



Full wwPDB EM Validation Report ⓘ

Jan 17, 2023 – 06:38 PM JST

PDB ID : 7W2K
EMDB ID : EMD-32263
Title : Deactive state CI from Rotenone-NADH dataset, Subclass 1
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-24
Resolution : 2.90 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:

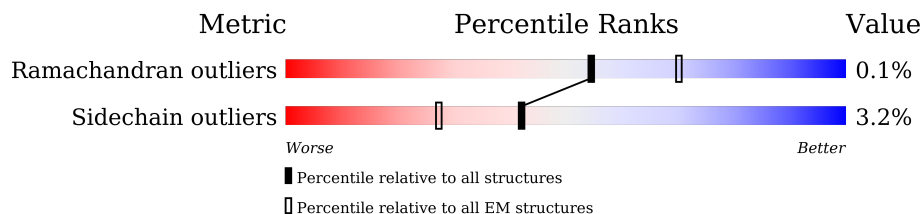
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.90 Å.

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



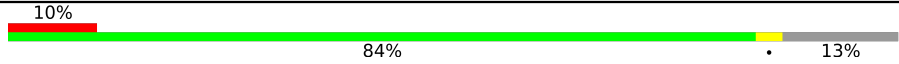

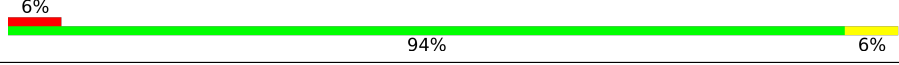
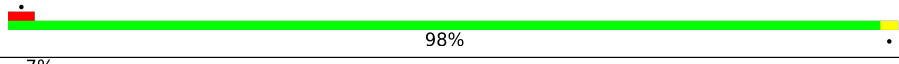
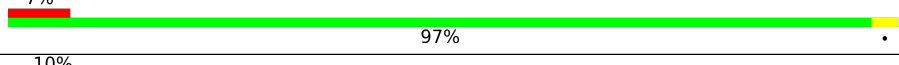
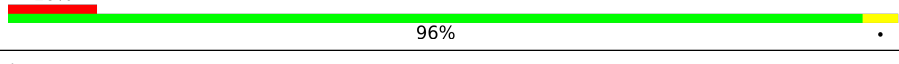
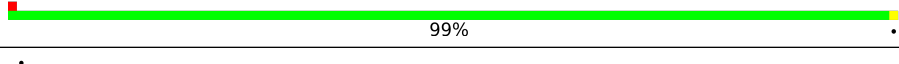
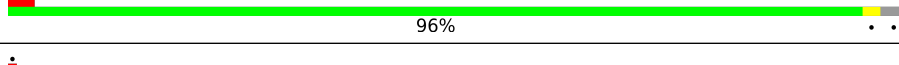
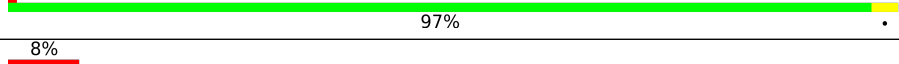
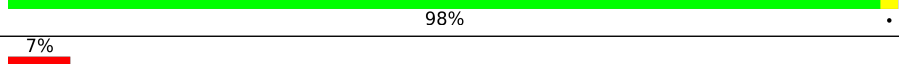
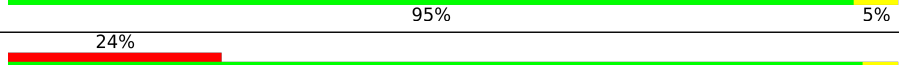
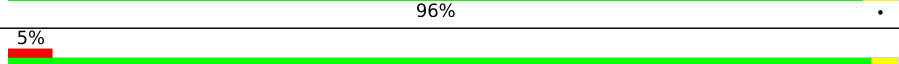
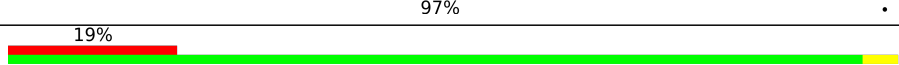
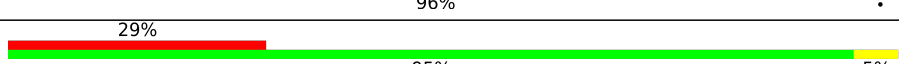
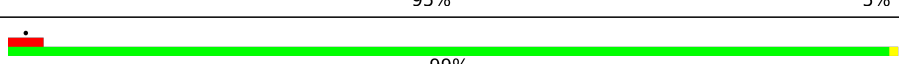
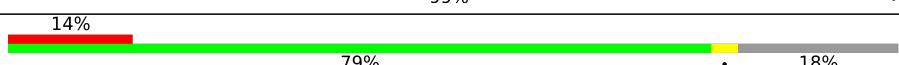
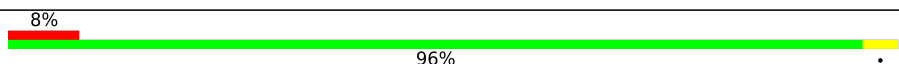
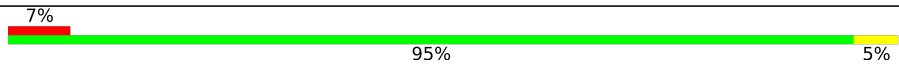
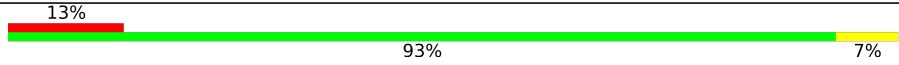
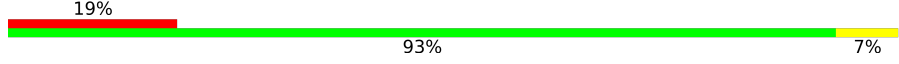
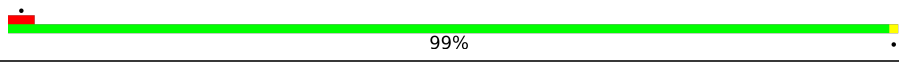
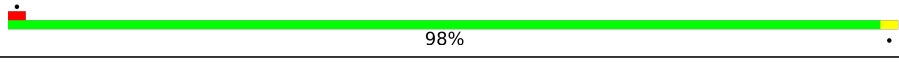
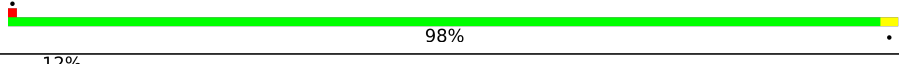


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	431	97%
2	B	176	98%
3	C	156	96%
4	E	115	10% 97%
5	F	86	13% 98%
6	G	88	52% 94% 6%
6	X	88	6% 97%
7	H	112	5% 99%
8	I	112	9% 83% 13%

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Mol	Chain	Length	Quality of chain
9	J	342	
10	K	42	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	70	
23	Z	84	
24	a	140	
25	b	126	
26	c	156	
27	d	175	
28	e	107	
29	f	42	
30	g	121	
31	h	105	
32	i	347	
33	j	113	

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Mol	Chain	Length	Quality of chain
34	k	98	<p>7% 98%</p>
35	l	603	<p>98%</p>
36	m	175	<p>9% 71% 26%</p>
37	n	56	<p>23% 96%</p>
38	o	128	<p>6% 98%</p>
39	p	178	<p>97%</p>
40	r	459	<p>98%</p>
41	s	318	<p>94% 5%</p>
42	u	171	<p>97%</p>
43	v	131	<p>18% 89% 6% 5%</p>
44	w	320	<p>8% 98%</p>

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 66522 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	156	1235	788	221	212	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	965	616	176	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	688	433	129	124	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
			696	449	103	139	5		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	97	Total	C	N	O	S	0	0
			762	479	144	136	3		

- Molecule 9 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	297	Total	C	N	O	S	0	0
			2352	1511	420	413	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	377	VAL	ILE	conflict	UNP F1SL07

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	217	1648	1054	277	308	9	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	419	3364	2153	574	613	24	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			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 Complex I-AGGG.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Y	70	583	386	98	98	1	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	a	140	1152	754	196	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	103	875	571	158	145	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	107	890	568	145	173	4	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	l	603	4782	3171	741	820	50	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	m	129	948	636	138	166	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	n	56	456	295	83	77	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	o	128	1058	688	181	189	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	v	124	1020	637	189	185	9	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	1	MYR	-	acetylation	UNP F1SCH1
v	126	ALA	GLN	conflict	UNP F1SCH1
v	128	ALA	PRO	conflict	UNP F1SCH1
v	130	ALA	GLU	conflict	UNP F1SCH1
v	131	ALA	VAL	conflict	UNP F1SCH1

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

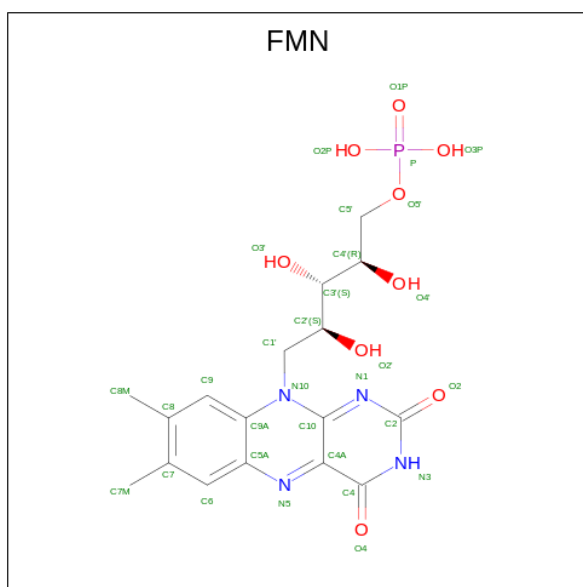
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	w	320	2574	1638	437	489	10	0	0

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



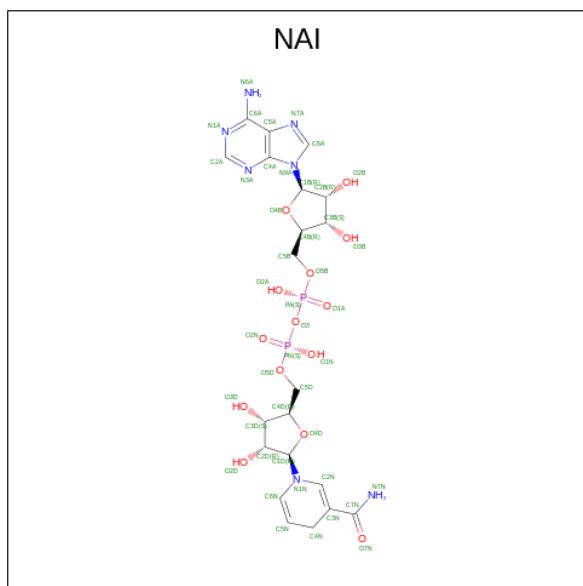
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	A	1	8	4	4	0
45	B	1	16	8	8	0
45	B	1	16	8	8	0
45	C	1	8	4	4	0
45	M	1	16	8	8	0
45	M	1	16	8	8	0

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



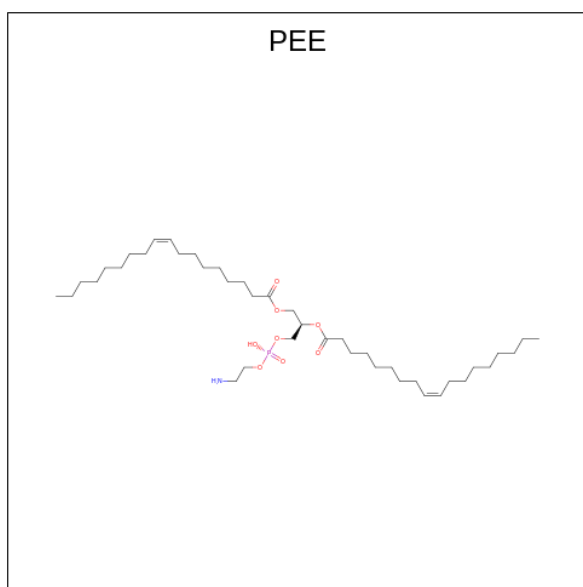
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	A	1	31	17	4	9	1	0

- 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).



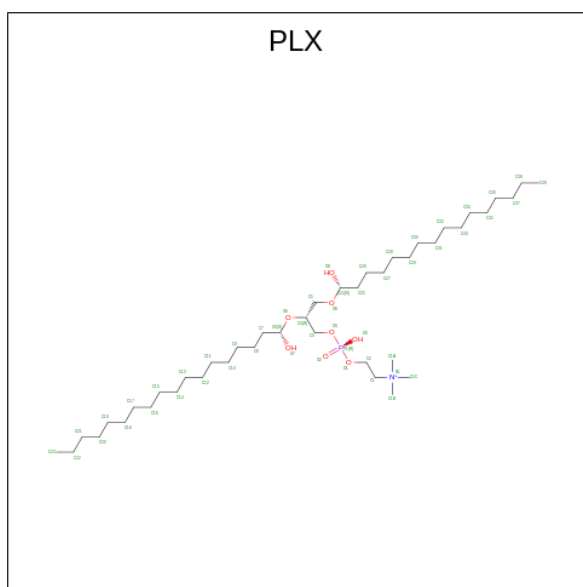
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	A	1	44	21	7	14	2	0

- 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).



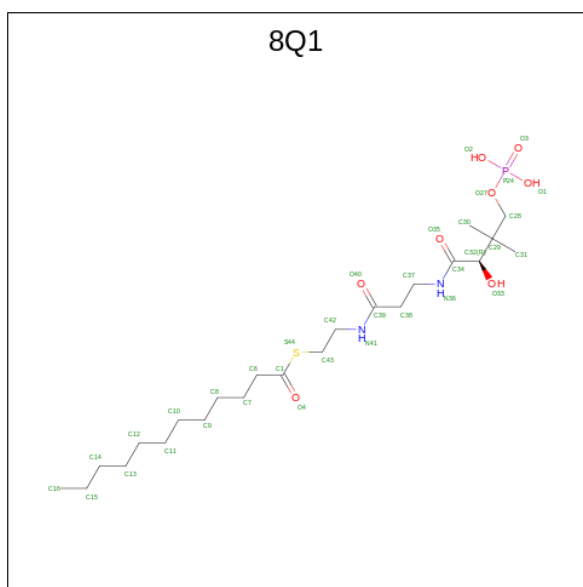
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	B	1	Total 51	41	1	8	1	0
48	C	1	Total 47	37	1	8	1	0
48	Q	1	Total 47	37	1	8	1	0
48	b	1	Total 46	36	1	8	1	0
48	j	1	Total 51	41	1	8	1	0
48	l	1	Total 46	36	1	8	1	0
48	r	1	Total 51	41	1	8	1	0
48	s	1	Total 41	31	1	8	1	0

- 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-TRIOXOL (three-letter code: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



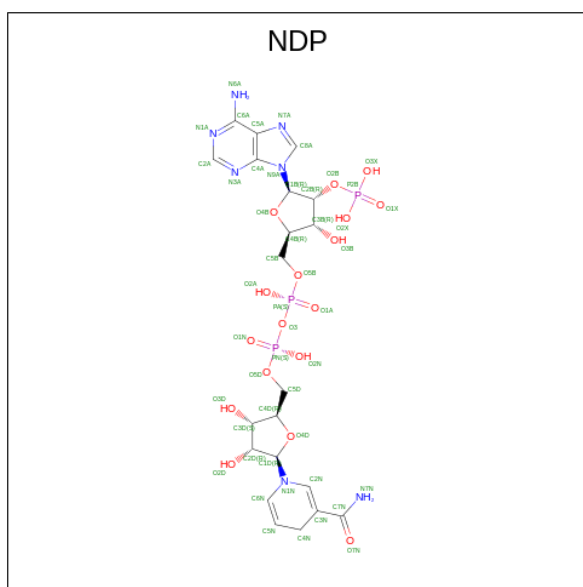
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	C	1	Total 52	42	1	8	1	0
49	a	1	Total 52	42	1	8	1	0
49	e	1	Total 52	42	1	8	1	0
49	g	1	Total 52	42	1	8	1	0
49	j	1	Total 52	42	1	8	1	0
49	r	1	Total 52	42	1	8	1	0

- Molecule 50 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).



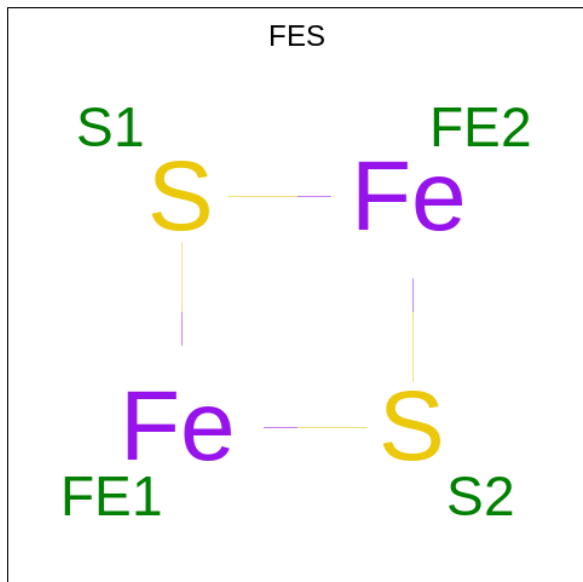
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
50	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
50	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 51 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



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

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



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

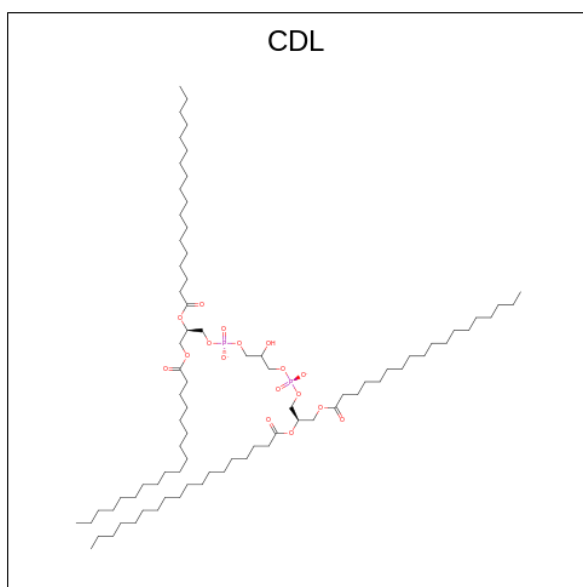
- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

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

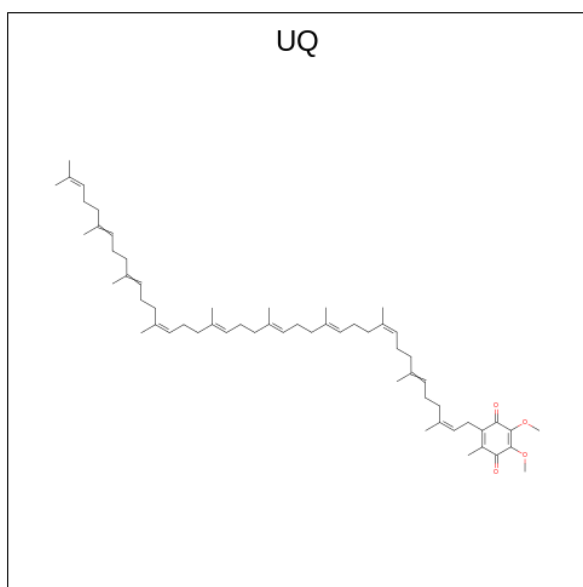
Mol	Chain	Residues	Atoms	AltConf
54	T	1	Total Zn 1 1	0

- Molecule 55 is CARDIOLIPIN (three-letter code: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



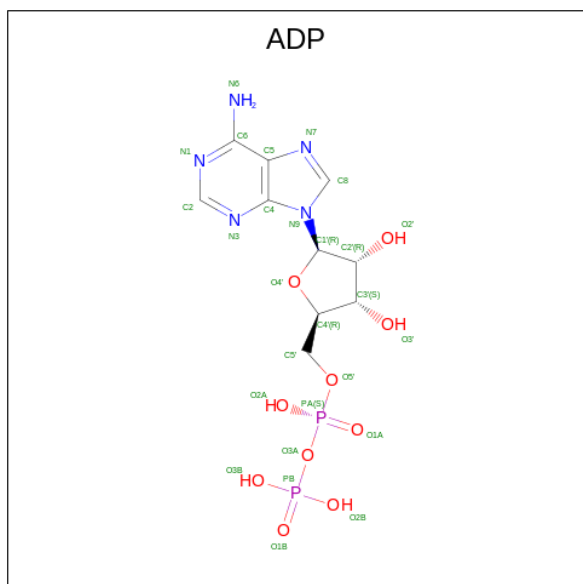
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
55	a	1	Total 91	C 72	O 17	P 2	0
55	i	1	Total 66	C 47	O 17	P 2	0
55	l	1	Total 199	C 161	O 34	P 4	0
55	l	1	Total 199	C 161	O 34	P 4	0
55	r	1	Total 100	C 81	O 17	P 2	0
55	u	1	Total 78	C 59	O 17	P 2	0

