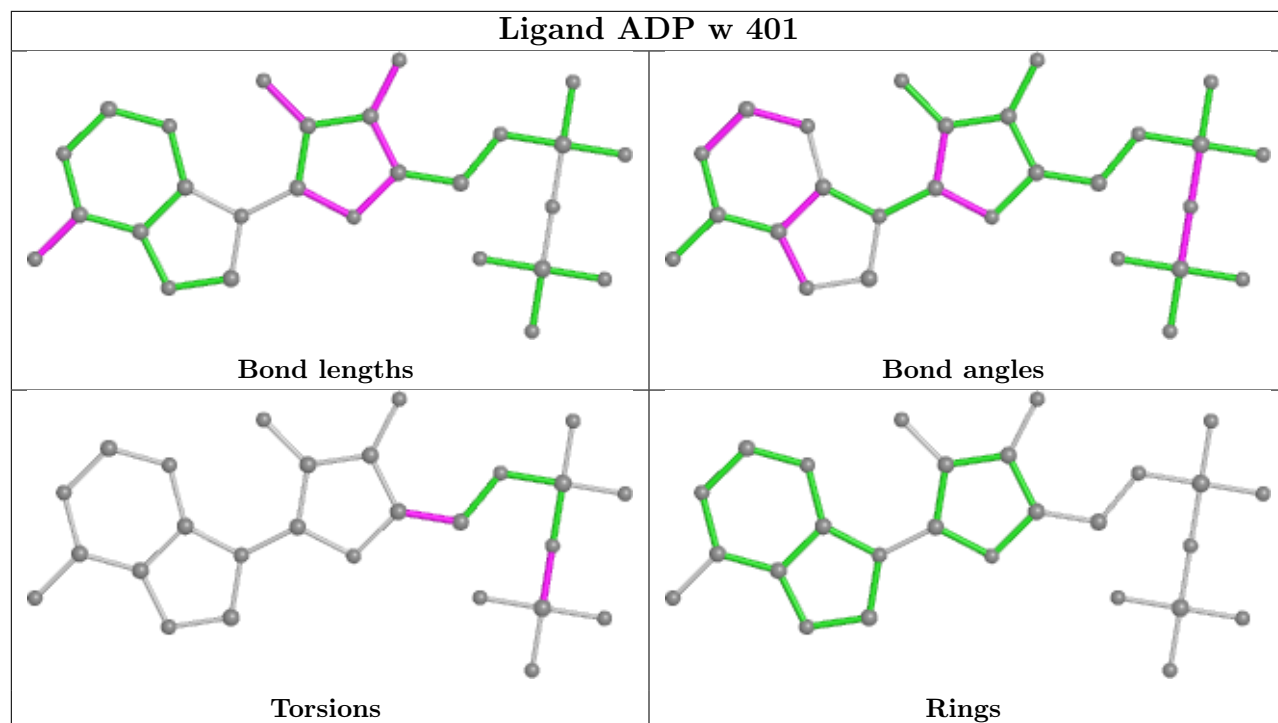


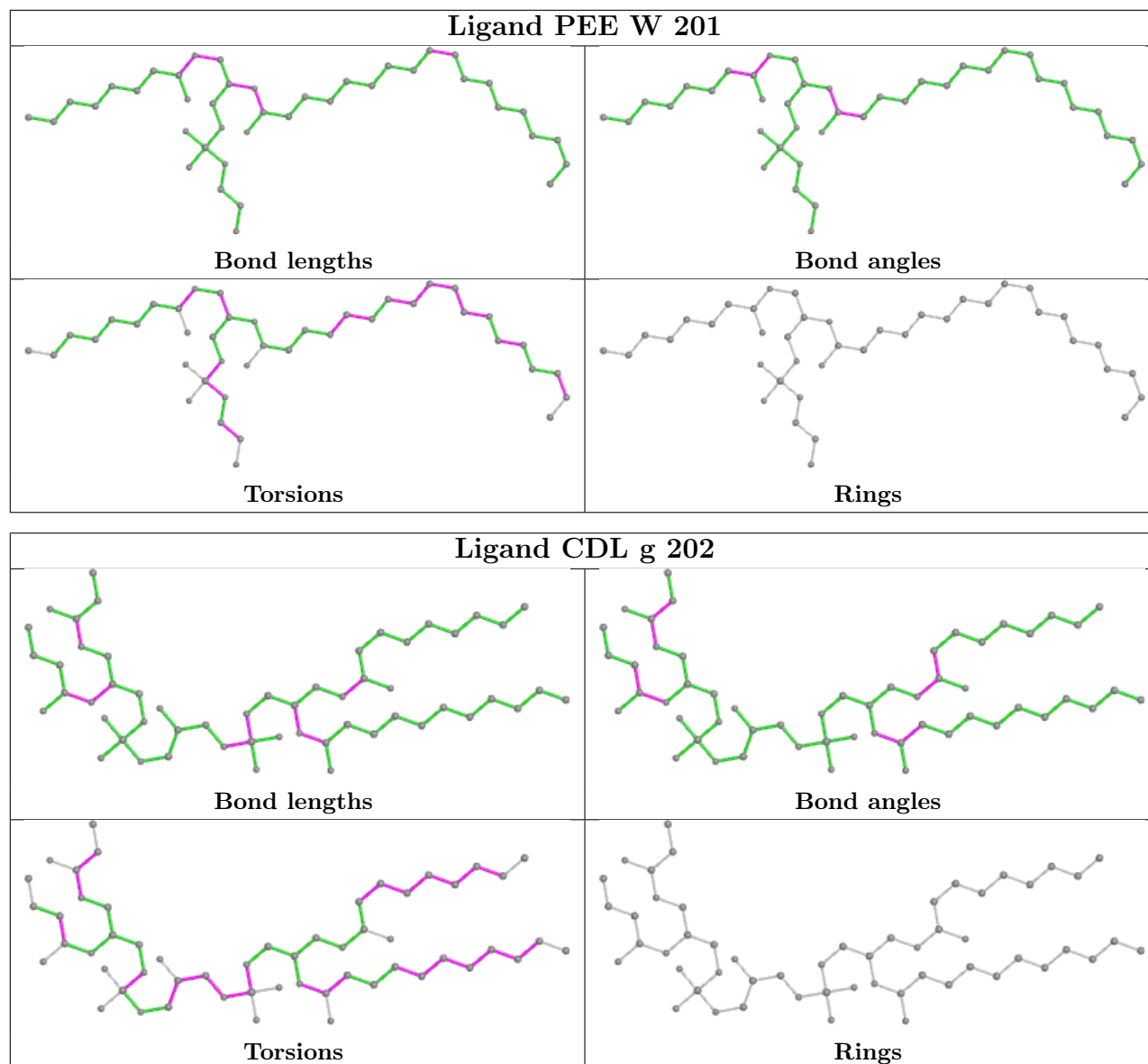












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

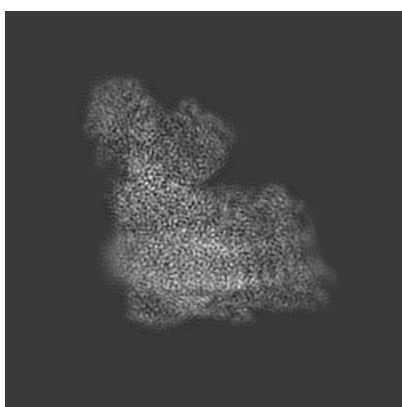
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32257. These allow visual inspection of the internal detail of the map and identification of artifacts.

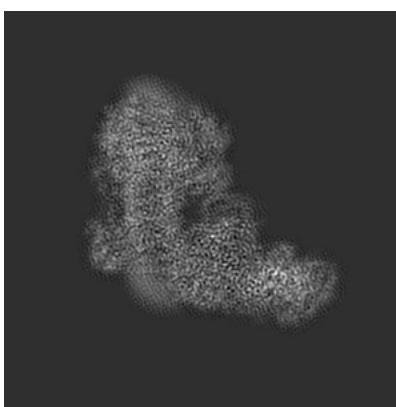
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