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



Mol	Chain	Residues	Atoms			AltConf
56	s	1	Total	C	O	0
			28	24	4	

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

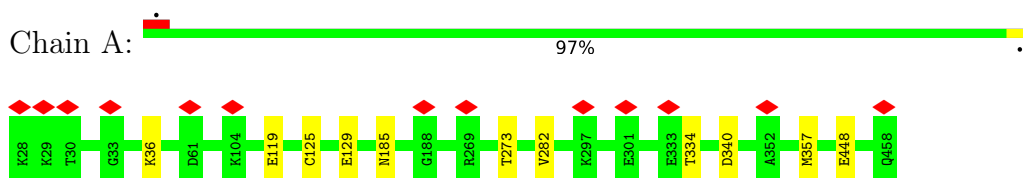


Mol	Chain	Residues	Atoms					AltConf
57	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

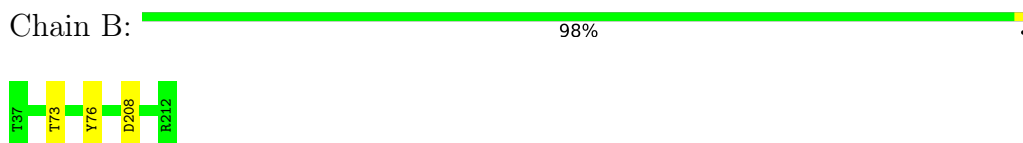
3 Residue-property plots [i](#)

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

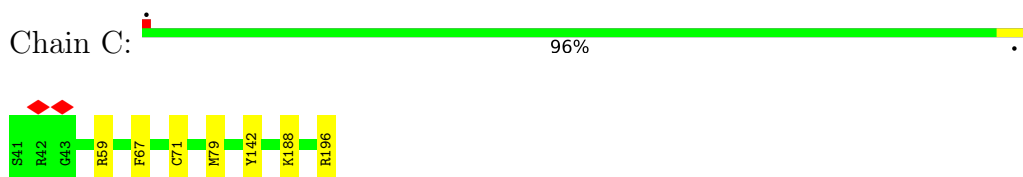
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



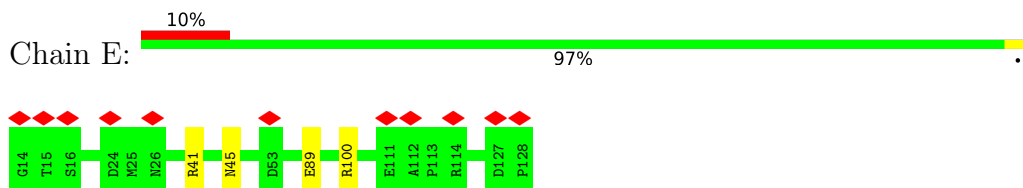
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



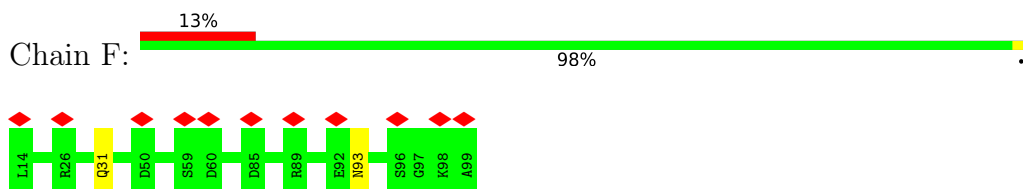
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



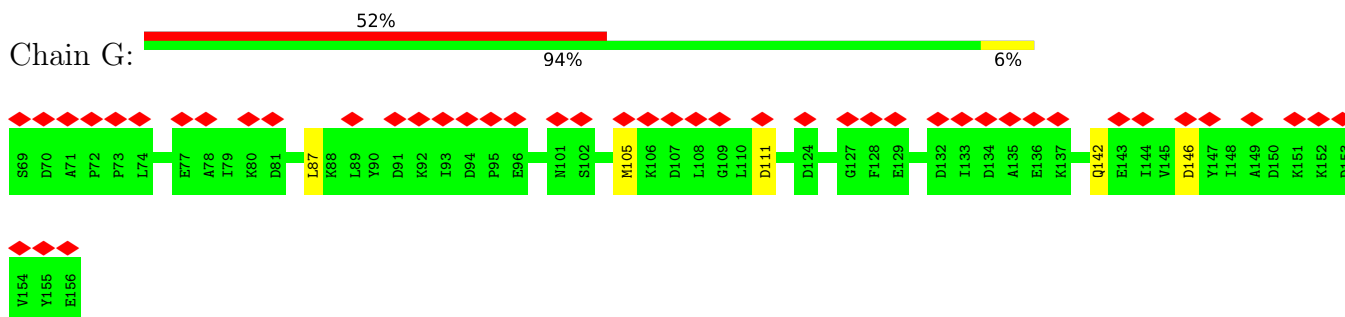
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



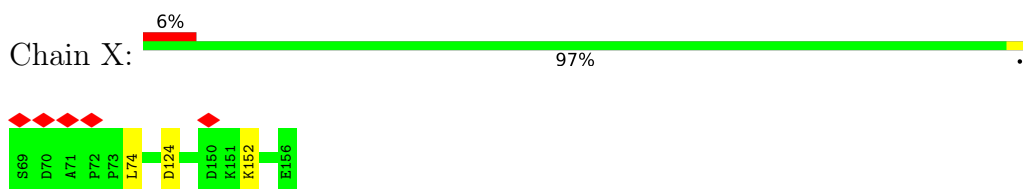
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



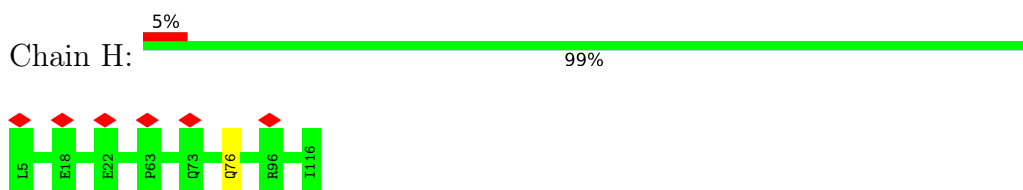
- Molecule 6: Acyl carrier protein



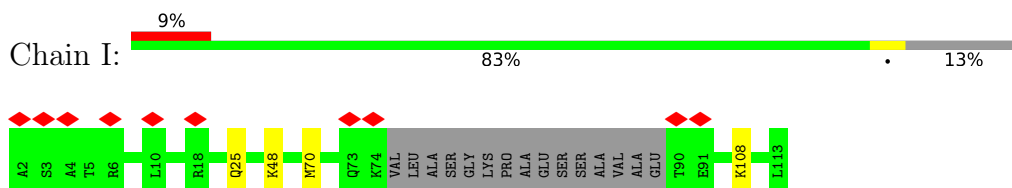
- Molecule 6: Acyl carrier protein



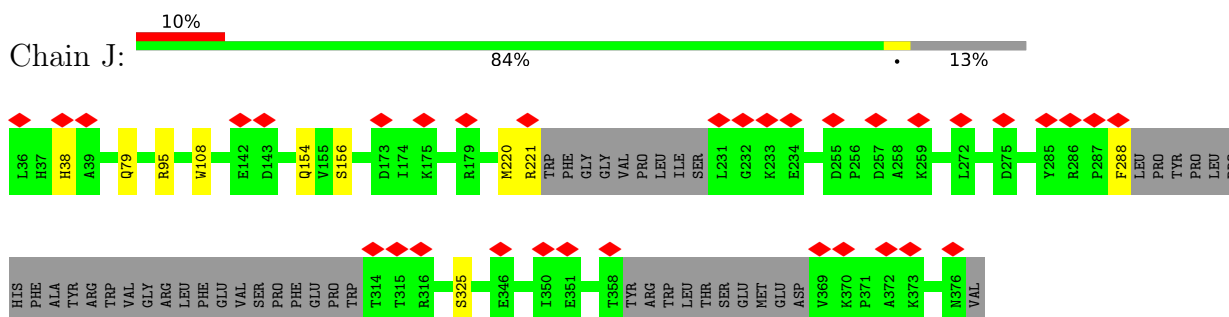
- Molecule 7: Complex I subunit B13



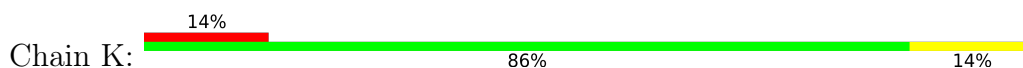
- Molecule 8: Complex I-B14.5a



- Molecule 9: NADH:ubiquinone oxidoreductase subunit A9

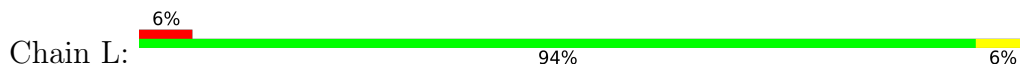


- Molecule 10: Complex I-9kD

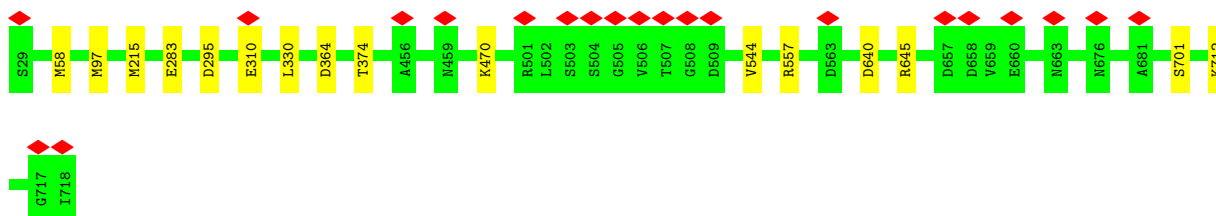




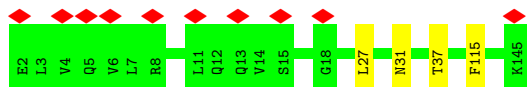
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



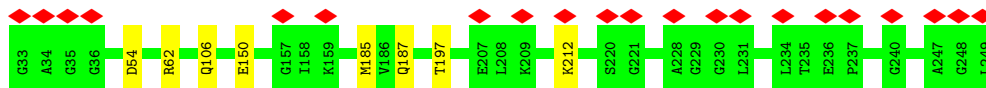
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



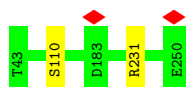
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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

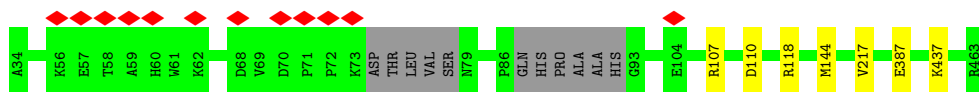


- Molecule 15: Complex I-30kD



- Molecule 16: Complex I-49kD

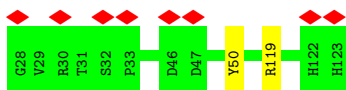




- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



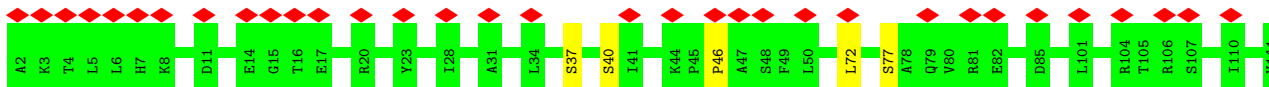
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



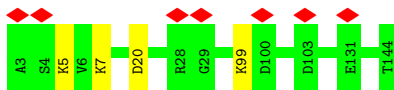
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



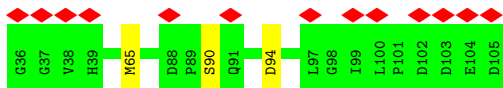
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



- Molecule 21: Complex I-B16.6



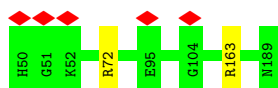
- Molecule 22: Complex I-AGGG



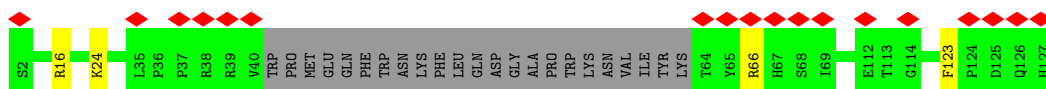
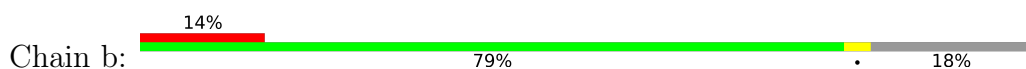
- Molecule 23: Complex I-B12



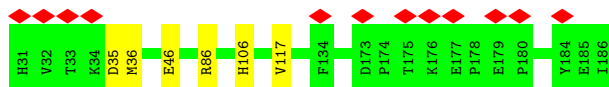
- Molecule 24: Complex I-SGDH



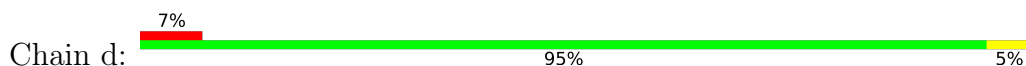
- Molecule 25: Complex I-B17



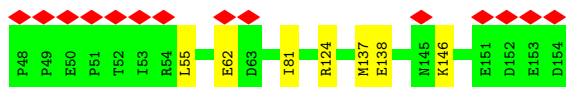
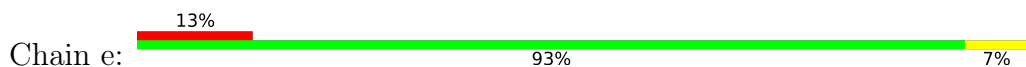
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



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

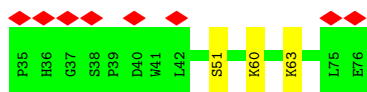


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



- Molecule 29: Complex I-KFYI

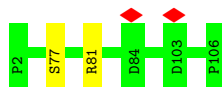




- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



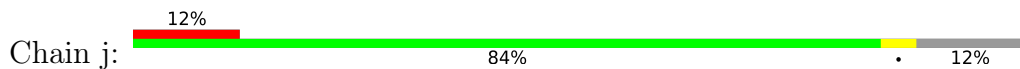
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



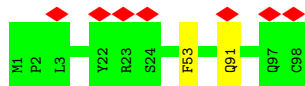
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



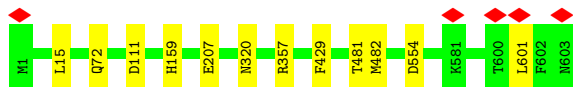
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3



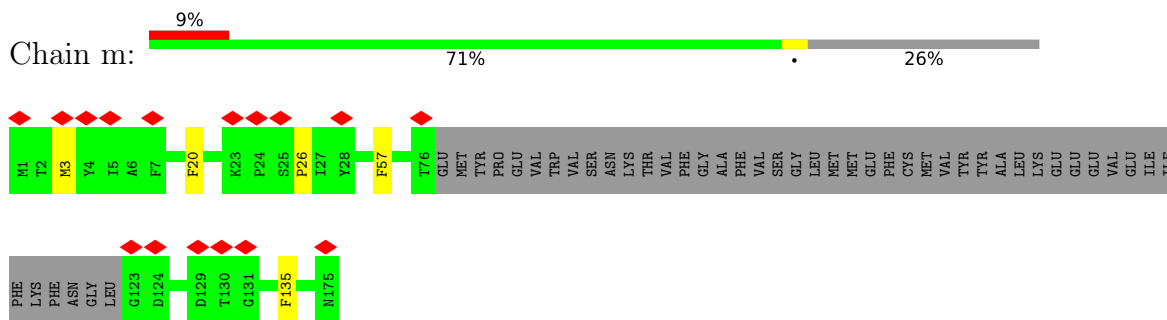
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L



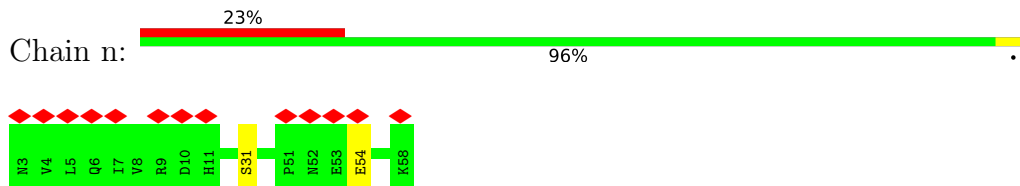
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5



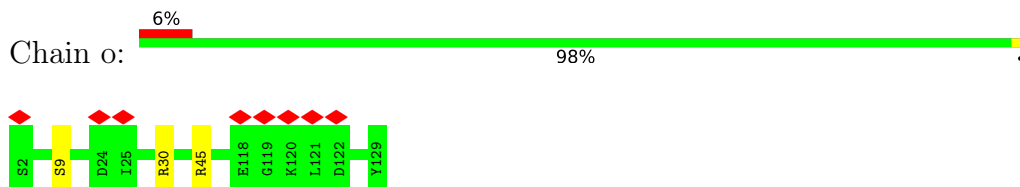
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6



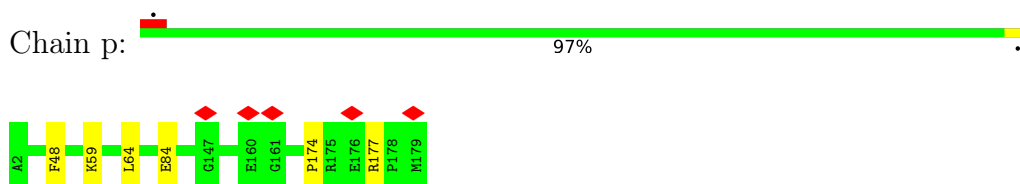
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



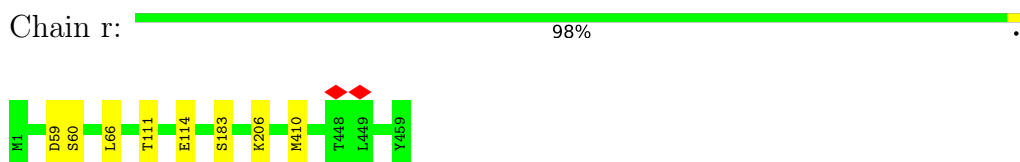
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



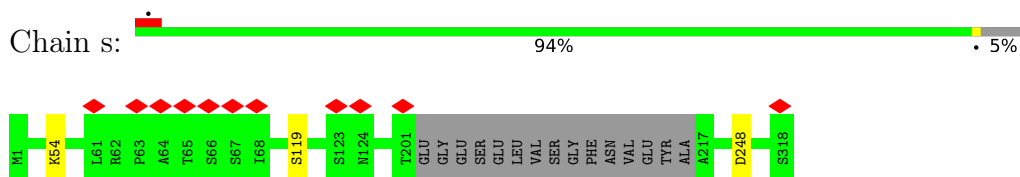
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4



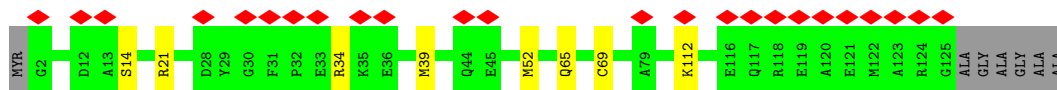
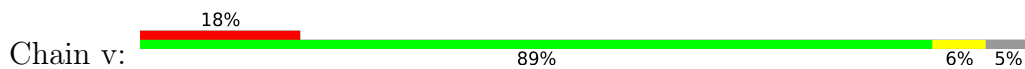
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1



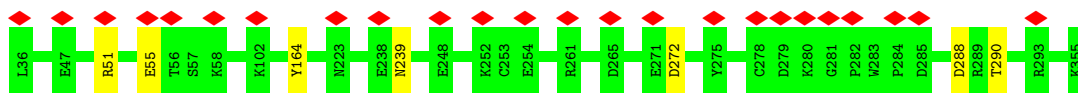
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99503	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	0.196	Depositor
Minimum map value	-0.112	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0279	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: ADP, CDL, SF4, 8Q1, UQ, 2MR, NAI, PLX, FMN, MG, NDP, FES, ZN, PEE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/3393	0.50	0/4584
2	B	0.26	0/1443	0.50	0/1952
3	C	0.26	0/1266	0.51	0/1715
4	E	0.27	0/989	0.52	0/1333
5	F	0.26	0/699	0.59	0/941
6	G	0.27	0/705	0.47	0/956
6	X	0.25	0/708	0.44	0/959
7	H	0.24	0/929	0.43	0/1258
8	I	0.25	0/780	0.53	0/1059
9	J	0.25	0/2404	0.49	0/3245
10	K	0.24	0/365	0.49	0/493
11	L	0.25	0/1039	0.51	0/1403
12	M	0.25	0/5381	0.50	0/7291
13	N	0.25	0/1245	0.51	0/1694
14	O	0.26	0/1688	0.50	0/2301
15	P	0.27	0/1789	0.51	0/2436
16	Q	0.27	0/3437	0.50	0/4656
17	S	0.26	0/582	0.47	0/783
18	T	0.24	0/755	0.51	0/1018
19	U	0.25	0/664	0.45	0/912
20	V	0.27	0/1042	0.48	0/1411
21	W	0.26	0/1192	0.47	0/1610
22	Y	0.26	0/609	0.47	0/835
23	Z	0.26	0/695	0.53	1/939 (0.1%)
24	a	0.26	0/1185	0.48	0/1606
25	b	0.26	0/902	0.52	0/1227
26	c	0.27	0/1371	0.51	0/1875
27	d	0.25	0/1494	0.49	0/2015
28	e	0.26	0/916	0.49	0/1246
29	f	0.28	0/350	0.47	0/473
30	g	0.28	0/1031	0.51	0/1394
31	h	0.25	0/889	0.51	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.26	0/2769	0.45	0/3764
33	j	0.26	0/819	0.45	0/1117
34	k	0.26	0/759	0.46	0/1029
35	l	0.26	0/4911	0.45	0/6680
36	m	0.27	0/970	0.47	0/1316
37	n	0.23	0/468	0.48	0/633
38	o	0.27	0/1088	0.51	0/1477
39	p	0.26	0/1590	0.51	0/2155
40	r	0.26	0/3723	0.46	0/5078
41	s	0.26	0/2464	0.46	0/3369
42	u	0.24	0/1436	0.47	0/1938
43	v	0.28	0/1044	0.58	0/1403
44	w	0.26	0/2634	0.48	0/3571
All	All	0.26	0/66612	0.49	1/90340 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Z	43	ASP	CB-CG-OD1	5.26	123.04	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	415 (97%)	14 (3%)	0	100	100
2	B	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
3	C	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
4	E	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
5	F	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
6	G	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
6	X	86/88 (98%)	86 (100%)	0	0	100	100
7	H	110/112 (98%)	103 (94%)	7 (6%)	0	100	100
8	I	93/112 (83%)	83 (89%)	10 (11%)	0	100	100
9	J	289/342 (84%)	281 (97%)	7 (2%)	1 (0%)	41	71
10	K	40/42 (95%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	666 (97%)	21 (3%)	1 (0%)	51	82
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
15	P	206/208 (99%)	194 (94%)	12 (6%)	0	100	100
16	Q	412/430 (96%)	398 (97%)	14 (3%)	0	100	100
17	S	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
18	T	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
19	U	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
20	V	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	22	54
21	W	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
22	Y	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
23	Z	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
24	a	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
25	b	99/126 (79%)	93 (94%)	6 (6%)	0	100	100
26	c	154/156 (99%)	145 (94%)	8 (5%)	1 (1%)	25	58
27	d	173/175 (99%)	172 (99%)	1 (1%)	0	100	100
28	e	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
29	f	40/42 (95%)	38 (95%)	2 (5%)	0	100	100
30	g	119/121 (98%)	114 (96%)	5 (4%)	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%)	336 (97%)	9 (3%)	0	100	100
33	j	95/113 (84%)	87 (92%)	8 (8%)	0	100	100
34	k	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
35	l	601/603 (100%)	573 (95%)	27 (4%)	1 (0%)	47	78
36	m	125/175 (71%)	112 (90%)	12 (10%)	1 (1%)	19	51
37	n	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
38	o	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
39	p	176/178 (99%)	166 (94%)	9 (5%)	1 (1%)	25	58
40	r	457/459 (100%)	446 (98%)	11 (2%)	0	100	100
41	s	299/318 (94%)	290 (97%)	9 (3%)	0	100	100
42	u	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
43	v	122/131 (93%)	114 (93%)	8 (7%)	0	100	100
44	w	318/320 (99%)	305 (96%)	13 (4%)	0	100	100
All	All	8029/8316 (96%)	7731 (96%)	291 (4%)	7 (0%)	54	82

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	38	HIS
12	M	283	GLU
26	c	106	HIS
20	V	46	PRO
35	l	15	LEU
36	m	26	PRO
39	p	174	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/345 (100%)	334 (97%)	11 (3%)	39	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	151/151 (100%)	148 (98%)	3 (2%)	55	82
3	C	129/132 (98%)	122 (95%)	7 (5%)	22	54
4	E	106/107 (99%)	102 (96%)	4 (4%)	33	67
5	F	75/76 (99%)	73 (97%)	2 (3%)	44	77
6	G	76/81 (94%)	71 (93%)	5 (7%)	16	44
6	X	77/81 (95%)	74 (96%)	3 (4%)	32	66
7	H	99/99 (100%)	98 (99%)	1 (1%)	76	92
8	I	82/97 (84%)	78 (95%)	4 (5%)	25	57
9	J	253/296 (86%)	244 (96%)	9 (4%)	35	69
10	K	41/41 (100%)	35 (85%)	6 (15%)	3	9
11	L	113/113 (100%)	106 (94%)	7 (6%)	18	47
12	M	579/580 (100%)	564 (97%)	15 (3%)	46	77
13	N	130/130 (100%)	126 (97%)	4 (3%)	40	74
14	O	176/183 (96%)	168 (96%)	8 (4%)	27	61
15	P	190/190 (100%)	188 (99%)	2 (1%)	73	92
16	Q	358/370 (97%)	352 (98%)	6 (2%)	60	86
17	S	58/58 (100%)	56 (97%)	2 (3%)	37	71
18	T	79/79 (100%)	77 (98%)	2 (2%)	47	78
19	U	69/69 (100%)	65 (94%)	4 (6%)	20	50
20	V	101/101 (100%)	97 (96%)	4 (4%)	31	65
21	W	121/123 (98%)	117 (97%)	4 (3%)	38	72
22	Y	58/63 (92%)	55 (95%)	3 (5%)	23	55
23	Z	65/65 (100%)	62 (95%)	3 (5%)	27	60
24	a	119/122 (98%)	117 (98%)	2 (2%)	60	86
25	b	97/119 (82%)	93 (96%)	4 (4%)	30	64
26	c	141/141 (100%)	136 (96%)	5 (4%)	36	70
27	d	155/155 (100%)	146 (94%)	9 (6%)	20	50
28	e	99/99 (100%)	92 (93%)	7 (7%)	14	40
29	f	35/38 (92%)	32 (91%)	3 (9%)	10	30
30	g	108/108 (100%)	107 (99%)	1 (1%)	78	93
31	h	93/93 (100%)	91 (98%)	2 (2%)	52	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	i	310/311 (100%)	302 (97%)	8 (3%)	46	77
33	j	88/99 (89%)	84 (96%)	4 (4%)	27	61
34	k	85/85 (100%)	83 (98%)	2 (2%)	49	79
35	l	536/537 (100%)	525 (98%)	11 (2%)	53	81
36	m	98/141 (70%)	94 (96%)	4 (4%)	30	64
37	n	46/53 (87%)	44 (96%)	2 (4%)	29	62
38	o	112/113 (99%)	109 (97%)	3 (3%)	44	77
39	p	159/159 (100%)	154 (97%)	5 (3%)	40	74
40	r	410/410 (100%)	402 (98%)	8 (2%)	55	82
41	s	263/275 (96%)	260 (99%)	3 (1%)	73	92
42	u	153/153 (100%)	148 (97%)	5 (3%)	38	72
43	v	103/111 (93%)	95 (92%)	8 (8%)	12	34
44	w	279/283 (99%)	272 (98%)	7 (2%)	47	78
All	All	7020/7235 (97%)	6798 (97%)	222 (3%)	42	73

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	119	GLU
1	A	125	CYS
1	A	129	GLU
1	A	185	ASN
1	A	273	THR
1	A	282	VAL
1	A	334	THR
1	A	340	ASP
1	A	357	MET
1	A	448	GLU
2	B	73	THR
2	B	76	TYR
2	B	208	ASP
3	C	59	ARG
3	C	67	PHE
3	C	71	CYS
3	C	79	MET
3	C	142	TYR

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Mol	Chain	Res	Type
3	C	188	LYS
3	C	196	ARG
4	E	41	ARG
4	E	45	ASN
4	E	89	GLU
4	E	100	ARG
5	F	31	GLN
5	F	93	ASN
6	G	87	LEU
6	G	105	MET
6	G	111	ASP
6	G	142	GLN
6	G	146	ASP
7	H	76	GLN
8	I	25	GLN
8	I	48	LYS
8	I	70	MET
8	I	108	LYS
9	J	79	GLN
9	J	95	ARG
9	J	108	TRP
9	J	154	GLN
9	J	156	SER
9	J	220	MET
9	J	221	ARG
9	J	288	PHE
9	J	325	SER
10	K	76	LEU
10	K	83	THR
10	K	94	SER
10	K	95	LYS
10	K	97	ARG
10	K	107	SER
11	L	78	ARG
11	L	86	ASN
11	L	89	SER
11	L	124	LEU
11	L	130	THR
11	L	144	SER
11	L	157	SER
12	M	58	MET
12	M	97	MET

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Mol	Chain	Res	Type
12	M	215	MET
12	M	295	ASP
12	M	310	GLU
12	M	330	LEU
12	M	364	ASP
12	M	374	THR
12	M	470	LYS
12	M	544	VAL
12	M	557	ARG
12	M	640	ASP
12	M	645	ARG
12	M	701	SER
12	M	712	LYS
13	N	27	LEU
13	N	31	ASN
13	N	37	THR
13	N	115	PHE
14	O	54	ASP
14	O	62	ARG
14	O	106	GLN
14	O	150	GLU
14	O	185	MET
14	O	187	GLN
14	O	197	THR
14	O	212	LYS
15	P	110	SER
15	P	231	ARG
16	Q	107	ARG
16	Q	110	ASP
16	Q	144	MET
16	Q	217	VAL
16	Q	387	GLU
16	Q	437	LYS
17	S	12	MET
17	S	67	GLU
18	T	50	TYR
18	T	119	ARG
19	U	34	SER
19	U	41	TYR
19	U	47	ARG
19	U	68	SER
20	V	37	SER

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Mol	Chain	Res	Type
20	V	40	SER
20	V	72	LEU
20	V	77	SER
21	W	5	LYS
21	W	7	LYS
21	W	20	ASP
21	W	99	LYS
6	X	74	LEU
6	X	124	ASP
6	X	152	LYS
22	Y	65	MET
22	Y	90	SER
22	Y	94	ASP
23	Z	14	MET
23	Z	19	TYR
23	Z	47	ARG
24	a	72	ARG
24	a	163	ARG
25	b	16	ARG
25	b	24	LYS
25	b	66	ARG
25	b	123	PHE
26	c	35	ASP
26	c	36	MET
26	c	46	GLU
26	c	86	ARG
26	c	117	VAL
27	d	6	ASP
27	d	8	ASP
27	d	15	ARG
27	d	17	THR
27	d	60	ARG
27	d	120	SER
27	d	136	SER
27	d	144	SER
27	d	150	TYR
28	e	55	LEU
28	e	62	GLU
28	e	81	ILE
28	e	124	ARG
28	e	137	MET
28	e	138	GLU

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Mol	Chain	Res	Type
28	e	146	LYS
29	f	51	SER
29	f	60	LYS
29	f	63	LYS
30	g	36	MET
31	h	77	SER
31	h	81	ARG
32	i	97	MET
32	i	104	MET
32	i	187	MET
32	i	257	LEU
32	i	261	MET
32	i	300	SER
32	i	323	MET
32	i	324	LYS
33	j	8	LEU
33	j	22	PHE
33	j	85	LYS
33	j	87	MET
34	k	53	PHE
34	k	91	GLN
35	l	72	GLN
35	l	111	ASP
35	l	159	HIS
35	l	207	GLU
35	l	320	ASN
35	l	357	ARG
35	l	429	PHE
35	l	481	THR
35	l	482	MET
35	l	554	ASP
35	l	601	LEU
36	m	3	MET
36	m	20	PHE
36	m	57	PHE
36	m	135	PHE
37	n	31	SER
37	n	54	GLU
38	o	9	SER
38	o	30	ARG
38	o	45	ARG
39	p	48	PHE

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Mol	Chain	Res	Type
39	p	59	LYS
39	p	64	LEU
39	p	84	GLU
39	p	177	ARG
40	r	59	ASP
40	r	60	SER
40	r	66	LEU
40	r	111	THR
40	r	114	GLU
40	r	183	SER
40	r	206	LYS
40	r	410	MET
41	s	54	LYS
41	s	119	SER
41	s	248	ASP
42	u	6	GLU
42	u	48	TRP
42	u	64	ASN
42	u	87	THR
42	u	108	ASP
43	v	14	SER
43	v	21	ARG
43	v	34	ARG
43	v	39	MET
43	v	52	MET
43	v	65	GLN
43	v	69	CYS
43	v	112	LYS
44	w	51	ARG
44	w	55	GLU
44	w	164	TYR
44	w	239	ASN
44	w	272	ASP
44	w	288	ASP
44	w	290	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
12	M	336	ASN
15	P	107	GLN
16	Q	182	ASN

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Mol	Chain	Res	Type
16	Q	190	HIS
25	b	14	GLN
26	c	106	HIS
33	j	83	ASN
35	l	135	ASN
35	l	199	GLN
39	p	76	HIS
44	w	127	ASN
44	w	132	GLN
44	w	202	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	2MR	Q	118	16	10,12,13	1.98	1 (10%)	5,13,15	6.05	3 (60%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.64	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	12.39	130.84	119.48
16	Q	118	2MR	CD-NE-CZ	4.37	131.60	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.01	130.51	123.86

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

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 37 ligands modelled in this entry, 2 are monoatomic - leaving 35 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	$\# Z > 2$
55	CDL	a	201	-	90,90,99	1.14	8 (8%)	96,102,111	0.92	4 (4%)
48	PEE	j	201	-	50,50,50	1.16	6 (12%)	53,55,55	0.95	2 (3%)
48	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	0.97	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	PLX	g	201	-	51,51,51	1.14	3 (5%)	55,59,59	0.61	1 (1%)
45	SF4	B	302	2	0,12,12	-	-	-	-	-
47	NAI	A	503	-	42,48,48	4.95	19 (45%)	47,73,73	1.31	7 (14%)
49	PLX	e	201	-	51,51,51	1.14	4 (7%)	55,59,59	0.60	1 (1%)
55	CDL	i	401	-	65,65,99	1.28	8 (12%)	71,77,111	0.97	4 (5%)
56	UQ	s	402	-	28,28,63	3.27	7 (25%)	34,37,79	2.79	10 (29%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
48	PEE	l	703	-	45,45,50	1.23	6 (13%)	48,50,55	0.99	2 (4%)
48	PEE	b	201	-	45,45,50	1.22	6 (13%)	48,50,55	0.98	2 (4%)
48	PEE	Q	501	-	46,46,50	1.21	6 (13%)	49,51,55	1.00	2 (4%)
49	PLX	r	502	-	51,51,51	1.14	4 (7%)	55,59,59	0.62	1 (1%)
46	FMN	A	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.21	8 (16%)
49	PLX	C	303	-	51,51,51	1.15	4 (7%)	55,59,59	0.59	1 (1%)
55	CDL	l	701	-	98,98,99	1.09	8 (8%)	104,110,111	0.88	4 (3%)
57	ADP	w	401	-	24,29,29	3.11	6 (25%)	29,45,45	1.43	4 (13%)
52	FES	M	803	12	0,4,4	-	-	-	-	-
45	SF4	B	301	2	0,12,12	-	-	-	-	-
45	SF4	M	801	12	0,12,12	-	-	-	-	-
48	PEE	s	401	-	40,40,50	1.15	5 (12%)	43,45,55	1.01	2 (4%)
50	8Q1	X	201	-	31,34,34	1.71	6 (19%)	40,43,43	1.60	6 (15%)
55	CDL	l	702	-	99,99,99	1.09	9 (9%)	105,111,111	0.85	4 (3%)
45	SF4	C	301	16,3	0,12,12	-	-	-	-	-
49	PLX	a	202	-	51,51,51	1.14	4 (7%)	55,59,59	0.60	1 (1%)
55	CDL	r	503	-	99,99,99	1.09	8 (8%)	105,111,111	0.85	4 (3%)
55	CDL	u	201	-	77,77,99	1.20	9 (11%)	83,89,111	0.95	4 (4%)
45	SF4	A	501	1	0,12,12	-	-	-	-	-
48	PEE	B	303	-	50,50,50	1.16	6 (12%)	53,55,55	0.98	2 (3%)
50	8Q1	G	201	6	31,34,34	1.69	6 (19%)	40,43,43	1.52	6 (15%)
51	NDP	J	401	-	45,52,52	4.57	20 (44%)	53,80,80	2.04	7 (13%)
52	FES	O	301	14	0,4,4	-	-	-	-	-
48	PEE	C	302	-	46,46,50	1.21	6 (13%)	49,51,55	0.94	2 (4%)
49	PLX	j	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.59	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	CDL	a	201	-	-	49/101/101/110	-
48	PEE	j	201	-	-	21/54/54/54	-
48	PEE	r	501	-	-	23/54/54/54	-
49	PLX	g	201	-	-	28/55/55/55	-
47	NAI	A	503	-	-	7/25/72/72	0/5/5/5
45	SF4	B	302	2	-	-	0/6/5/5
49	PLX	e	201	-	-	33/55/55/55	-
55	CDL	i	401	-	-	35/76/76/110	-
56	UQ	s	402	-	-	8/21/45/87	0/1/1/1
45	SF4	M	802	12	-	-	0/6/5/5
48	PEE	l	703	-	-	21/49/49/54	-
48	PEE	b	201	-	-	22/49/49/54	-
48	PEE	Q	501	-	-	25/50/50/54	-
49	PLX	r	502	-	-	21/55/55/55	-
46	FMN	A	502	-	-	8/18/18/18	0/3/3/3
49	PLX	C	303	-	-	24/55/55/55	-
55	CDL	l	701	-	-	50/109/109/110	-
57	ADP	w	401	-	-	3/12/32/32	0/3/3/3
52	FES	M	803	12	-	-	0/1/1/1
45	SF4	B	301	2	-	-	0/6/5/5
45	SF4	M	801	12	-	-	0/6/5/5
48	PEE	s	401	-	-	16/44/44/54	-
50	8Q1	X	201	-	-	20/41/41/41	-
55	CDL	l	702	-	-	58/110/110/110	-
45	SF4	C	301	16,3	-	-	0/6/5/5
49	PLX	a	202	-	-	31/55/55/55	-
55	CDL	r	503	-	-	71/110/110/110	-
55	CDL	u	201	-	-	41/88/88/110	-
45	SF4	A	501	1	-	-	0/6/5/5
48	PEE	B	303	-	-	22/54/54/54	-
50	8Q1	G	201	6	-	18/41/41/41	-
51	NDP	J	401	-	-	7/30/77/77	0/4/5/5
52	FES	O	301	14	-	-	0/1/1/1
48	PEE	C	302	-	-	24/50/50/54	-
49	PLX	j	202	-	-	32/55/55/55	-