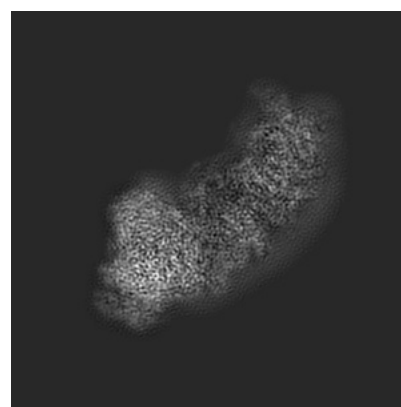
6.1.1 Primary map



X



Y

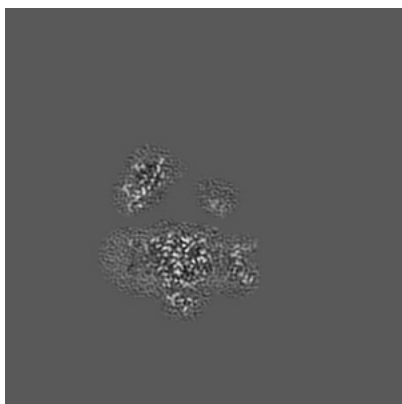


Z

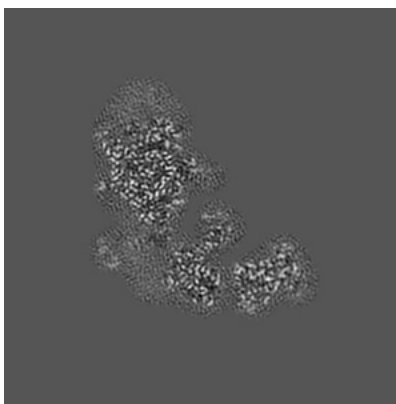
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

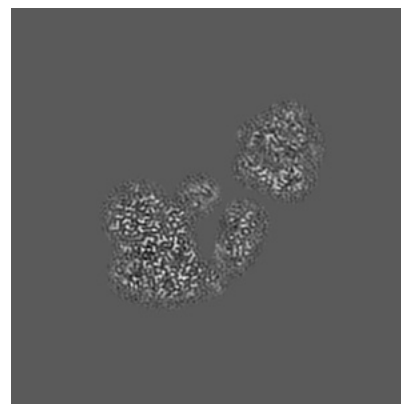
6.2.1 Primary map



X Index: 155



Y Index: 155

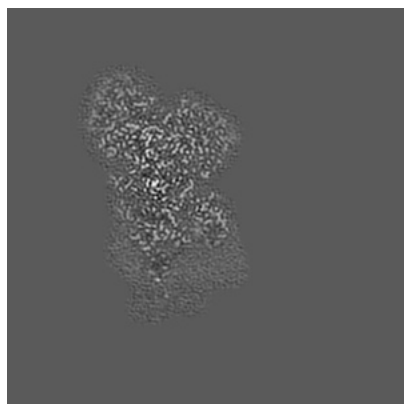


Z Index: 155

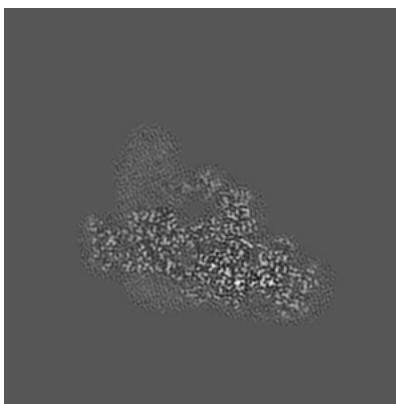
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

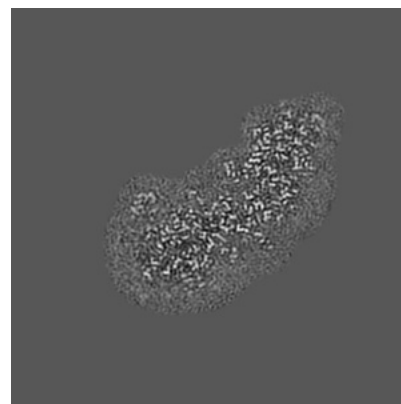
6.3.1 Primary map



X Index: 105



Y Index: 112

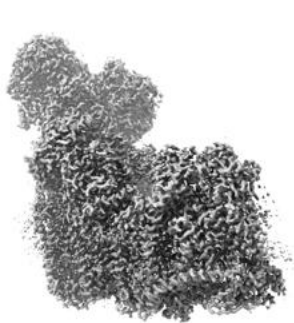


Z Index: 128

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

6.4 Orthogonal surface views [i](#)

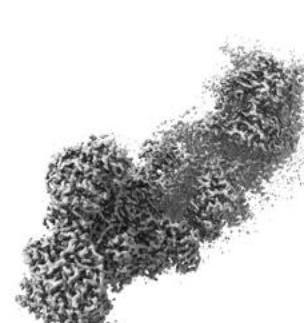
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0336. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