All (186) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	O4B-C1B	16.20	1.63	1.41
47	A	503	NAI	C2B-C1B	-15.42	1.30	1.53
51	J	401	NDP	C3B-C2B	-12.77	1.24	1.52
51	J	401	NDP	C6N-C5N	12.54	1.55	1.33
51	J	401	NDP	O4D-C4D	10.71	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.25	1.26	1.53
51	J	401	NDP	C3D-C4D	-9.84	1.27	1.53
56	s	402	UQ	C13-C14	9.24	1.55	1.33
56	s	402	UQ	C8-C9	8.94	1.54	1.33
57	w	401	ADP	C3'-C4'	-8.85	1.30	1.53
47	A	503	NAI	O4B-C4B	-8.29	1.26	1.45
51	J	401	NDP	O4B-C1B	8.23	1.52	1.41
56	s	402	UQ	C18-C19	8.23	1.56	1.32
51	J	401	NDP	O4B-C4B	-7.97	1.27	1.45
57	w	401	ADP	O4'-C4'	7.74	1.62	1.45
47	A	503	NAI	C2D-C1D	-7.58	1.29	1.53
51	J	401	NDP	C2N-C3N	7.35	1.55	1.34
47	A	503	NAI	O4D-C4D	7.03	1.60	1.45
57	w	401	ADP	O4'-C1'	-6.80	1.31	1.41
47	A	503	NAI	C2D-C3D	5.92	1.69	1.53
51	J	401	NDP	P2B-O2B	5.77	1.70	1.59
47	A	503	NAI	C7N-N7N	5.74	1.48	1.33
47	A	503	NAI	O4D-C1D	5.50	1.55	1.42
50	X	201	8Q1	C34-N36	5.49	1.45	1.33
51	J	401	NDP	C3B-C4B	5.48	1.67	1.53
50	G	201	8Q1	C34-N36	5.43	1.45	1.33
50	X	201	8Q1	C39-N41	5.42	1.45	1.33
50	G	201	8Q1	C39-N41	5.29	1.45	1.33
47	A	503	NAI	C4N-C3N	-5.06	1.40	1.49
51	J	401	NDP	O4D-C1D	-4.88	1.30	1.42
51	J	401	NDP	C6N-N1N	4.78	1.49	1.37
47	A	503	NAI	O2B-C2B	4.54	1.53	1.43
51	J	401	NDP	C7N-N7N	4.20	1.44	1.33
51	J	401	NDP	O2D-C2D	-4.15	1.33	1.43
51	J	401	NDP	C6A-N6A	4.11	1.49	1.34
47	A	503	NAI	C6N-C5N	3.94	1.40	1.33
46	A	502	FMN	C4A-N5	3.86	1.38	1.30
57	w	401	ADP	C6-N6	3.82	1.48	1.34
48	C	302	PEE	C18-C19	3.75	1.53	1.31
48	s	401	PEE	C18-C19	3.74	1.53	1.31
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	r	501	PEE	C18-C19	3.73	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	Q	501	PEE	C18-C19	3.72	1.53	1.31
48	j	201	PEE	C18-C19	3.71	1.53	1.31
48	b	201	PEE	C18-C19	3.71	1.53	1.31
48	b	201	PEE	C39-C38	3.65	1.52	1.31
48	C	302	PEE	C39-C38	3.65	1.52	1.31
48	r	501	PEE	C39-C38	3.65	1.52	1.31
48	j	201	PEE	C39-C38	3.65	1.52	1.31
48	l	703	PEE	C39-C38	3.64	1.52	1.31
48	Q	501	PEE	C39-C38	3.64	1.52	1.31
48	B	303	PEE	C39-C38	3.64	1.52	1.31
47	A	503	NAI	C7N-C3N	3.62	1.56	1.48
47	A	503	NAI	C6A-N6A	3.61	1.47	1.34
55	i	401	CDL	OA8-CA7	3.47	1.43	1.33
55	u	201	CDL	OA8-CA7	3.46	1.43	1.33
55	l	702	CDL	OA8-CA7	3.45	1.43	1.33
55	a	201	CDL	OA8-CA7	3.43	1.43	1.33
55	r	503	CDL	OA8-CA7	3.40	1.43	1.33
55	l	701	CDL	OA8-CA7	3.37	1.43	1.33
57	w	401	ADP	O2'-C2'	-3.34	1.35	1.43
47	A	503	NAI	C4N-C5N	-3.31	1.40	1.48
55	r	503	CDL	OB6-CB5	3.11	1.43	1.34
51	J	401	NDP	O3D-C3D	3.10	1.50	1.43
57	w	401	ADP	O3'-C3'	3.10	1.50	1.43
55	l	701	CDL	OB6-CB5	3.05	1.42	1.34
55	i	401	CDL	OB8-CB7	3.05	1.42	1.33
55	i	401	CDL	OB6-CB5	3.05	1.42	1.34
55	a	201	CDL	OB6-CB5	3.04	1.42	1.34
55	l	702	CDL	OB6-CB5	3.04	1.42	1.34
51	J	401	NDP	C7N-C3N	3.02	1.55	1.48
55	u	201	CDL	OB6-CB5	3.01	1.42	1.34
55	u	201	CDL	OB8-CB7	3.01	1.42	1.33
55	l	702	CDL	OB8-CB7	3.00	1.42	1.33
55	a	201	CDL	OB8-CB7	3.00	1.42	1.33
55	r	503	CDL	OB8-CB7	3.00	1.42	1.33
55	a	201	CDL	OA6-CA5	2.99	1.42	1.34
55	l	702	CDL	OA6-CA5	2.97	1.42	1.34
55	i	401	CDL	OA6-CA5	2.95	1.42	1.34
55	l	701	CDL	OB8-CB7	2.94	1.41	1.33
55	u	201	CDL	OA6-CA5	2.94	1.42	1.34
55	r	503	CDL	OA6-CA5	2.92	1.42	1.34
55	l	701	CDL	OA6-CA5	2.91	1.42	1.34
49	C	303	PLX	O6-C4	-2.77	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	g	201	PLX	O6-C4	-2.73	1.41	1.44
49	e	201	PLX	O6-C4	-2.72	1.41	1.44
56	s	402	UQ	C6-C1	2.66	1.54	1.46
49	a	202	PLX	O6-C4	-2.62	1.41	1.44
49	j	202	PLX	O6-C4	-2.56	1.41	1.44
48	C	302	PEE	O3-C30	2.51	1.40	1.33
48	Q	501	PEE	O3-C30	2.49	1.40	1.33
46	A	502	FMN	C10-N1	2.48	1.38	1.33
48	b	201	PEE	O3-C30	2.48	1.40	1.33
48	j	201	PEE	O3-C30	2.47	1.40	1.33
47	A	503	NAI	PN-O5D	2.47	1.69	1.59
47	A	503	NAI	O3B-C3B	-2.46	1.37	1.43
55	r	503	CDL	OA6-CA4	-2.45	1.40	1.46
55	l	701	CDL	OA6-CA4	-2.45	1.40	1.46
48	r	501	PEE	O3-C30	2.44	1.40	1.33
48	B	303	PEE	O3-C30	2.43	1.40	1.33
51	J	401	NDP	O2B-C2B	2.43	1.52	1.44
48	j	201	PEE	O2-C2	-2.43	1.40	1.46
49	r	502	PLX	C7-C6	2.43	1.55	1.50
55	a	201	CDL	OA6-CA4	-2.43	1.40	1.46
48	l	703	PEE	O3-C30	2.42	1.40	1.33
48	Q	501	PEE	O2-C2	-2.42	1.40	1.46
55	u	201	CDL	OA6-CA4	-2.41	1.40	1.46
50	X	201	8Q1	C1-S44	2.41	1.82	1.76
48	s	401	PEE	O3-C30	2.41	1.40	1.33
55	i	401	CDL	OA6-CA4	-2.40	1.40	1.46
48	r	501	PEE	O2-C2	-2.40	1.40	1.46
48	B	303	PEE	O2-C2	-2.39	1.40	1.46
51	J	401	NDP	C2D-C3D	2.39	1.59	1.53
50	G	201	8Q1	C6-C1	2.38	1.53	1.50
48	l	703	PEE	O2-C2	-2.38	1.40	1.46
49	j	202	PLX	C7-C6	2.38	1.55	1.50
48	C	302	PEE	O2-C10	2.38	1.41	1.34
48	l	703	PEE	O2-C10	2.37	1.41	1.34
50	G	201	8Q1	C1-S44	2.37	1.81	1.76
48	C	302	PEE	O2-C2	-2.36	1.40	1.46
49	C	303	PLX	C7-C6	2.35	1.55	1.50
48	s	401	PEE	O2-C10	2.35	1.40	1.34
48	b	201	PEE	O2-C2	-2.35	1.40	1.46
49	e	201	PLX	C7-C6	2.34	1.55	1.50
55	l	702	CDL	OA6-CA4	-2.33	1.40	1.46
49	a	202	PLX	C7-C6	2.32	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	b	201	PEE	O2-C10	2.32	1.40	1.34
48	s	401	PEE	O2-C2	-2.28	1.40	1.46
47	A	503	NAI	C5B-C4B	2.28	1.58	1.51
49	g	201	PLX	C7-C6	2.27	1.55	1.50
48	r	501	PEE	O2-C10	2.26	1.40	1.34
48	j	201	PEE	O2-C10	2.26	1.40	1.34
48	Q	501	PEE	O2-C10	2.25	1.40	1.34
48	B	303	PEE	O2-C10	2.25	1.40	1.34
50	X	201	8Q1	O35-C34	-2.25	1.18	1.23
50	G	201	8Q1	O35-C34	-2.24	1.18	1.23
55	i	401	CDL	OB6-CB4	-2.22	1.41	1.46
50	G	201	8Q1	O40-C39	-2.21	1.18	1.23
55	a	201	CDL	PB2-OB2	2.21	1.68	1.59
55	l	702	CDL	PB2-OB2	2.20	1.68	1.59
55	r	503	CDL	PB2-OB5	2.20	1.68	1.59
55	l	701	CDL	PB2-OB5	2.20	1.68	1.59
55	i	401	CDL	PB2-OB2	2.20	1.68	1.59
55	r	503	CDL	PB2-OB2	2.19	1.68	1.59
55	u	201	CDL	PB2-OB5	2.19	1.68	1.59
55	l	702	CDL	PB2-OB5	2.18	1.68	1.59
49	r	502	PLX	O6-C4	-2.18	1.41	1.44
50	X	201	8Q1	O40-C39	-2.18	1.18	1.23
50	X	201	8Q1	C6-C1	2.17	1.53	1.50
56	s	402	UQ	O4-C4	-2.17	1.18	1.23
55	u	201	CDL	PB2-OB2	2.17	1.68	1.59
55	a	201	CDL	PB2-OB5	2.17	1.68	1.59
55	l	701	CDL	PB2-OB2	2.16	1.68	1.59
55	a	201	CDL	OB6-CB4	-2.16	1.41	1.46
55	u	201	CDL	OB6-CB4	-2.16	1.41	1.46
56	s	402	UQ	C7-C8	2.16	1.53	1.50
49	a	202	PLX	P1-O4	2.15	1.68	1.59
49	j	202	PLX	P1-O4	2.15	1.68	1.59
55	i	401	CDL	PB2-OB5	2.15	1.68	1.59
49	g	201	PLX	P1-O4	2.14	1.68	1.59
49	r	502	PLX	P1-O4	2.14	1.68	1.59
48	r	501	PEE	O3-C3	-2.13	1.40	1.45
55	l	702	CDL	OB6-CB4	-2.13	1.41	1.46
48	B	303	PEE	O3-C3	-2.13	1.40	1.45
49	C	303	PLX	P1-O4	2.13	1.67	1.59
55	l	701	CDL	OB6-CB4	-2.12	1.41	1.46
48	l	703	PEE	O3-C3	-2.12	1.40	1.45
51	J	401	NDP	O7N-C7N	-2.11	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	s	402	UQ	O1-C1	-2.11	1.18	1.23
51	J	401	NDP	PA-O5B	2.09	1.67	1.59
48	b	201	PEE	O3-C3	-2.09	1.40	1.45
49	e	201	PLX	P1-O4	2.08	1.67	1.59
48	j	201	PEE	O3-C3	-2.08	1.40	1.45
48	s	401	PEE	O3-C3	-2.07	1.40	1.45
49	j	202	PLX	P1-O1	2.07	1.67	1.59
48	C	302	PEE	O3-C3	-2.07	1.40	1.45
48	Q	501	PEE	O3-C3	-2.07	1.40	1.45
49	a	202	PLX	P1-O1	2.05	1.67	1.59
49	r	502	PLX	P1-O1	2.04	1.67	1.59
55	r	503	CDL	OB6-CB4	-2.03	1.41	1.46
49	e	201	PLX	P1-O1	2.03	1.67	1.59
49	C	303	PLX	P1-O1	2.02	1.67	1.59
47	A	503	NAI	C2N-C3N	2.02	1.40	1.34
55	u	201	CDL	C11-CA5	2.01	1.56	1.50
55	l	702	CDL	C11-CA5	2.01	1.56	1.50

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	s	402	UQ	C7-C8-C9	-9.19	111.50	126.79
51	J	401	NDP	C3N-C2N-N1N	-9.10	110.12	123.10
51	J	401	NDP	C1D-N1N-C2N	-6.61	110.11	121.11
50	X	201	8Q1	C6-C1-S44	6.17	120.64	113.46
56	s	402	UQ	C12-C13-C14	-5.94	113.36	127.66
50	G	201	8Q1	C6-C1-S44	5.71	120.11	113.46
51	J	401	NDP	C1D-N1N-C6N	-5.08	109.89	120.83
56	s	402	UQ	C11-C9-C8	-4.72	111.56	121.12
57	w	401	ADP	N3-C2-N1	-4.48	121.68	128.68
56	s	402	UQ	C10-C9-C8	-4.41	112.36	123.68
47	A	503	NAI	N3A-C2A-N1A	-4.34	121.89	128.68
56	s	402	UQ	C15-C14-C13	-4.31	112.61	123.68
56	s	402	UQ	C16-C14-C13	-4.31	112.39	121.12
56	s	402	UQ	C17-C18-C19	-4.18	113.47	127.75
55	a	201	CDL	OA6-CA5-C11	4.16	120.47	111.50
55	l	701	CDL	OA6-CA5-C11	4.11	120.37	111.50
55	a	201	CDL	OB6-CB5-C51	4.10	120.35	111.50
48	B	303	PEE	O2-C10-C11	4.09	120.31	111.50
48	s	401	PEE	O2-C10-C11	4.08	120.30	111.50
55	r	503	CDL	OB6-CB5-C51	4.03	120.20	111.50
55	l	702	CDL	OA6-CA5-C11	4.03	120.18	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	J	401	NDP	N3A-C2A-N1A	-4.02	122.40	128.68
48	r	501	PEE	O2-C10-C11	4.00	120.13	111.50
55	u	201	CDL	OB6-CB5-C51	3.99	120.10	111.50
48	Q	501	PEE	O2-C10-C11	3.97	120.06	111.50
55	l	701	CDL	OB6-CB5-C51	3.93	119.98	111.50
48	l	703	PEE	O2-C10-C11	3.91	119.94	111.50
48	b	201	PEE	O2-C10-C11	3.91	119.92	111.50
55	l	702	CDL	OB6-CB5-C51	3.90	119.90	111.50
55	u	201	CDL	OA6-CA5-C11	3.89	119.89	111.50
55	r	503	CDL	OA6-CA5-C11	3.86	119.82	111.50
55	i	401	CDL	OA6-CA5-C11	3.81	119.71	111.50
48	j	201	PEE	O2-C10-C11	3.80	119.69	111.50
48	C	302	PEE	O2-C10-C11	3.73	119.53	111.50
55	i	401	CDL	OB6-CB5-C51	3.58	119.22	111.50
50	X	201	8Q1	O4-C1-C6	-3.56	119.78	123.99
56	s	402	UQ	C21-C19-C18	-3.42	112.75	122.65
50	X	201	8Q1	C37-C38-C39	3.32	117.88	112.36
50	G	201	8Q1	O4-C1-C6	-3.15	120.27	123.99
47	A	503	NAI	C3D-C2D-C1D	3.13	107.37	101.43
56	s	402	UQ	C20-C19-C18	-3.09	113.71	122.65
46	A	502	FMN	C4-N3-C2	-3.04	120.03	125.64
56	s	402	UQ	CM5-C5-C6	-2.94	119.60	124.40
50	G	201	8Q1	C37-C38-C39	2.80	117.01	112.36
47	A	503	NAI	C4D-O4D-C1D	-2.79	103.32	109.47
47	A	503	NAI	C2D-C3D-C4D	2.75	107.98	102.64
48	l	703	PEE	O3-C30-C31	2.71	120.42	111.91
55	i	401	CDL	OA8-CA7-C31	2.69	120.35	111.91
48	B	303	PEE	O3-C30-C31	2.68	120.32	111.91
55	a	201	CDL	OB8-CB7-C71	2.68	120.32	111.91
46	A	502	FMN	C4A-C4-N3	2.66	119.94	113.19
55	l	701	CDL	OB8-CB7-C71	2.65	120.22	111.91
51	J	401	NDP	C2B-C3B-C4B	2.65	107.75	101.99
55	i	401	CDL	OB8-CB7-C71	2.65	120.21	111.91
57	w	401	ADP	PA-O3A-PB	-2.64	123.77	132.83
55	u	201	CDL	OB8-CB7-C71	2.63	120.17	111.91
48	Q	501	PEE	O3-C30-C31	2.63	120.16	111.91
48	j	201	PEE	O3-C30-C31	2.61	120.11	111.91
55	l	702	CDL	OB8-CB7-C71	2.60	120.05	111.91
48	r	501	PEE	O3-C30-C31	2.59	120.05	111.91
51	J	401	NDP	PN-O3-PA	-2.59	123.93	132.83
47	A	503	NAI	C4A-C5A-N7A	-2.59	106.70	109.40
48	s	401	PEE	O3-C30-C31	2.59	120.02	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	u	201	CDL	OA8-CA7-C31	2.57	119.97	111.91
55	l	702	CDL	OA8-CA7-C31	2.56	119.94	111.91
55	a	201	CDL	OA8-CA7-C31	2.54	119.89	111.91
48	C	302	PEE	O3-C30-C31	2.53	119.86	111.91
49	e	201	PLX	C1A-N1-C1	2.53	120.28	109.92
48	b	201	PEE	O3-C30-C31	2.52	119.81	111.91
47	A	503	NAI	PN-O3-PA	-2.51	124.23	132.83
55	l	701	CDL	OA8-CA7-C31	2.50	119.77	111.91
55	r	503	CDL	OB8-CB7-C71	2.47	119.66	111.91
46	A	502	FMN	O4-C4-C4A	-2.46	120.07	126.60
55	r	503	CDL	OA8-CA7-C31	2.46	119.62	111.91
46	A	502	FMN	C4A-C10-N10	2.44	120.05	116.48
49	g	201	PLX	C1A-N1-C1	2.44	119.91	109.92
57	w	401	ADP	O4'-C1'-C2'	-2.39	103.44	106.93
50	G	201	8Q1	C38-C39-N41	2.38	120.44	116.42
49	r	502	PLX	C1A-N1-C1	2.37	119.61	109.92
49	j	202	PLX	C1A-N1-C1	2.35	119.52	109.92
50	X	201	8Q1	O4-C1-S44	-2.34	119.57	122.61
50	G	201	8Q1	O4-C1-S44	-2.30	119.62	122.61
49	C	303	PLX	C1A-N1-C1	2.29	119.27	109.92
51	J	401	NDP	C4A-C5A-N7A	-2.26	107.05	109.40
49	a	202	PLX	C1A-N1-C1	2.26	119.14	109.92
46	A	502	FMN	C9A-C5A-N5	-2.25	119.99	122.43
46	A	502	FMN	C10-C4A-N5	-2.22	120.15	124.86
50	X	201	8Q1	C38-C39-N41	2.19	120.12	116.42
46	A	502	FMN	C4A-C10-N1	-2.18	119.66	124.73
50	G	201	8Q1	C43-S44-C1	2.16	108.60	101.87
50	X	201	8Q1	C43-S44-C1	2.15	108.56	101.87
47	A	503	NAI	C3B-C2B-C1B	2.13	104.19	100.98
46	A	502	FMN	C5A-C9A-N10	2.11	120.13	117.95
57	w	401	ADP	C4-C5-N7	-2.08	107.23	109.40

There are no chirality outliers.

All (718) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C1'-C2'-C3'-O3'
46	A	502	FMN	C3'-C4'-C5'-O5'
47	A	503	NAI	C5D-O5D-PN-O3
48	C	302	PEE	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
48	C	302	PEE	O4P-C4-C5-N
48	Q	501	PEE	C11-C10-O2-C2
48	b	201	PEE	C1-O3P-P-O1P
48	b	201	PEE	C37-C38-C39-C40
48	l	703	PEE	C11-C10-O2-C2
48	l	703	PEE	O3P-C1-C2-O2
48	l	703	PEE	C4-O4P-P-O2P
48	r	501	PEE	C17-C18-C19-C20
48	r	501	PEE	O3P-C1-C2-O2
48	s	401	PEE	C11-C10-O2-C2
49	C	303	PLX	C3-O4-P1-O3
49	C	303	PLX	N1-C1-C2-O1
49	a	202	PLX	O7-C6-C7-C8
49	a	202	PLX	O7-C6-O6-C4
49	a	202	PLX	O4-C3-C4-O6
49	a	202	PLX	C3-O4-P1-O1
49	a	202	PLX	C3-O4-P1-O2
49	a	202	PLX	C2-O1-P1-O2
49	a	202	PLX	C2-O1-P1-O3
49	a	202	PLX	C25-C24-O8-C5
49	e	201	PLX	C3-O4-P1-O1
49	e	201	PLX	C3-O4-P1-O2
49	e	201	PLX	C3-O4-P1-O3
49	e	201	PLX	O9-C24-O8-C5
49	e	201	PLX	O9-C24-C25-C26
49	g	201	PLX	O7-C6-C7-C8
49	g	201	PLX	O7-C6-O6-C4
49	g	201	PLX	O9-C24-C25-C26
49	j	202	PLX	O7-C6-C7-C8
49	j	202	PLX	C3-O4-P1-O3
49	r	502	PLX	O7-C6-O6-C4
49	r	502	PLX	C5-C4-O6-C6
49	r	502	PLX	O9-C24-C25-C26
50	G	201	8Q1	O27-C28-C29-C31
50	G	201	8Q1	O27-C28-C29-C32
50	G	201	8Q1	N36-C37-C38-C39
50	G	201	8Q1	N41-C42-C43-S44
50	G	201	8Q1	C42-C43-S44-C1
50	G	201	8Q1	C28-O27-P24-O1
50	X	201	8Q1	O4-C1-S44-C43
50	X	201	8Q1	C6-C1-S44-C43
50	X	201	8Q1	C28-C29-C32-C34

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Mol	Chain	Res	Type	Atoms
50	X	201	8Q1	C28-C29-C32-O33
50	X	201	8Q1	C30-C29-C32-C34
50	X	201	8Q1	C30-C29-C32-O33
50	X	201	8Q1	N36-C37-C38-C39
50	X	201	8Q1	C42-C43-S44-C1
50	X	201	8Q1	C28-O27-P24-O2
50	X	201	8Q1	C28-O27-P24-O1
51	J	401	NDP	C5B-O5B-PA-O1A
51	J	401	NDP	C2B-O2B-P2B-O1X
55	a	201	CDL	CA3-OA5-PA1-OA4
55	a	201	CDL	CB2-OB2-PB2-OB3
55	a	201	CDL	CB3-OB5-PB2-OB3
55	i	401	CDL	CA3-OA5-PA1-OA4
55	i	401	CDL	CB3-OB5-PB2-OB3
55	i	401	CDL	CB3-OB5-PB2-OB4
55	l	701	CDL	O1-C1-CA2-OA2
55	l	701	CDL	O1-C1-CB2-OB2
55	l	701	CDL	CA2-C1-CB2-OB2
55	l	701	CDL	CB3-OB5-PB2-OB2
55	l	702	CDL	O1-C1-CA2-OA2
55	l	702	CDL	CA2-C1-CB2-OB2
55	l	702	CDL	CA2-OA2-PA1-OA3
55	l	702	CDL	CA3-OA5-PA1-OA2
55	l	702	CDL	CB2-OB2-PB2-OB4
55	l	702	CDL	CB2-OB2-PB2-OB5
55	l	702	CDL	OB6-CB4-CB6-OB8
55	r	503	CDL	CA2-OA2-PA1-OA3
55	r	503	CDL	CA2-OA2-PA1-OA4
55	r	503	CDL	CA3-OA5-PA1-OA2
55	r	503	CDL	CA3-OA5-PA1-OA3
55	r	503	CDL	CA3-OA5-PA1-OA4
55	u	201	CDL	CB2-C1-CA2-OA2
55	u	201	CDL	CA3-OA5-PA1-OA3
55	u	201	CDL	CA3-OA5-PA1-OA4
56	s	402	UQ	C7-C8-C9-C10
56	s	402	UQ	C7-C8-C9-C11
56	s	402	UQ	C12-C11-C9-C10
57	w	401	ADP	C5'-O5'-PA-O1A
57	w	401	ADP	C5'-O5'-PA-O2A
57	w	401	ADP	C5'-O5'-PA-O3A
56	s	402	UQ	C17-C18-C19-C21
48	s	401	PEE	O5-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
55	i	401	CDL	OA9-CA7-OA8-CA6
55	l	701	CDL	OA9-CA7-OA8-CA6
48	C	302	PEE	O4-C10-O2-C2
48	Q	501	PEE	O4-C10-O2-C2
48	l	703	PEE	O4-C10-O2-C2
48	s	401	PEE	O4-C10-O2-C2
55	l	702	CDL	C71-CB7-OB8-CB6
48	C	302	PEE	C11-C10-O2-C2
48	l	703	PEE	O5-C30-O3-C3
49	r	502	PLX	C9-C10-C11-C12
48	b	201	PEE	C31-C30-O3-C3
48	l	703	PEE	C31-C30-O3-C3
48	s	401	PEE	C31-C30-O3-C3
55	i	401	CDL	C31-CA7-OA8-CA6
55	l	701	CDL	C31-CA7-OA8-CA6
48	B	303	PEE	C37-C38-C39-C40
48	j	201	PEE	C17-C18-C19-C20
56	s	402	UQ	C12-C13-C14-C15
55	l	701	CDL	C32-C33-C34-C35
55	r	503	CDL	OB9-CB7-OB8-CB6
49	a	202	PLX	C10-C11-C12-C13
55	a	201	CDL	O1-C1-CB2-OB2
55	l	702	CDL	O1-C1-CB2-OB2
55	r	503	CDL	O1-C1-CA2-OA2
55	l	702	CDL	OB9-CB7-OB8-CB6
49	g	201	PLX	C7-C8-C9-C10
55	i	401	CDL	C31-C32-C33-C34
55	l	702	CDL	C11-C12-C13-C14
49	j	202	PLX	C28-C29-C30-C31
55	l	702	CDL	C59-C60-C61-C62
55	l	701	CDL	C55-C56-C57-C58
47	A	503	NAI	C3D-C4D-C5D-O5D
51	J	401	NDP	O4B-C4B-C5B-O5B
55	r	503	CDL	C71-CB7-OB8-CB6
48	b	201	PEE	O5-C30-O3-C3
49	g	201	PLX	C12-C13-C14-C15
55	u	201	CDL	C71-C72-C73-C74
48	j	201	PEE	C31-C30-O3-C3
55	l	702	CDL	C75-C76-C77-C78
48	r	501	PEE	C11-C10-O2-C2
55	a	201	CDL	CB2-C1-CA2-OA2
55	a	201	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
55	r	503	CDL	CB2-C1-CA2-OA2
55	u	201	CDL	CA2-C1-CB2-OB2
55	l	701	CDL	C71-CB7-OB8-CB6
49	j	202	PLX	C32-C33-C34-C35
55	l	702	CDL	CB7-C71-C72-C73
55	l	702	CDL	C35-C36-C37-C38
55	u	201	CDL	C75-C76-C77-C78
55	i	401	CDL	C14-C15-C16-C17
55	u	201	CDL	O1-C1-CA2-OA2
55	u	201	CDL	O1-C1-CB2-OB2
55	r	503	CDL	C51-CB5-OB6-CB4
49	a	202	PLX	C11-C10-C9-C8
51	J	401	NDP	C2D-C1D-N1N-C6N
48	r	501	PEE	C10-C11-C12-C13
55	a	201	CDL	CA7-C31-C32-C33
55	r	503	CDL	CB5-C51-C52-C53
49	C	303	PLX	C28-C29-C30-C31
55	l	702	CDL	C39-C40-C41-C42
48	C	302	PEE	C10-C11-C12-C13
55	i	401	CDL	CB5-C51-C52-C53
55	l	701	CDL	CB5-C51-C52-C53
55	l	702	CDL	CB5-C51-C52-C53
55	r	503	CDL	CB7-C71-C72-C73
47	A	503	NAI	O4D-C4D-C5D-O5D
49	e	201	PLX	C2-C1-N1-C1A
55	a	201	CDL	CB7-C71-C72-C73
55	l	701	CDL	OB9-CB7-OB8-CB6
55	i	401	CDL	O1-C1-CA2-OA2
48	r	501	PEE	O4-C10-O2-C2
55	r	503	CDL	OB7-CB5-OB6-CB4
55	r	503	CDL	C74-C75-C76-C77
48	j	201	PEE	O5-C30-O3-C3
49	r	502	PLX	C30-C31-C32-C33
48	b	201	PEE	C17-C18-C19-C20
48	j	201	PEE	C11-C10-O2-C2
48	l	703	PEE	C4-O4P-P-O3P
49	C	303	PLX	C3-O4-P1-O1
49	a	202	PLX	C2-O1-P1-O4
49	e	201	PLX	C2-O1-P1-O4
49	j	202	PLX	C3-O4-P1-O1
55	a	201	CDL	CA2-OA2-PA1-OA5
55	a	201	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	CB3-OB5-PB2-OB2
55	i	401	CDL	CA3-OA5-PA1-OA2
55	i	401	CDL	CB3-OB5-PB2-OB2
55	l	701	CDL	CA2-OA2-PA1-OA5
55	l	702	CDL	CA2-OA2-PA1-OA5
55	l	702	CDL	CB3-OB5-PB2-OB2
55	r	503	CDL	CA2-OA2-PA1-OA5
55	r	503	CDL	CB2-OB2-PB2-OB5
55	r	503	CDL	CB3-OB5-PB2-OB2
55	u	201	CDL	CA3-OA5-PA1-OA2
55	r	503	CDL	CA7-C31-C32-C33
55	i	401	CDL	CB2-C1-CA2-OA2
55	l	702	CDL	CB2-C1-CA2-OA2
48	j	201	PEE	O4-C10-O2-C2
49	r	502	PLX	C11-C12-C13-C14
49	a	202	PLX	O6-C6-C7-C8
49	e	201	PLX	O8-C24-C25-C26
48	s	401	PEE	C13-C14-C15-C16
49	j	202	PLX	C12-C13-C14-C15
55	u	201	CDL	C14-C15-C16-C17
48	b	201	PEE	C12-C13-C14-C15
49	a	202	PLX	C33-C34-C35-C36
49	a	202	PLX	C34-C35-C36-C37
55	l	702	CDL	C72-C73-C74-C75
50	G	201	8Q1	O27-C28-C29-C30
48	b	201	PEE	C33-C34-C35-C36
48	j	201	PEE	C21-C22-C23-C24
48	r	501	PEE	C13-C14-C15-C16
49	C	303	PLX	C33-C34-C35-C36
49	r	502	PLX	C12-C13-C14-C15
55	l	702	CDL	C56-C57-C58-C59
55	r	503	CDL	C17-C18-C19-C20
55	r	503	CDL	C35-C36-C37-C38
48	Q	501	PEE	C10-C11-C12-C13
48	l	703	PEE	C30-C31-C32-C33
55	a	201	CDL	C13-C14-C15-C16
55	l	701	CDL	C56-C57-C58-C59
48	C	302	PEE	C37-C38-C39-C40
48	r	501	PEE	C12-C13-C14-C15
49	a	202	PLX	C28-C29-C30-C31
49	r	502	PLX	C15-C16-C17-C18
49	r	502	PLX	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	C72-C73-C74-C75
55	l	701	CDL	C81-C82-C83-C84
55	a	201	CDL	O1-C1-CA2-OA2
49	j	202	PLX	C27-C28-C29-C30
55	r	503	CDL	C41-C42-C43-C44
55	r	503	CDL	OA6-CA4-CA6-OA8
55	a	201	CDL	C71-CB7-OB8-CB6
55	i	401	CDL	C71-CB7-OB8-CB6
49	g	201	PLX	C28-C29-C30-C31
49	j	202	PLX	C13-C14-C15-C16
55	l	702	CDL	C37-C38-C39-C40
55	l	702	CDL	C60-C61-C62-C63
55	r	503	CDL	C12-C13-C14-C15
55	r	503	CDL	C62-C63-C64-C65
55	u	201	CDL	C56-C57-C58-C59
49	g	201	PLX	C9-C10-C11-C12
49	r	502	PLX	C28-C29-C30-C31
50	G	201	8Q1	C12-C13-C14-C15
55	a	201	CDL	C32-C33-C34-C35
55	r	503	CDL	C63-C64-C65-C66
55	u	201	CDL	C57-C58-C59-C60
55	i	401	CDL	CA7-C31-C32-C33
48	C	302	PEE	C43-C44-C45-C46
49	e	201	PLX	C27-C28-C29-C30
49	g	201	PLX	C25-C26-C27-C28
49	g	201	PLX	C27-C28-C29-C30
55	i	401	CDL	C36-C37-C38-C39
55	i	401	CDL	C52-C53-C54-C55
55	r	503	CDL	C73-C74-C75-C76
49	a	202	PLX	C7-C8-C9-C10
50	X	201	8Q1	C7-C8-C9-C10
55	r	503	CDL	C37-C38-C39-C40
48	Q	501	PEE	C21-C22-C23-C24
55	l	701	CDL	C12-C13-C14-C15
55	l	701	CDL	C35-C36-C37-C38
48	B	303	PEE	C23-C24-C25-C26
48	C	302	PEE	C13-C14-C15-C16
48	s	401	PEE	C11-C12-C13-C14
49	a	202	PLX	C31-C32-C33-C34
49	e	201	PLX	C14-C15-C16-C17
49	e	201	PLX	C28-C29-C30-C31
49	e	201	PLX	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
49	g	201	PLX	C10-C11-C12-C13
55	r	503	CDL	C75-C76-C77-C78
49	e	201	PLX	C2-C1-N1-C1C
48	Q	501	PEE	C22-C23-C24-C25
48	l	703	PEE	C21-C22-C23-C24
49	C	303	PLX	C16-C17-C18-C19
49	j	202	PLX	C25-C26-C27-C28
55	l	702	CDL	C73-C74-C75-C76
48	s	401	PEE	O4P-C4-C5-N
49	j	202	PLX	C7-C8-C9-C10
55	a	201	CDL	C52-C53-C54-C55
49	j	202	PLX	C9-C10-C11-C12
49	e	201	PLX	C11-C12-C13-C14
46	A	502	FMN	O4'-C4'-C5'-O5'
55	r	503	CDL	C34-C35-C36-C37
55	r	503	CDL	C52-C53-C54-C55
55	r	503	CDL	C55-C56-C57-C58
55	u	201	CDL	C54-C55-C56-C57
48	B	303	PEE	C32-C33-C34-C35
49	a	202	PLX	C12-C13-C14-C15
49	e	201	PLX	C25-C26-C27-C28
55	r	503	CDL	CB3-CB4-CB6-OB8
48	Q	501	PEE	C37-C38-C39-C40
55	l	701	CDL	C20-C21-C22-C23
55	r	503	CDL	C11-C12-C13-C14
48	r	501	PEE	C30-C31-C32-C33
48	C	302	PEE	C32-C33-C34-C35
49	a	202	PLX	C35-C36-C37-C38
49	C	303	PLX	O7-C6-C7-C8
49	e	201	PLX	O7-C6-C7-C8
49	j	202	PLX	O9-C24-C25-C26
49	e	201	PLX	C29-C30-C31-C32
55	r	503	CDL	C43-C44-C45-C46
55	u	201	CDL	CA7-C31-C32-C33
55	l	702	CDL	C55-C56-C57-C58
48	B	303	PEE	C34-C35-C36-C37
49	j	202	PLX	C34-C35-C36-C37
49	j	202	PLX	C19-C20-C21-C22
55	r	503	CDL	C33-C34-C35-C36
55	r	503	CDL	C56-C57-C58-C59
55	l	701	CDL	CB2-C1-CA2-OA2
48	C	302	PEE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
55	r	503	CDL	C71-C72-C73-C74
48	B	303	PEE	C14-C15-C16-C17
49	e	201	PLX	C10-C11-C12-C13
49	j	202	PLX	C18-C19-C20-C21
49	r	502	PLX	C14-C15-C16-C17
50	G	201	8Q1	C11-C12-C13-C14
55	l	701	CDL	C75-C76-C77-C78
49	a	202	PLX	C29-C30-C31-C32
49	g	201	PLX	C15-C16-C17-C18
49	g	201	PLX	C14-C15-C16-C17
55	i	401	CDL	C71-C72-C73-C74
48	B	303	PEE	C12-C13-C14-C15
48	l	703	PEE	C22-C23-C24-C25
49	j	202	PLX	C14-C15-C16-C17
48	Q	501	PEE	C31-C30-O3-C3
49	a	202	PLX	C25-C26-C27-C28
55	a	201	CDL	C42-C43-C44-C45
55	l	702	CDL	C54-C55-C56-C57
55	a	201	CDL	OB9-CB7-OB8-CB6
55	i	401	CDL	OB9-CB7-OB8-CB6
49	a	202	PLX	C9-C10-C11-C12
48	b	201	PEE	C21-C22-C23-C24
48	j	201	PEE	C34-C35-C36-C37
49	C	303	PLX	C31-C32-C33-C34
48	Q	501	PEE	C35-C36-C37-C38
48	B	303	PEE	C30-C31-C32-C33
48	r	501	PEE	C31-C32-C33-C34
48	l	703	PEE	C31-C32-C33-C34
55	a	201	CDL	C21-C22-C23-C24
48	s	401	PEE	C33-C34-C35-C36
55	l	701	CDL	C52-C53-C54-C55
48	B	303	PEE	C10-C11-C12-C13
55	i	401	CDL	CB7-C71-C72-C73
49	r	502	PLX	C16-C17-C18-C19
48	r	501	PEE	C41-C42-C43-C44
55	l	702	CDL	C52-C53-C54-C55
48	b	201	PEE	C11-C10-O2-C2
55	l	701	CDL	C11-CA5-OA6-CA4
55	u	201	CDL	C11-CA5-OA6-CA4
55	i	401	CDL	C35-C36-C37-C38
55	u	201	CDL	C60-C61-C62-C63
48	j	201	PEE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
48	b	201	PEE	O4-C10-O2-C2
55	l	701	CDL	OA7-CA5-OA6-CA4
55	u	201	CDL	OA7-CA5-OA6-CA4
55	l	702	CDL	C62-C63-C64-C65
55	l	701	CDL	OB6-CB4-CB6-OB8
55	r	503	CDL	OB6-CB4-CB6-OB8
55	r	503	CDL	C15-C16-C17-C18
49	e	201	PLX	C2-C1-N1-C1B
50	X	201	8Q1	C10-C11-C12-C13
48	Q	501	PEE	C19-C20-C21-C22
48	s	401	PEE	C19-C20-C21-C22
55	l	701	CDL	C58-C59-C60-C61
49	C	303	PLX	C13-C14-C15-C16
48	b	201	PEE	C31-C32-C33-C34
55	l	701	CDL	C77-C78-C79-C80
55	r	503	CDL	C59-C60-C61-C62
48	Q	501	PEE	O5-C30-O3-C3
55	l	701	CDL	C39-C40-C41-C42
55	l	702	CDL	C40-C41-C42-C43
48	r	501	PEE	C36-C37-C38-C39
46	A	502	FMN	O2'-C2'-C3'-C4'
48	B	303	PEE	C4-O4P-P-O3P
48	C	302	PEE	C1-O3P-P-O4P
55	a	201	CDL	CB2-OB2-PB2-OB5
49	r	502	PLX	C13-C14-C15-C16
55	a	201	CDL	C73-C74-C75-C76
55	l	701	CDL	C62-C63-C64-C65
55	l	701	CDL	CA7-C31-C32-C33
48	l	703	PEE	O3P-C1-C2-C3
48	r	501	PEE	O3P-C1-C2-C3
55	a	201	CDL	OB5-CB3-CB4-CB6
55	l	701	CDL	CB7-C71-C72-C73
55	l	701	CDL	C14-C15-C16-C17
55	l	702	CDL	C11-CA5-OA6-CA4
55	a	201	CDL	C31-C32-C33-C34
48	Q	501	PEE	C12-C13-C14-C15
48	b	201	PEE	C1-C2-C3-O3
49	a	202	PLX	C3-C4-C5-O8
55	l	702	CDL	CB3-CB4-CB6-OB8
55	r	503	CDL	CA3-CA4-CA6-OA8
55	u	201	CDL	C17-C18-C19-C20
49	C	303	PLX	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
49	j	202	PLX	C26-C27-C28-C29
49	g	201	PLX	C11-C10-C9-C8
50	G	201	8Q1	C7-C8-C9-C10
55	r	503	CDL	C84-C85-C86-C87
49	j	202	PLX	C15-C16-C17-C18
49	r	502	PLX	O8-C24-C25-C26
48	l	703	PEE	C24-C25-C26-C27
49	g	201	PLX	C18-C19-C20-C21
55	l	701	CDL	C73-C74-C75-C76
49	a	202	PLX	C27-C28-C29-C30
55	i	401	CDL	C11-C12-C13-C14
48	B	303	PEE	C15-C16-C17-C18
48	C	302	PEE	C39-C40-C41-C42
49	C	303	PLX	C14-C15-C16-C17
55	r	503	CDL	C78-C79-C80-C81
48	Q	501	PEE	C24-C25-C26-C27
50	G	201	8Q1	C28-O27-P24-O3
50	X	201	8Q1	C28-O27-P24-O3
49	e	201	PLX	C16-C17-C18-C19
55	r	503	CDL	C31-CA7-OA8-CA6
49	g	201	PLX	O4-C3-C4-O6
50	X	201	8Q1	C6-C7-C8-C9
55	i	401	CDL	OB6-CB4-CB6-OB8
56	s	402	UQ	C17-C18-C19-C20
50	X	201	8Q1	C31-C29-C32-O33
48	j	201	PEE	C44-C45-C46-C47
48	r	501	PEE	C22-C23-C24-C25
49	a	202	PLX	C19-C20-C21-C22
49	a	202	PLX	C13-C14-C15-C16
55	l	702	CDL	C64-C65-C66-C67
55	a	201	CDL	C14-C15-C16-C17
48	Q	501	PEE	C32-C33-C34-C35
55	r	503	CDL	C32-C33-C34-C35
48	C	302	PEE	C31-C30-O3-C3
55	a	201	CDL	OA5-CA3-CA4-CA6
55	a	201	CDL	CA5-C11-C12-C13
49	g	201	PLX	C32-C33-C34-C35
55	a	201	CDL	C53-C54-C55-C56
49	g	201	PLX	C11-C12-C13-C14
50	G	201	8Q1	C11-C10-C9-C8
55	l	702	CDL	C31-C32-C33-C34
48	B	303	PEE	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
48	j	201	PEE	C38-C39-C40-C41
55	a	201	CDL	C60-C61-C62-C63
55	l	701	CDL	C31-C32-C33-C34
55	a	201	CDL	C31-CA7-OA8-CA6
48	r	501	PEE	C1-C2-C3-O3
49	g	201	PLX	C3-C4-C5-O8
55	l	701	CDL	CB3-CB4-CB6-OB8
55	u	201	CDL	CA3-CA4-CA6-OA8
49	j	202	PLX	C33-C34-C35-C36
48	B	303	PEE	C17-C18-C19-C20
49	r	502	PLX	C33-C34-C35-C36
55	l	701	CDL	C74-C75-C76-C77
48	l	703	PEE	C32-C33-C34-C35
49	g	201	PLX	C36-C37-C38-C39
49	C	303	PLX	C9-C10-C11-C12
49	C	303	PLX	C17-C18-C19-C20
48	s	401	PEE	C23-C24-C25-C26
48	b	201	PEE	C1-O3P-P-O4P
49	C	303	PLX	C27-C28-C29-C30
55	l	702	CDL	C22-C23-C24-C25
55	u	201	CDL	C76-C77-C78-C79
55	a	201	CDL	OA5-CA3-CA4-OA6
55	l	702	CDL	OA5-CA3-CA4-OA6
48	j	201	PEE	C22-C23-C24-C25
48	r	501	PEE	C15-C16-C17-C18
49	C	303	PLX	C11-C10-C9-C8
55	r	503	CDL	OA9-CA7-OA8-CA6
48	r	501	PEE	O2-C2-C3-O3
49	a	202	PLX	O6-C4-C5-O8
49	j	202	PLX	O6-C4-C5-O8
55	l	702	CDL	OA6-CA4-CA6-OA8
55	r	503	CDL	C31-C32-C33-C34
49	C	303	PLX	C26-C27-C28-C29
48	j	201	PEE	C11-C12-C13-C14
55	l	702	CDL	OA7-CA5-OA6-CA4
55	a	201	CDL	C75-C76-C77-C78
55	u	201	CDL	C79-C80-C81-C82
55	l	701	CDL	C71-C72-C73-C74
49	C	303	PLX	C30-C31-C32-C33
49	a	202	PLX	C14-C15-C16-C17
49	j	202	PLX	C30-C31-C32-C33
55	u	201	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
48	C	302	PEE	C18-C19-C20-C21
49	a	202	PLX	C15-C16-C17-C18
55	r	503	CDL	C79-C80-C81-C82
50	G	201	8Q1	O4-C1-S44-C43
55	u	201	CDL	CB7-C71-C72-C73
55	l	702	CDL	C17-C18-C19-C20
49	C	303	PLX	O6-C6-C7-C8
48	B	303	PEE	O3P-C1-C2-C3
48	Q	501	PEE	O3P-C1-C2-C3
49	a	202	PLX	O4-C3-C4-C5
49	g	201	PLX	O4-C3-C4-C5
55	i	401	CDL	OB5-CB3-CB4-CB6
55	a	201	CDL	C59-C60-C61-C62
55	u	201	CDL	C18-C19-C20-C21
55	l	701	CDL	C37-C38-C39-C40
55	l	702	CDL	C14-C15-C16-C17
50	G	201	8Q1	C28-O27-P24-O2
50	X	201	8Q1	O33-C32-C34-N36
48	Q	501	PEE	C16-C17-C18-C19
55	a	201	CDL	C41-C42-C43-C44
48	s	401	PEE	C3-C2-O2-C10
50	G	201	8Q1	C6-C1-S44-C43
48	j	201	PEE	C12-C13-C14-C15
55	r	503	CDL	C60-C61-C62-C63
48	r	501	PEE	C31-C30-O3-C3
55	r	503	CDL	C44-C45-C46-C47
48	Q	501	PEE	C1-C2-C3-O3
48	Q	501	PEE	C2-C1-O3P-P
49	g	201	PLX	C7-C6-O6-C4
49	j	202	PLX	C3-C4-C5-O8
55	r	503	CDL	CB4-CB3-OB5-PB2
48	C	302	PEE	O5-C30-O3-C3
48	B	303	PEE	O3P-C1-C2-O2
55	a	201	CDL	OB5-CB3-CB4-OB6
50	X	201	8Q1	C31-C29-C32-C34
48	B	303	PEE	C21-C22-C23-C24
49	j	202	PLX	C31-C32-C33-C34
48	b	201	PEE	O2-C2-C3-O3
49	r	502	PLX	O6-C4-C5-O8
55	a	201	CDL	OA9-CA7-OA8-CA6
48	j	201	PEE	C43-C44-C45-C46
49	e	201	PLX	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	C38-C39-C40-C41
51	J	401	NDP	C5B-O5B-PA-O3
49	r	502	PLX	C31-C32-C33-C34
49	C	303	PLX	C11-C12-C13-C14
55	l	701	CDL	C36-C37-C38-C39
55	r	503	CDL	C76-C77-C78-C79
55	l	702	CDL	C79-C80-C81-C82
48	r	501	PEE	O5-C30-O3-C3
51	J	401	NDP	C3B-C4B-C5B-O5B
49	e	201	PLX	C12-C13-C14-C15
49	C	303	PLX	C19-C20-C21-C22
50	G	201	8Q1	C6-C7-C8-C9
55	i	401	CDL	C74-C75-C76-C77
49	e	201	PLX	C24-C25-C26-C27
55	u	201	CDL	CA2-OA2-PA1-OA5
55	u	201	CDL	CB2-OB2-PB2-OB5
48	l	703	PEE	C13-C14-C15-C16
47	A	503	NAI	C5D-O5D-PN-O1N
48	B	303	PEE	C4-O4P-P-O2P
48	C	302	PEE	C1-O3P-P-O2P
48	Q	501	PEE	C1-O3P-P-O1P
48	r	501	PEE	C4-O4P-P-O1P
49	e	201	PLX	C2-O1-P1-O2
49	e	201	PLX	C2-O1-P1-O3
49	j	202	PLX	C3-O4-P1-O2
55	a	201	CDL	CA2-OA2-PA1-OA4
55	a	201	CDL	CB2-OB2-PB2-OB4
55	l	701	CDL	CA2-OA2-PA1-OA3
55	l	701	CDL	CB2-OB2-PB2-OB3
55	l	702	CDL	CB2-OB2-PB2-OB3
55	l	702	CDL	CB3-OB5-PB2-OB3
55	l	702	CDL	CB3-OB5-PB2-OB4
55	r	503	CDL	CB2-OB2-PB2-OB3
55	r	503	CDL	CB2-OB2-PB2-OB4
55	r	503	CDL	CB3-OB5-PB2-OB3
55	u	201	CDL	CB2-OB2-PB2-OB4
55	u	201	CDL	CB3-OB5-PB2-OB4
50	G	201	8Q1	C9-C10-C11-C12
55	l	702	CDL	OA5-CA3-CA4-CA6
49	j	202	PLX	C10-C11-C12-C13
55	l	702	CDL	C80-C81-C82-C83
49	j	202	PLX	C25-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
49	r	502	PLX	C25-C24-O8-C5
49	j	202	PLX	C16-C17-C18-C19
49	e	201	PLX	C36-C37-C38-C39
48	Q	501	PEE	O3P-C1-C2-O2
49	j	202	PLX	O4-C3-C4-O6
55	i	401	CDL	OB5-CB3-CB4-OB6
49	C	303	PLX	C25-C26-C27-C28
55	a	201	CDL	C22-C23-C24-C25
55	r	503	CDL	CA5-C11-C12-C13
55	l	701	CDL	C51-CB5-OB6-CB4
49	e	201	PLX	C9-C10-C11-C12
55	r	503	CDL	C20-C21-C22-C23
55	a	201	CDL	CB5-C51-C52-C53
46	A	502	FMN	C1'-C2'-C3'-C4'
48	B	303	PEE	C13-C14-C15-C16
49	e	201	PLX	C3-C4-C5-O8
55	i	401	CDL	CB3-CB4-CB6-OB8
55	u	201	CDL	C59-C60-C61-C62
49	e	201	PLX	O6-C4-C5-O8
49	g	201	PLX	O6-C4-C5-O8
55	u	201	CDL	OA6-CA4-CA6-OA8
48	B	303	PEE	C33-C34-C35-C36
48	Q	501	PEE	C17-C18-C19-C20
48	j	201	PEE	C37-C38-C39-C40
48	r	501	PEE	C38-C39-C40-C41
49	r	502	PLX	C18-C19-C20-C21
55	a	201	CDL	C32-C31-CA7-OA8
50	G	201	8Q1	C10-C11-C12-C13
49	j	202	PLX	O6-C6-C7-C8
55	i	401	CDL	C33-C34-C35-C36
55	r	503	CDL	C14-C15-C16-C17
48	b	201	PEE	C38-C39-C40-C41
55	l	702	CDL	C32-C33-C34-C35
49	j	202	PLX	O4-C3-C4-C5
55	l	701	CDL	OB7-CB5-OB6-CB4
55	l	702	CDL	C58-C59-C60-C61
48	Q	501	PEE	C30-C31-C32-C33
48	r	501	PEE	C24-C25-C26-C27
49	e	201	PLX	C7-C8-C9-C10
55	u	201	CDL	C19-C20-C21-C22
47	A	503	NAI	O4D-C1D-N1N-C2N
48	r	501	PEE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
49	C	303	PLX	C36-C37-C38-C39
46	A	502	FMN	O2'-C2'-C3'-O3'
48	C	302	PEE	C42-C43-C44-C45
55	l	701	CDL	C40-C41-C42-C43
55	l	702	CDL	C43-C44-C45-C46
48	l	703	PEE	C36-C37-C38-C39
48	B	303	PEE	O5-C30-O3-C3
48	Q	501	PEE	O2-C2-C3-O3
48	B	303	PEE	C31-C30-O3-C3
48	C	302	PEE	C4-O4P-P-O3P
49	g	201	PLX	C3-O4-P1-O1
55	i	401	CDL	CA2-OA2-PA1-OA5
55	r	503	CDL	C42-C43-C44-C45
55	a	201	CDL	C43-C44-C45-C46
48	Q	501	PEE	C31-C32-C33-C34
55	i	401	CDL	CA4-CA3-OA5-PA1
55	u	201	CDL	OB9-CB7-OB8-CB6
49	e	201	PLX	C31-C32-C33-C34
55	l	702	CDL	C15-C16-C17-C18
48	l	703	PEE	C14-C15-C16-C17
49	g	201	PLX	C30-C31-C32-C33
55	u	201	CDL	C71-CB7-OB8-CB6
55	l	701	CDL	C54-C55-C56-C57
48	j	201	PEE	C31-C32-C33-C34
48	l	703	PEE	C11-C12-C13-C14
48	C	302	PEE	C33-C34-C35-C36
48	b	201	PEE	C16-C17-C18-C19
48	C	302	PEE	O3P-C1-C2-C3
49	a	202	PLX	C24-C25-C26-C27
55	l	702	CDL	C53-C54-C55-C56
48	s	401	PEE	C20-C21-C22-C23
48	l	703	PEE	C15-C16-C17-C18
49	C	303	PLX	C18-C19-C20-C21
48	j	201	PEE	C40-C41-C42-C43
49	g	201	PLX	O8-C24-C25-C26
55	l	702	CDL	C51-C52-C53-C54
55	u	201	CDL	CB4-CB3-OB5-PB2
50	X	201	8Q1	N41-C42-C43-S44
48	Q	501	PEE	C36-C37-C38-C39
47	A	503	NAI	C2D-C1D-N1N-C2N
55	i	401	CDL	C32-C33-C34-C35
55	l	702	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
55	r	503	CDL	C40-C41-C42-C43
51	J	401	NDP	O4D-C1D-N1N-C6N
55	u	201	CDL	CB3-OB5-PB2-OB2
49	j	202	PLX	C17-C18-C19-C20
55	i	401	CDL	C15-C16-C17-C18
48	b	201	PEE	C24-C25-C26-C27
48	j	201	PEE	O2-C2-C3-O3
55	r	503	CDL	C64-C65-C66-C67
55	r	503	CDL	C39-C40-C41-C42
49	e	201	PLX	C18-C19-C20-C21
48	l	703	PEE	C37-C38-C39-C40
48	s	401	PEE	O3-C30-C31-C32
55	a	201	CDL	C17-C18-C19-C20
48	b	201	PEE	C18-C19-C20-C21
48	C	302	PEE	C38-C39-C40-C41
49	e	201	PLX	O4-C3-C4-O6
48	b	201	PEE	O4P-C4-C5-N
48	s	401	PEE	C24-C25-C26-C27
50	X	201	8Q1	C13-C14-C15-C16
56	s	402	UQ	C15-C14-C16-C17
56	s	402	UQ	C12-C11-C9-C8
55	l	701	CDL	C33-C34-C35-C36
55	l	701	CDL	C18-C19-C20-C21
55	r	503	CDL	C52-C51-CB5-OB6
48	j	201	PEE	C16-C17-C18-C19
48	s	401	PEE	C18-C19-C20-C21
48	b	201	PEE	C30-C31-C32-C33
48	B	303	PEE	C39-C40-C41-C42
49	j	202	PLX	C7-C6-O6-C4
49	r	502	PLX	C3-C4-C5-O8
55	a	201	CDL	CA4-CA3-OA5-PA1
55	l	701	CDL	OA5-CA3-CA4-OA6
48	Q	501	PEE	C38-C39-C40-C41
48	C	302	PEE	C15-C16-C17-C18
55	i	401	CDL	OA5-CA3-CA4-CA6
55	r	503	CDL	C82-C83-C84-C85
48	l	703	PEE	C16-C17-C18-C19
55	l	702	CDL	C32-C31-CA7-OA8
48	j	201	PEE	O3-C30-C31-C32
50	X	201	8Q1	C11-C10-C9-C8
55	u	201	CDL	C77-C78-C79-C80
48	B	303	PEE	C40-C41-C42-C43