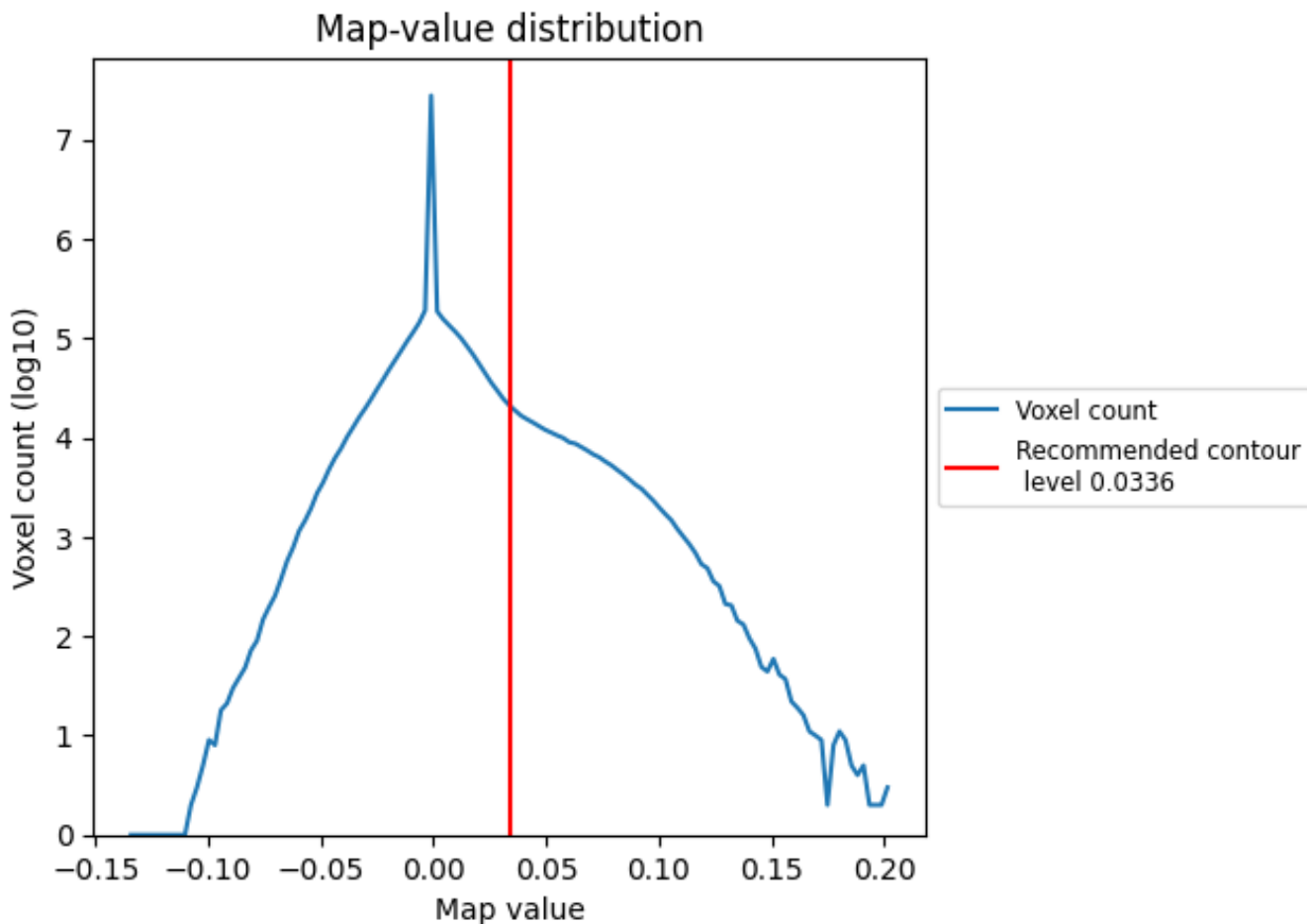
6.5 Mask visualisation

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

7 Map analysis [i](#)