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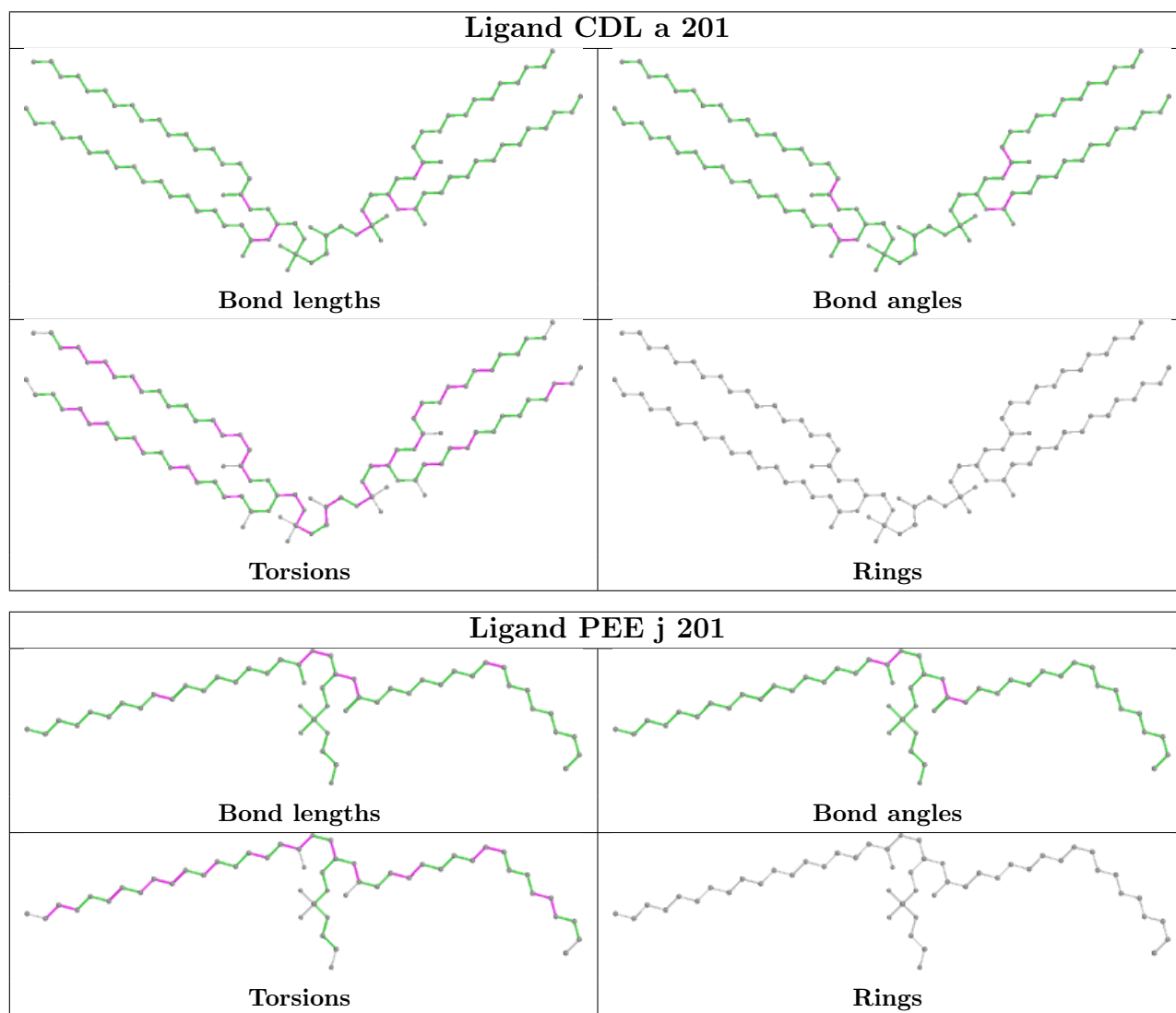
Continued from previous page...

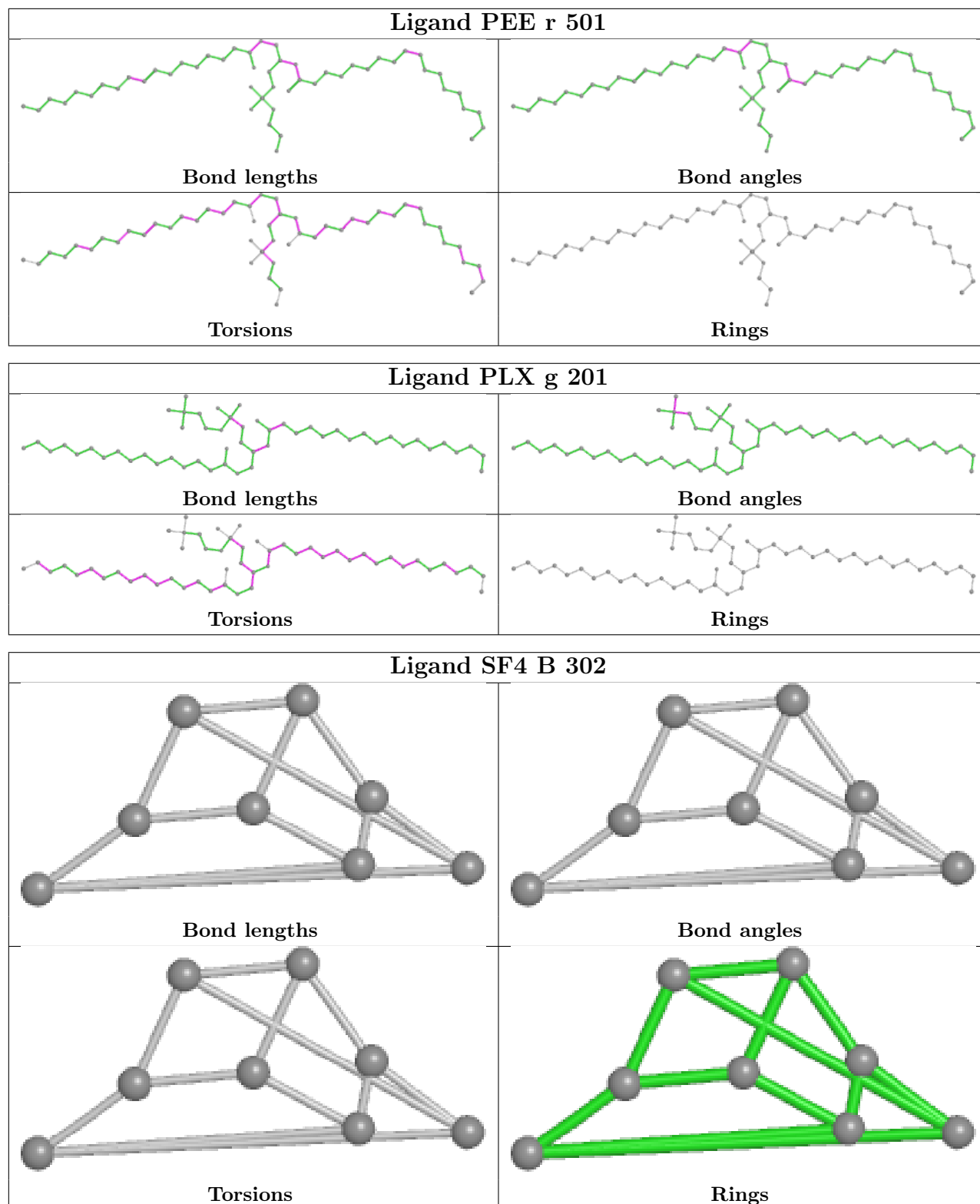
Mol	Chain	Res	Type	Atoms
48	C	302	PEE	C16-C17-C18-C19
48	s	401	PEE	C16-C17-C18-C19
48	b	201	PEE	C34-C35-C36-C37
49	g	201	PLX	C33-C34-C35-C36
55	u	201	CDL	C72-C71-CB7-OB8
48	C	302	PEE	C36-C37-C38-C39
55	r	503	CDL	C36-C37-C38-C39
55	a	201	CDL	C40-C41-C42-C43
55	a	201	CDL	C20-C21-C22-C23
55	r	503	CDL	C52-C51-CB5-OB7
55	i	401	CDL	CA3-CA4-CA6-OA8
49	r	502	PLX	C25-C26-C27-C28
55	l	701	CDL	CB2-OB2-PB2-OB5
55	r	503	CDL	C57-C58-C59-C60
55	l	702	CDL	C12-C11-CA5-OA6
55	r	503	CDL	CA4-CA3-OA5-PA1
47	A	503	NAI	C5D-O5D-PN-O2N
48	r	501	PEE	C1-O3P-P-O1P
49	g	201	PLX	C3-O4-P1-O2
55	a	201	CDL	CA3-OA5-PA1-OA3
55	l	702	CDL	CA3-OA5-PA1-OA4
55	u	201	CDL	CB2-OB2-PB2-OB3
55	a	201	CDL	OB6-CB4-CB6-OB8
55	i	401	CDL	C13-C14-C15-C16
55	l	701	CDL	C34-C35-C36-C37
55	u	201	CDL	C73-C74-C75-C76
55	r	503	CDL	C72-C71-CB7-OB8
55	u	201	CDL	C12-C11-CA5-OA6
48	b	201	PEE	C13-C14-C15-C16
49	g	201	PLX	C29-C30-C31-C32
55	r	503	CDL	C80-C81-C82-C83
55	l	702	CDL	C32-C31-CA7-OA9
55	u	201	CDL	C72-C71-CB7-OB9
49	C	303	PLX	C29-C30-C31-C32
55	i	401	CDL	OA5-CA3-CA4-OA6
55	r	503	CDL	OB5-CB3-CB4-OB6
55	l	701	CDL	C42-C43-C44-C45
55	l	702	CDL	C12-C11-CA5-OA7
55	l	701	CDL	C72-C71-CB7-OB8
48	j	201	PEE	O5-C30-C31-C32

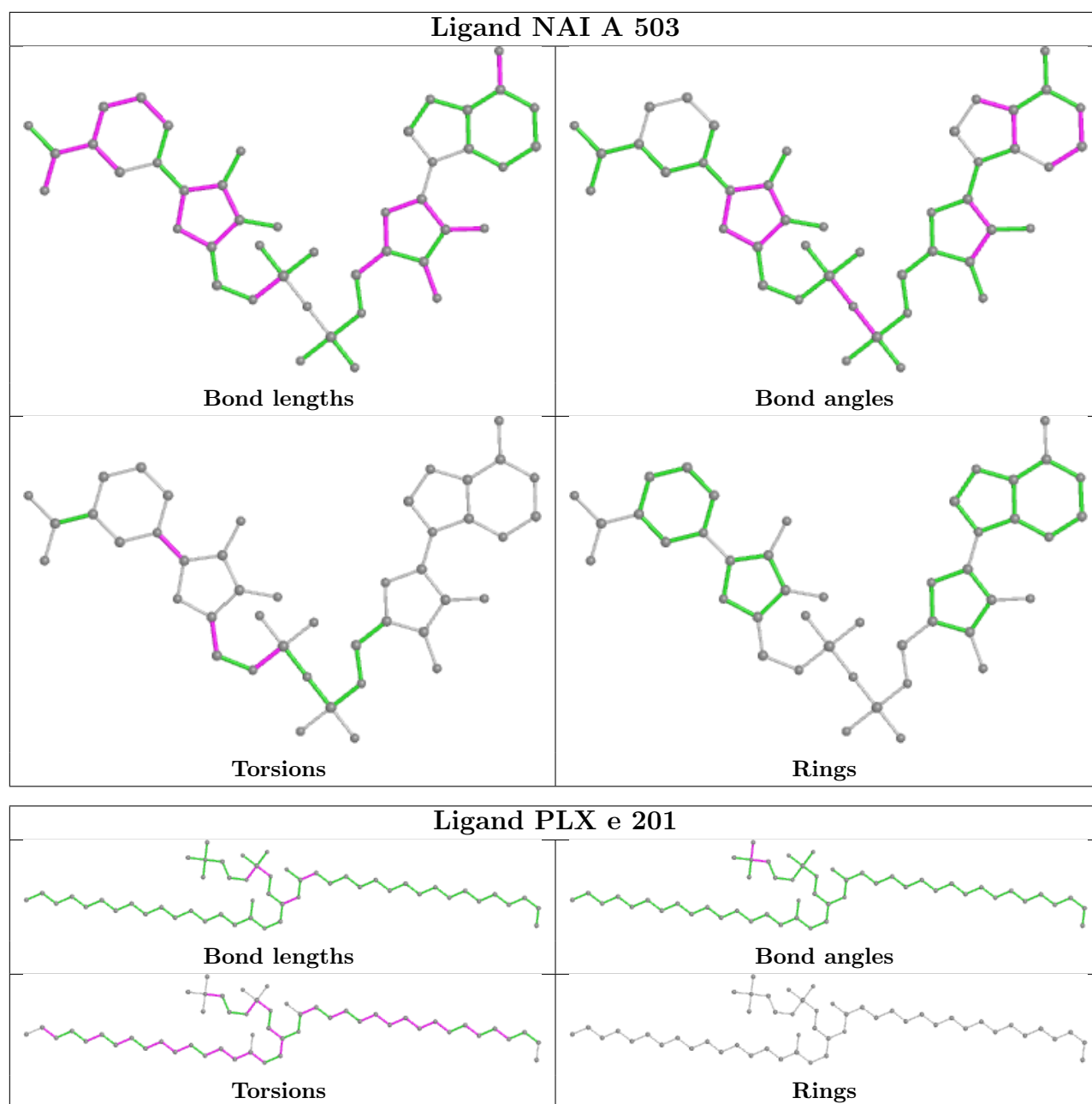
There are no ring outliers.

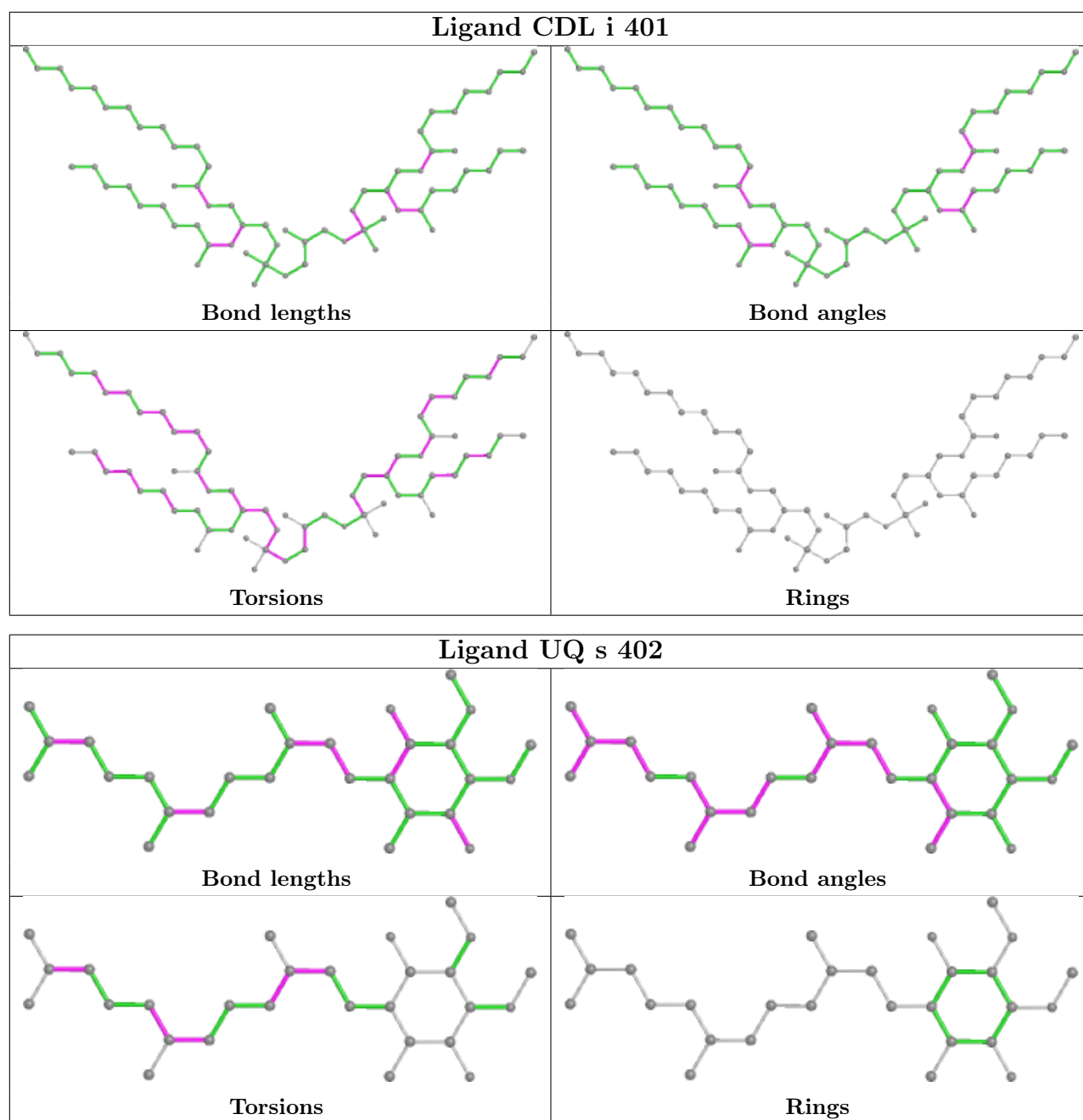
No monomer is involved in short contacts.

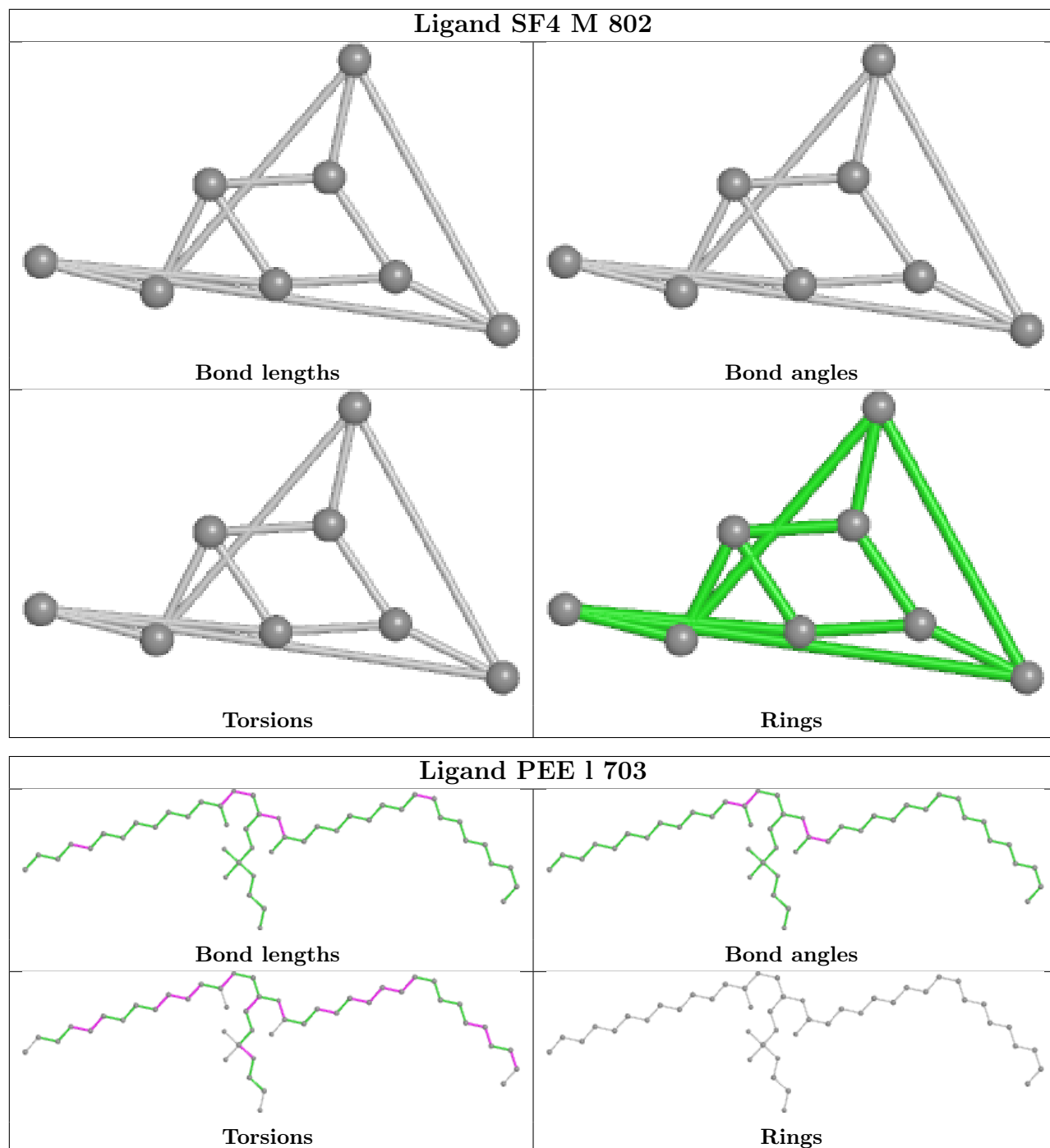
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