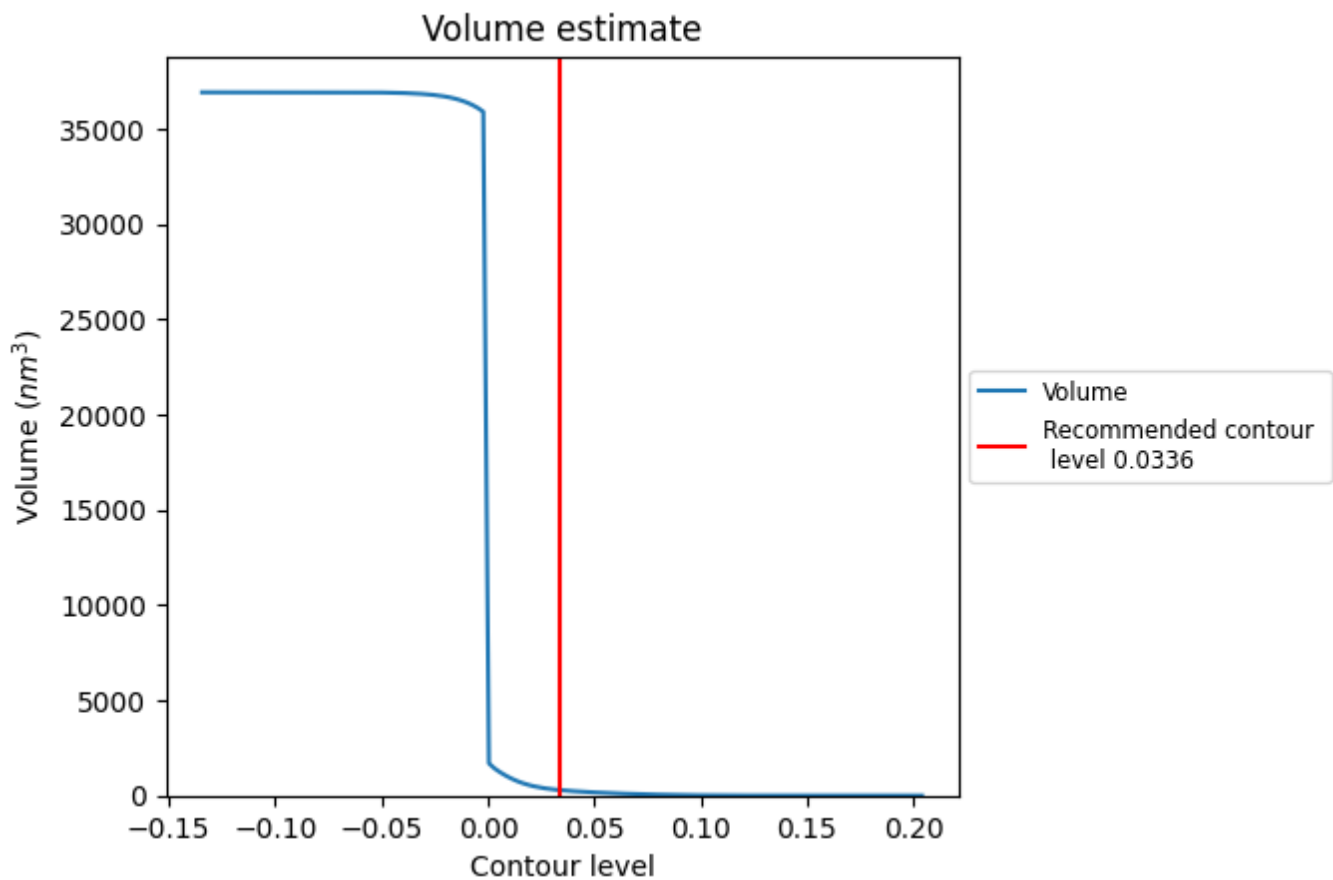
This section contains the results of statistical analysis of the map.

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.

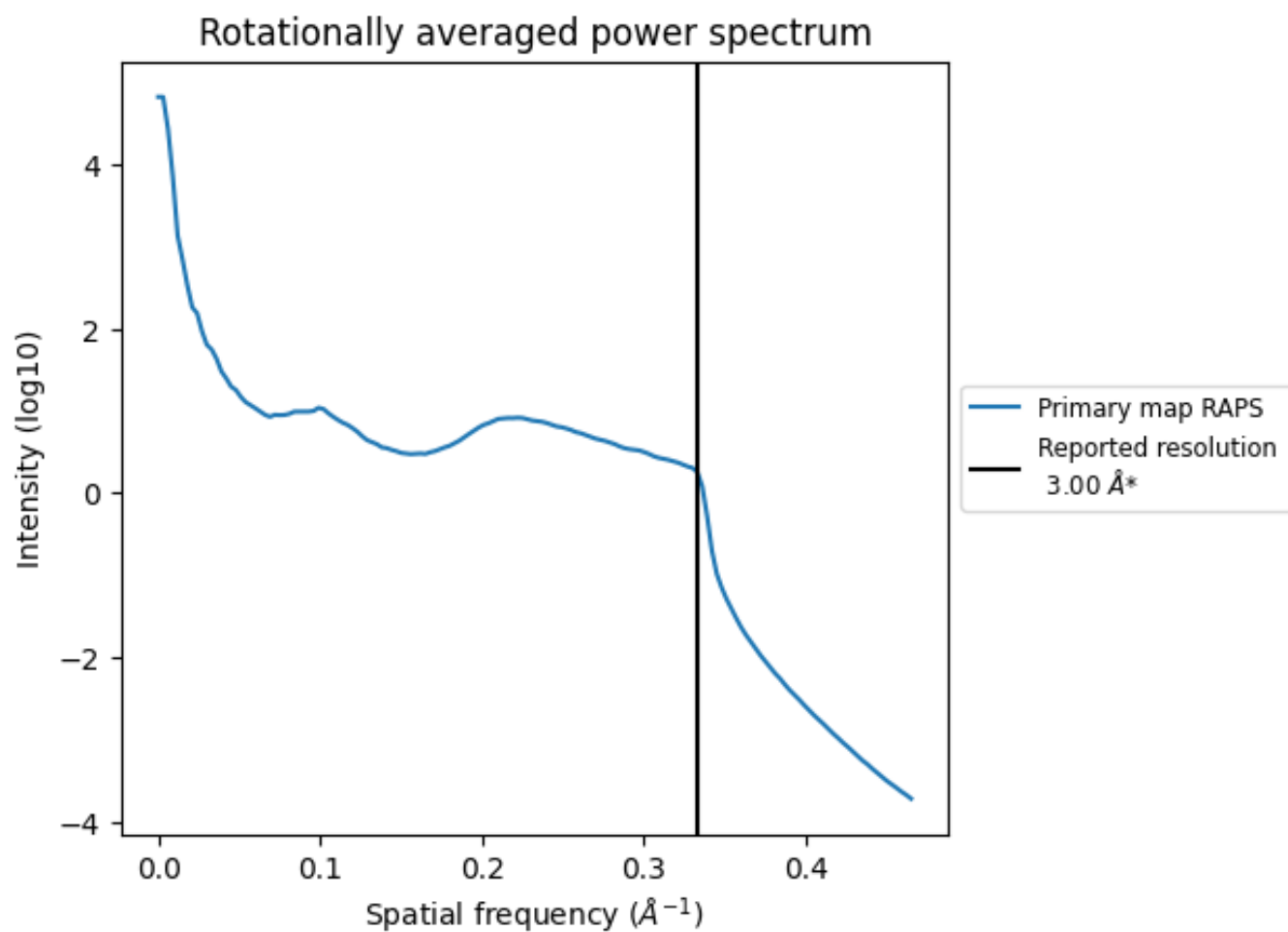
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 291 nm³; this corresponds to an approximate mass of 263 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

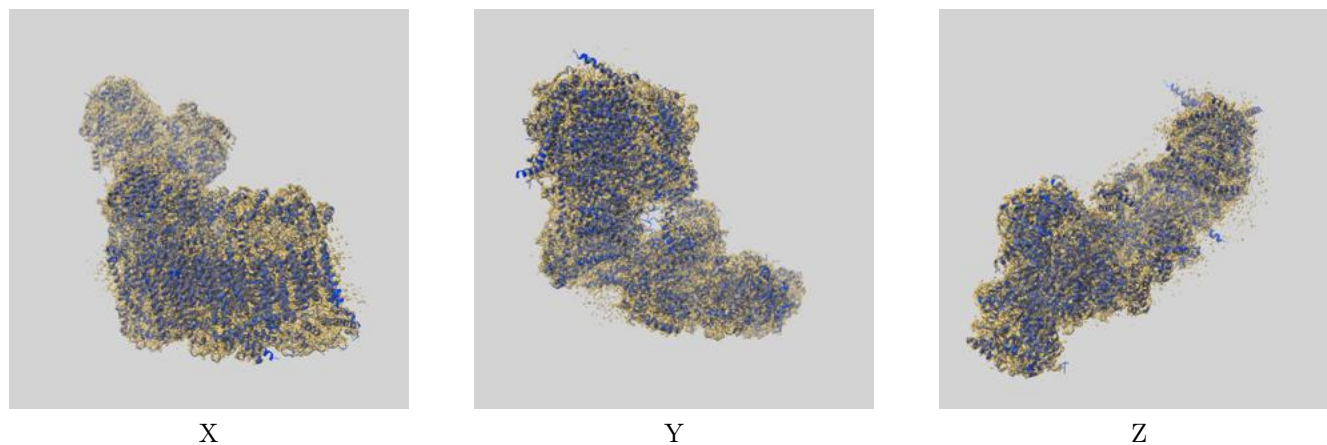
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

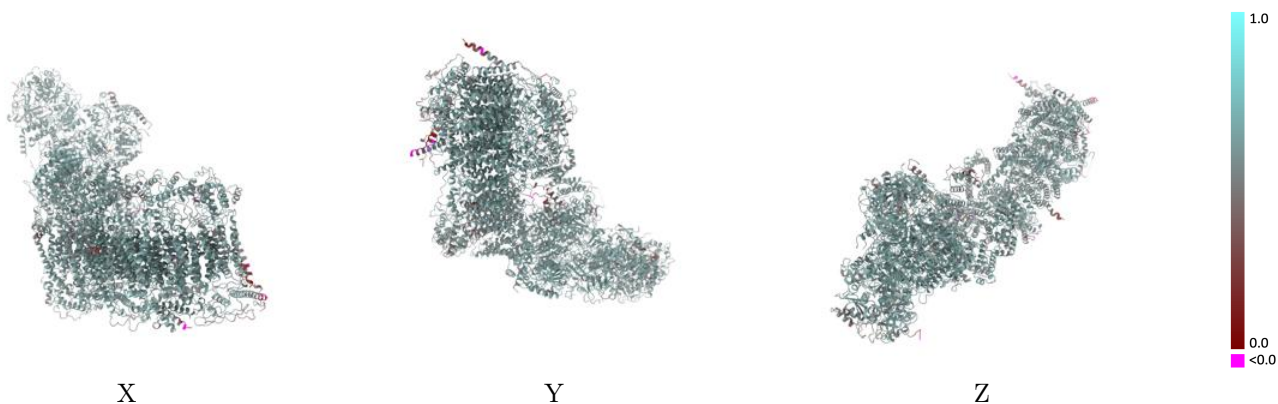
This section contains information regarding the fit between EMDB map EMD-32257 and PDB model 7W1V. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



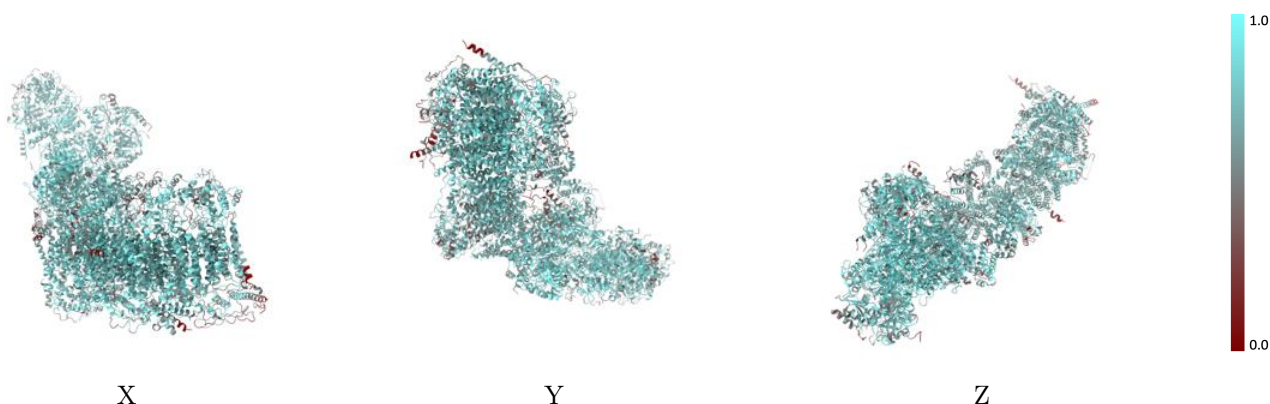
The images above show the 3D surface view of the map at the recommended contour level 0.0336 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



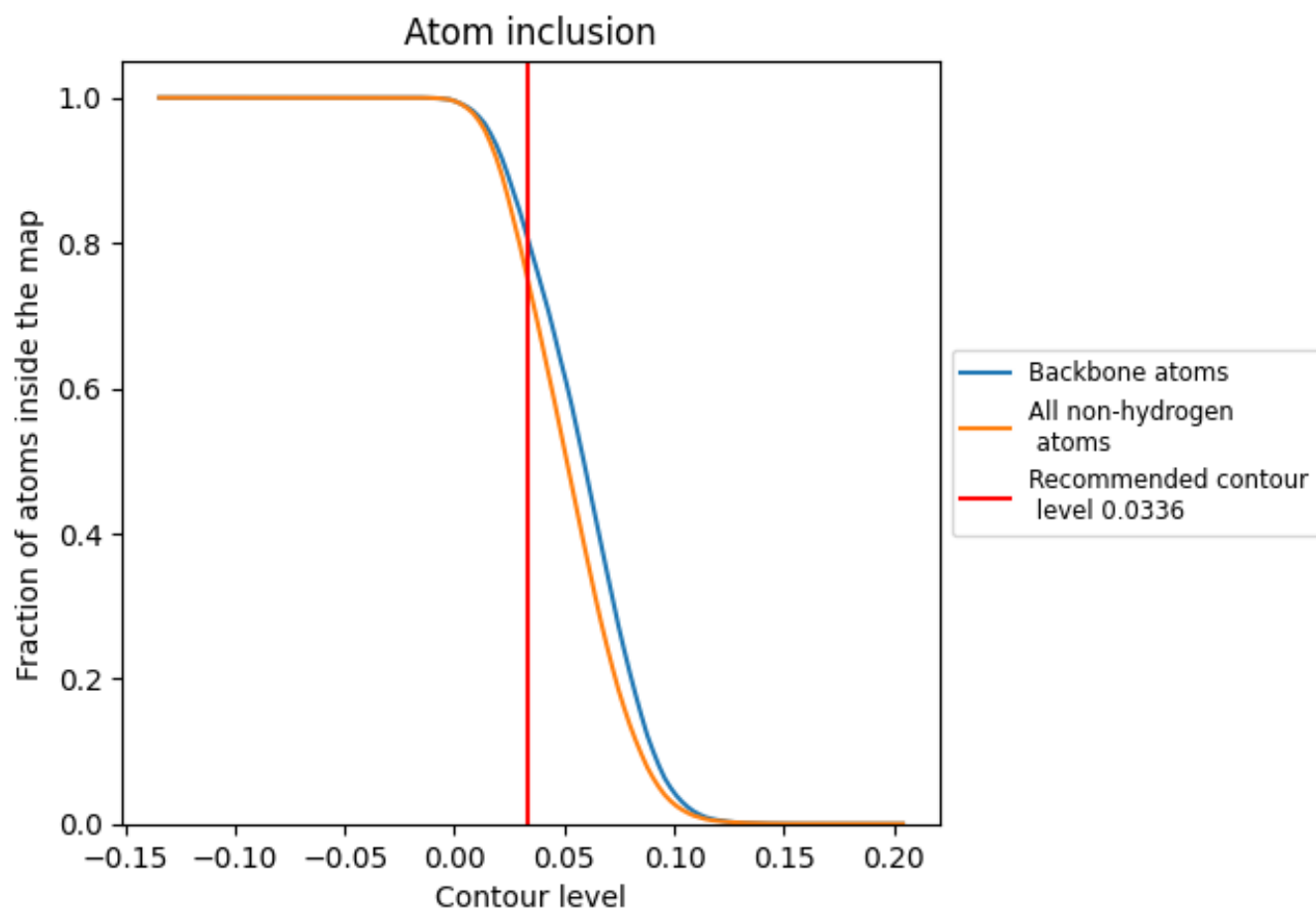
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0336).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 75% 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 (0.0336) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7468	 0.5790
A	 0.7401	 0.5720
B	 0.8568	 0.6170
C	 0.8585	 0.6170
E	 0.7856	 0.5940
F	 0.6406	 0.5260
G	 0.4723	 0.4590
H	 0.7531	 0.5850
I	 0.6171	 0.5480
J	 0.7819	 0.5930
K	 0.6394	 0.5370
L	 0.7897	 0.5950
M	 0.7977	 0.5910
N	 0.6977	 0.5790
O	 0.7230	 0.5570
P	 0.8711	 0.6220
Q	 0.8481	 0.6150
S	 0.7935	 0.5980
T	 0.7424	 0.5850
U	 0.6676	 0.5410
V	 0.6155	 0.5560
W	 0.7106	 0.5670
X	 0.6579	 0.5520
Y	 0.6134	 0.5150
Z	 0.5648	 0.4840
a	 0.7244	 0.5920
b	 0.6675	 0.5420
c	 0.7217	 0.5760
d	 0.6820	 0.5500
e	 0.6731	 0.5570
f	 0.5366	 0.4900
g	 0.7290	 0.5780
h	 0.7151	 0.5650
i	 0.7950	 0.5970
j	 0.7194	 0.5810



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Chain	Atom inclusion	Q-score
k	 0.8275	 0.6060
l	 0.7593	 0.5880
m	 0.6870	 0.5510
n	 0.5496	 0.5050
o	 0.6758	 0.5720
p	 0.7230	 0.5730
r	 0.8084	 0.6010
s	 0.8014	 0.5970
u	 0.7350	 0.5760
v	 0.6004	 0.5160
w	 0.7234	 0.5710