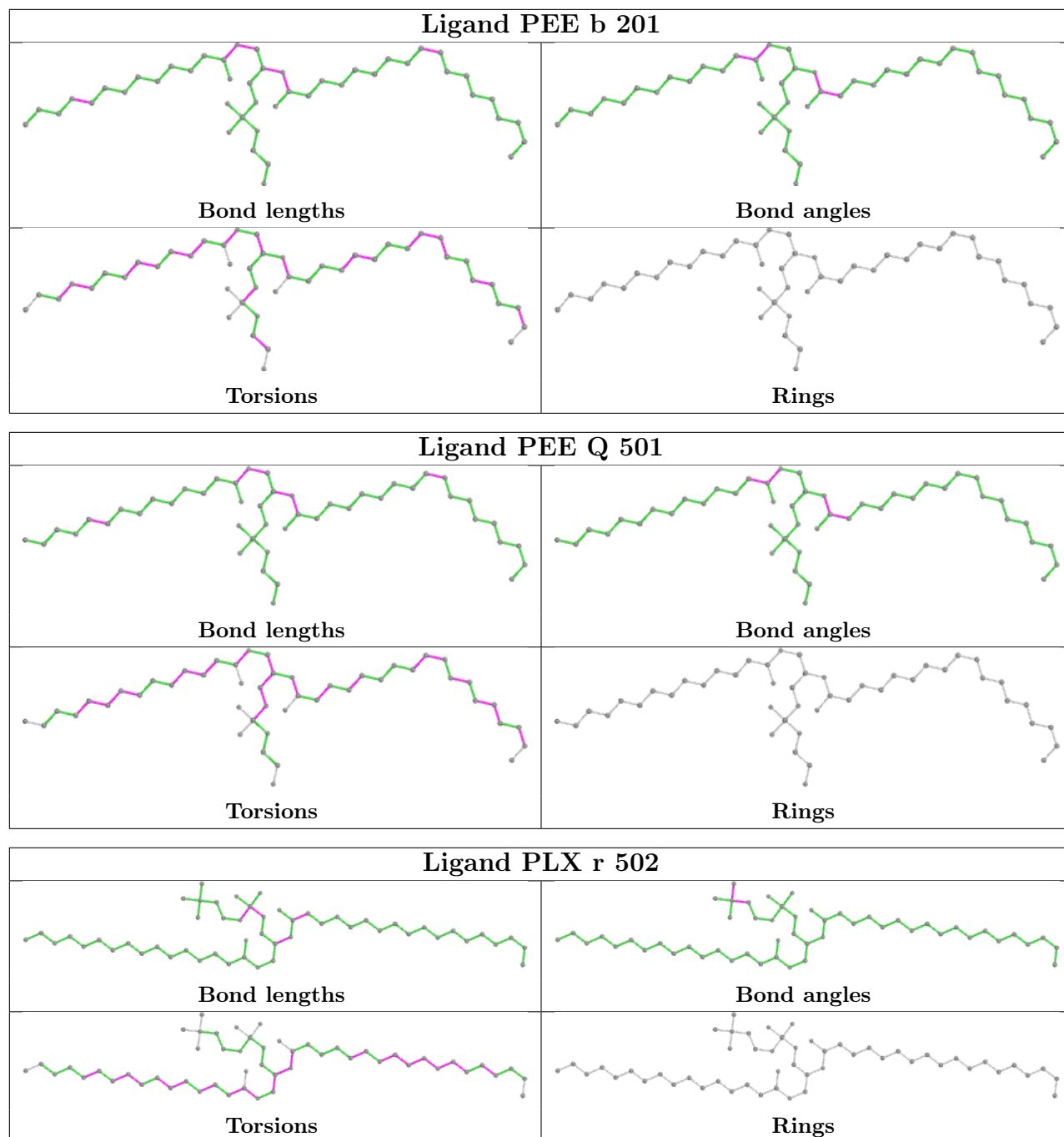


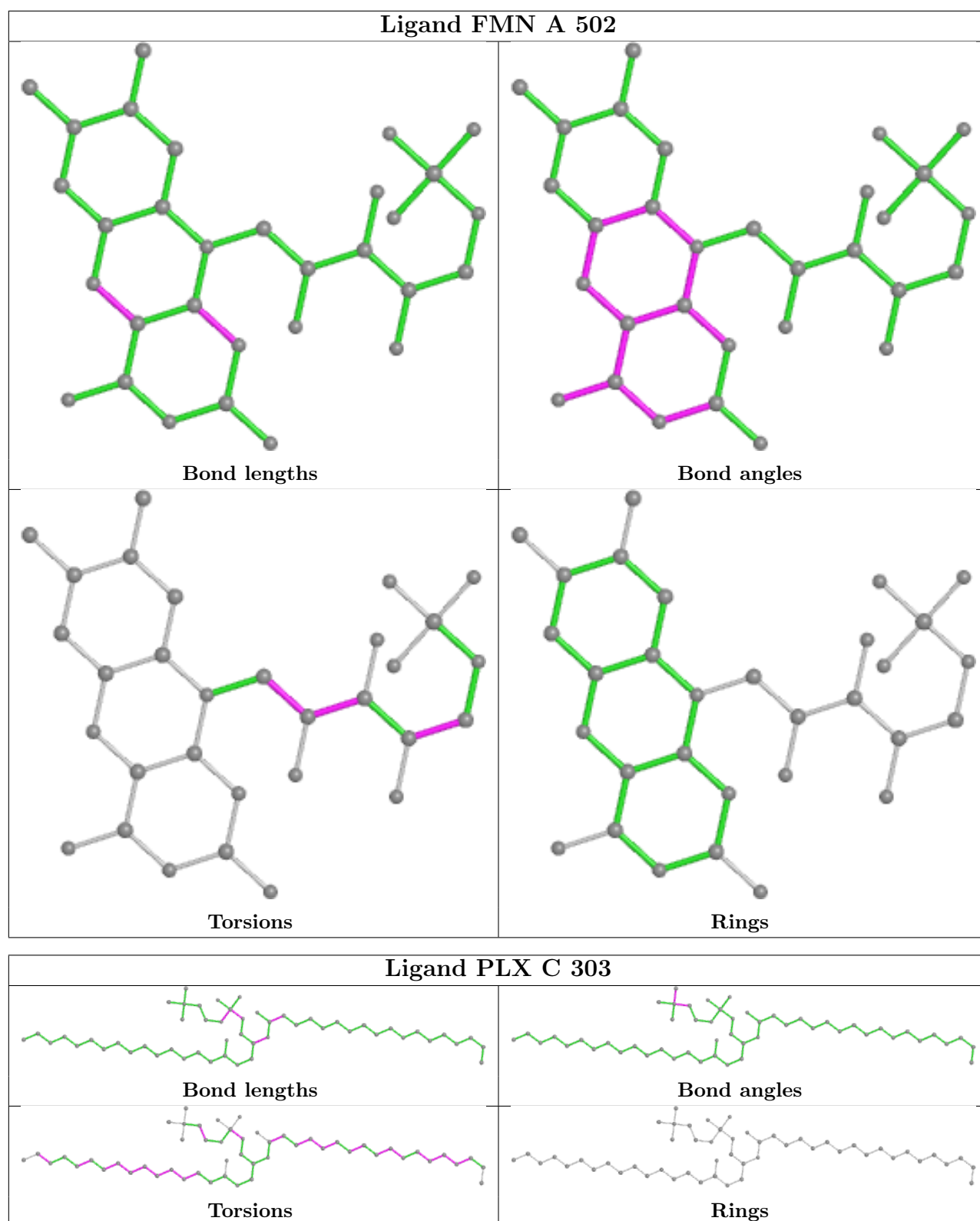


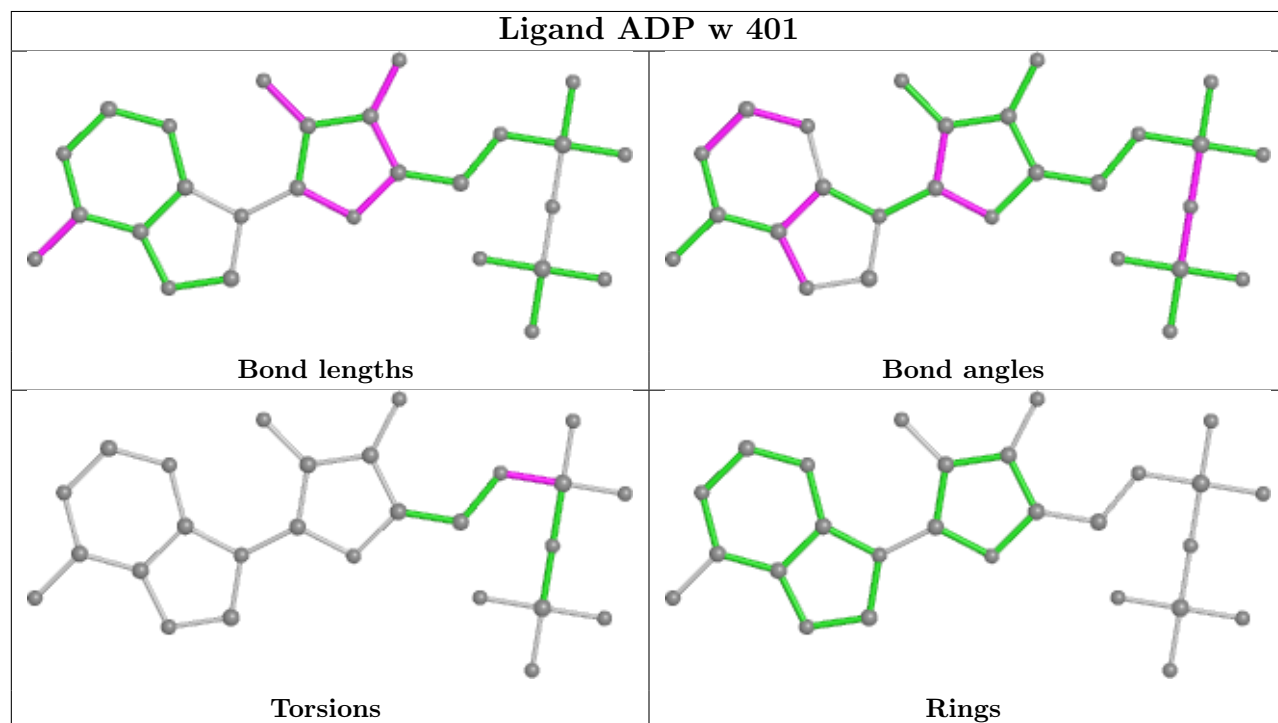
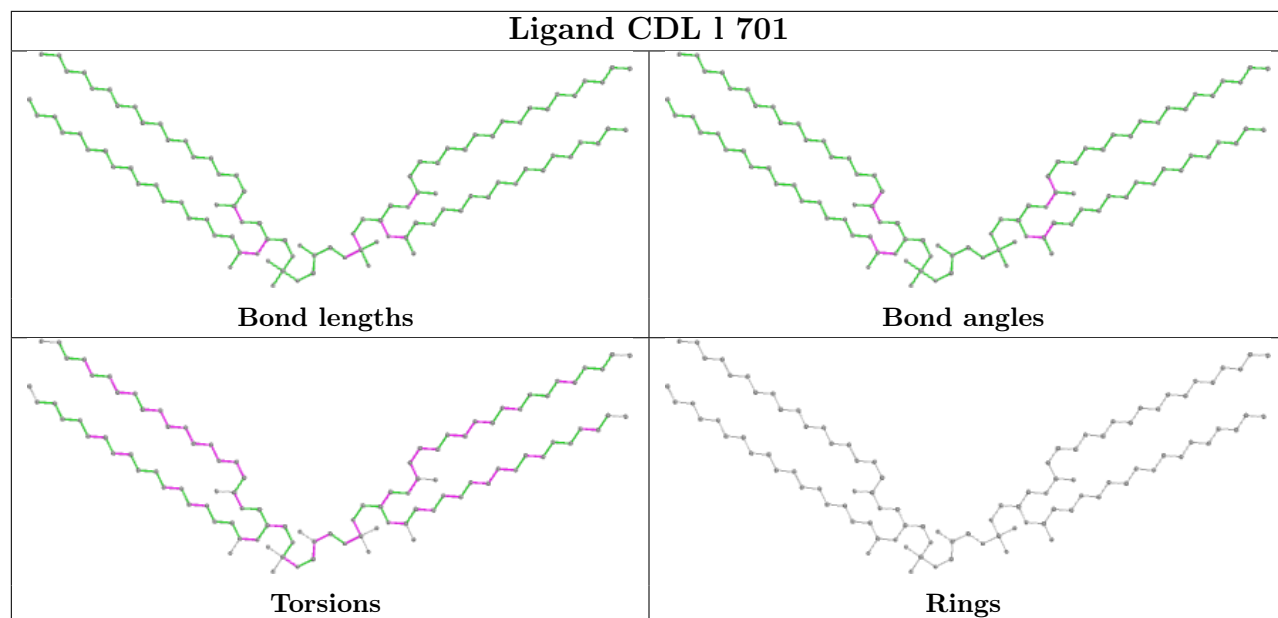


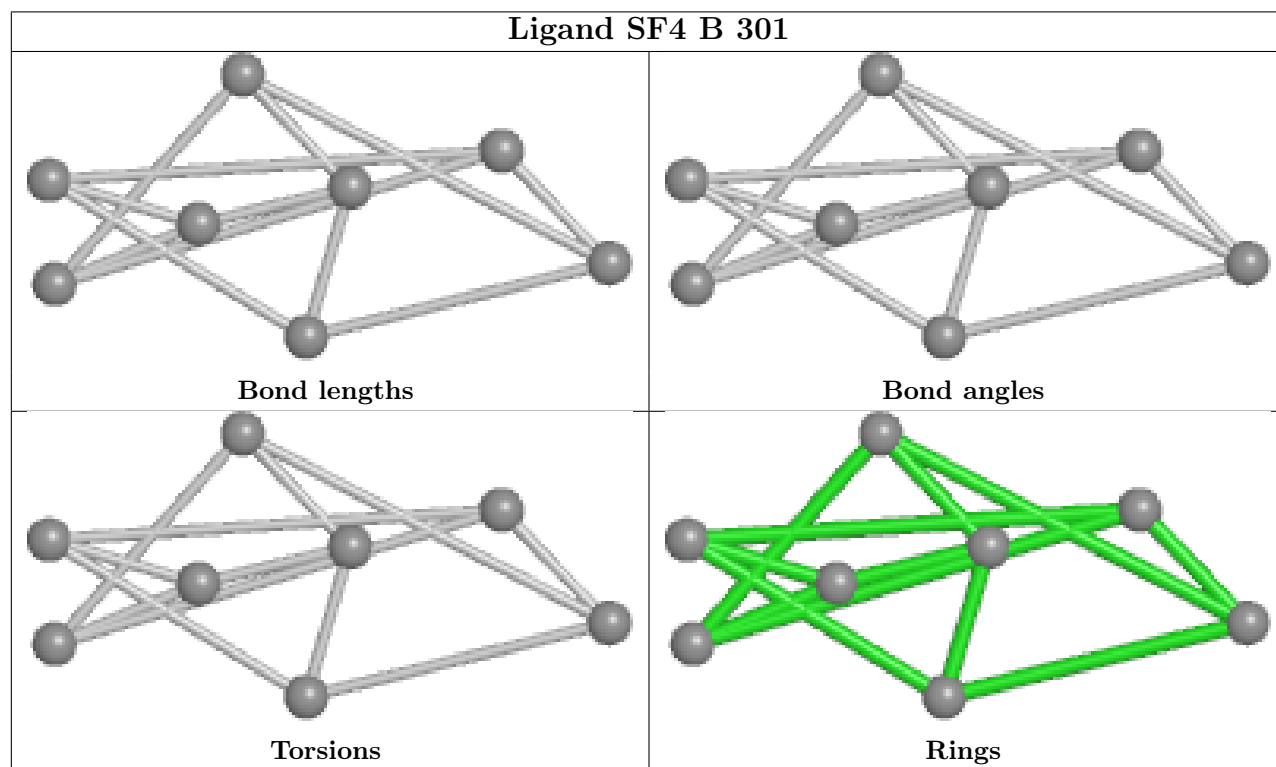
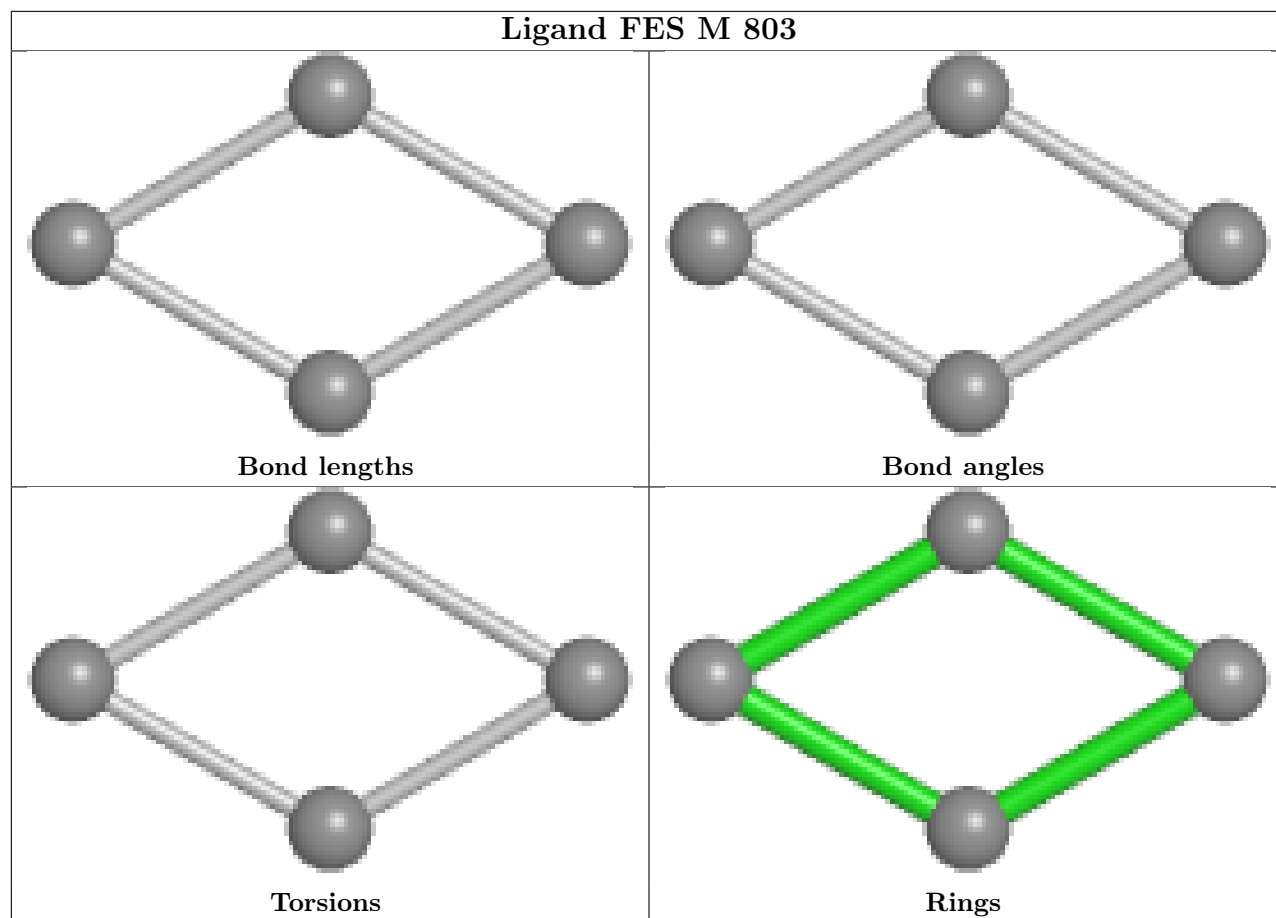


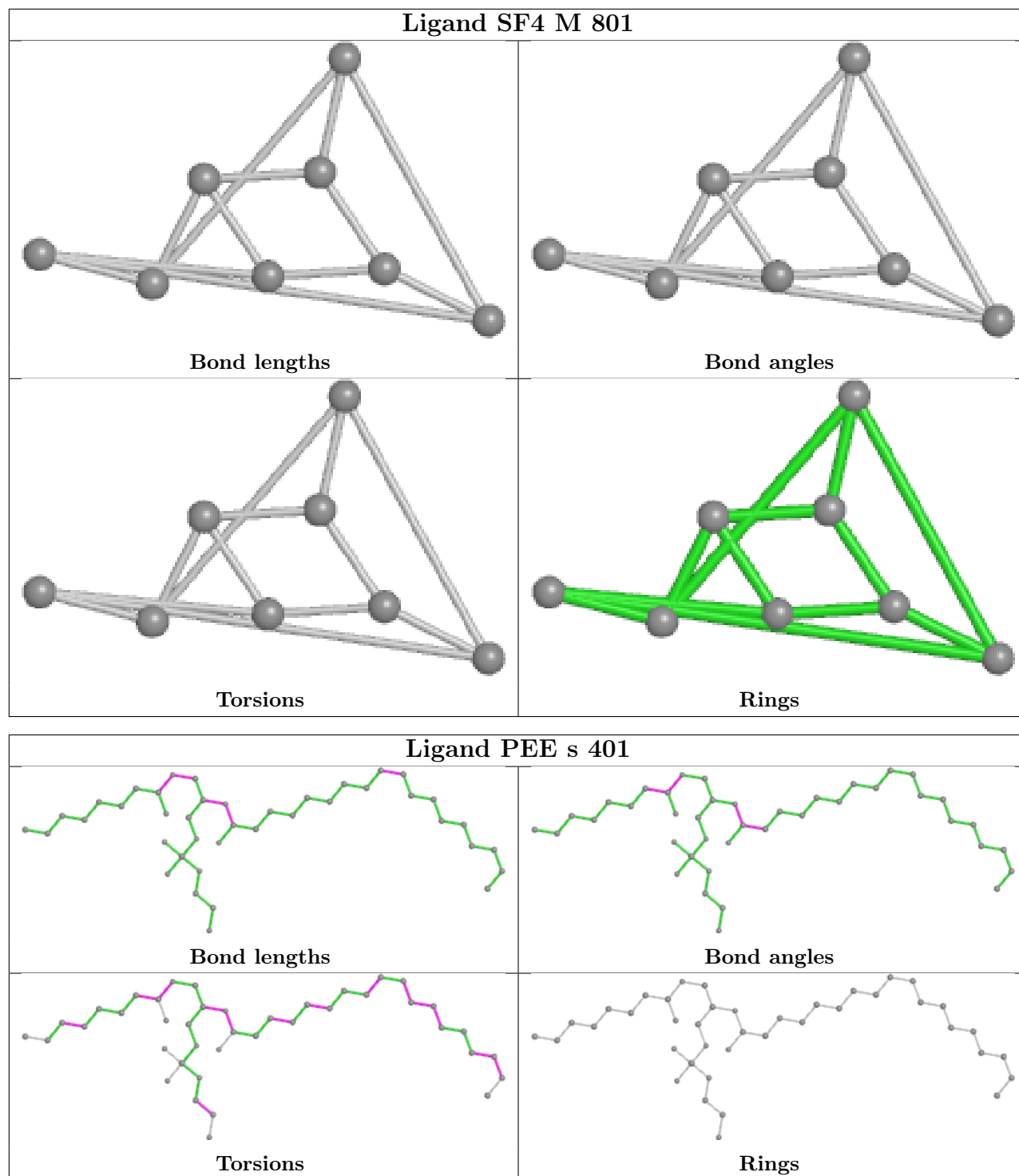


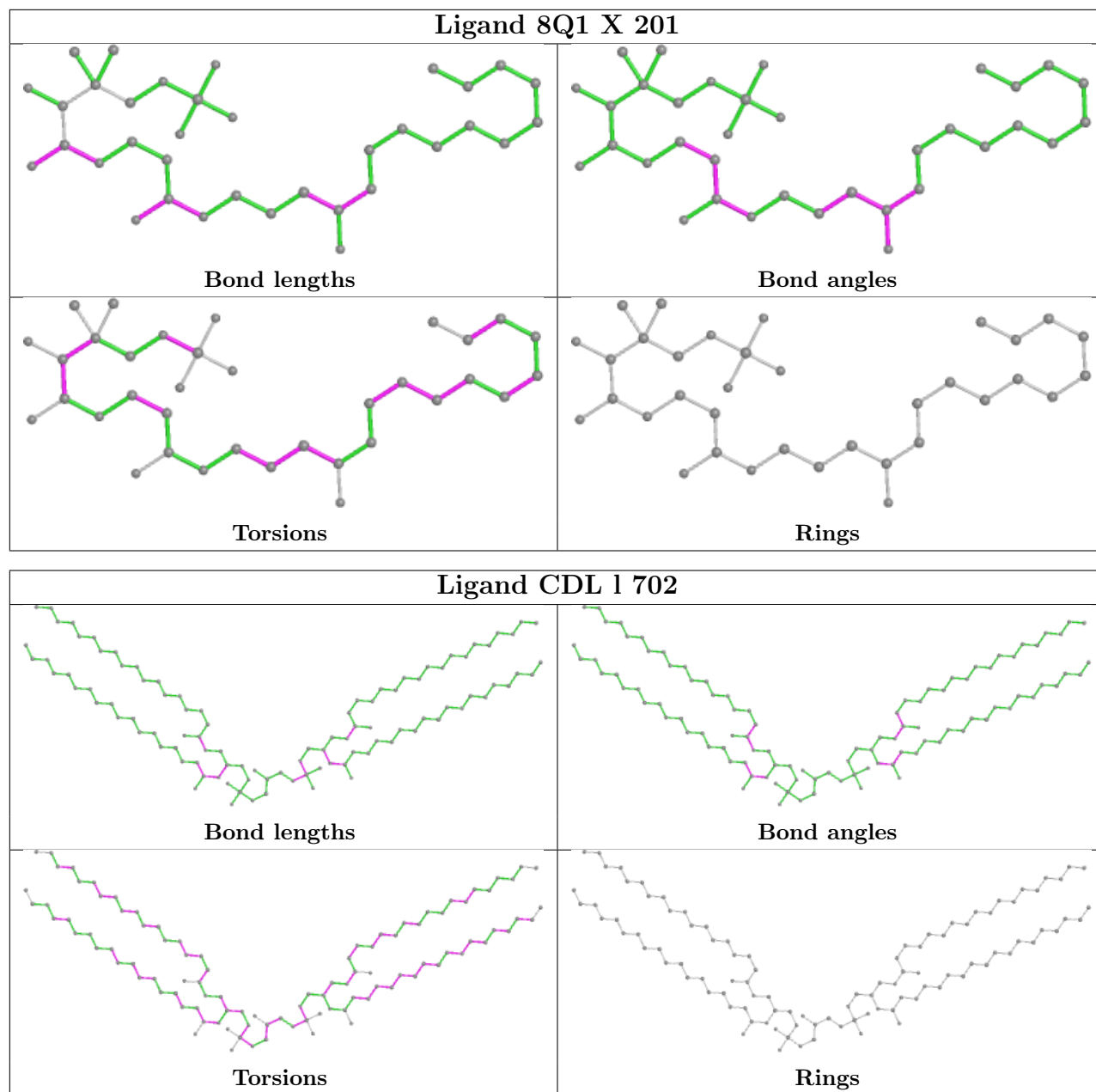


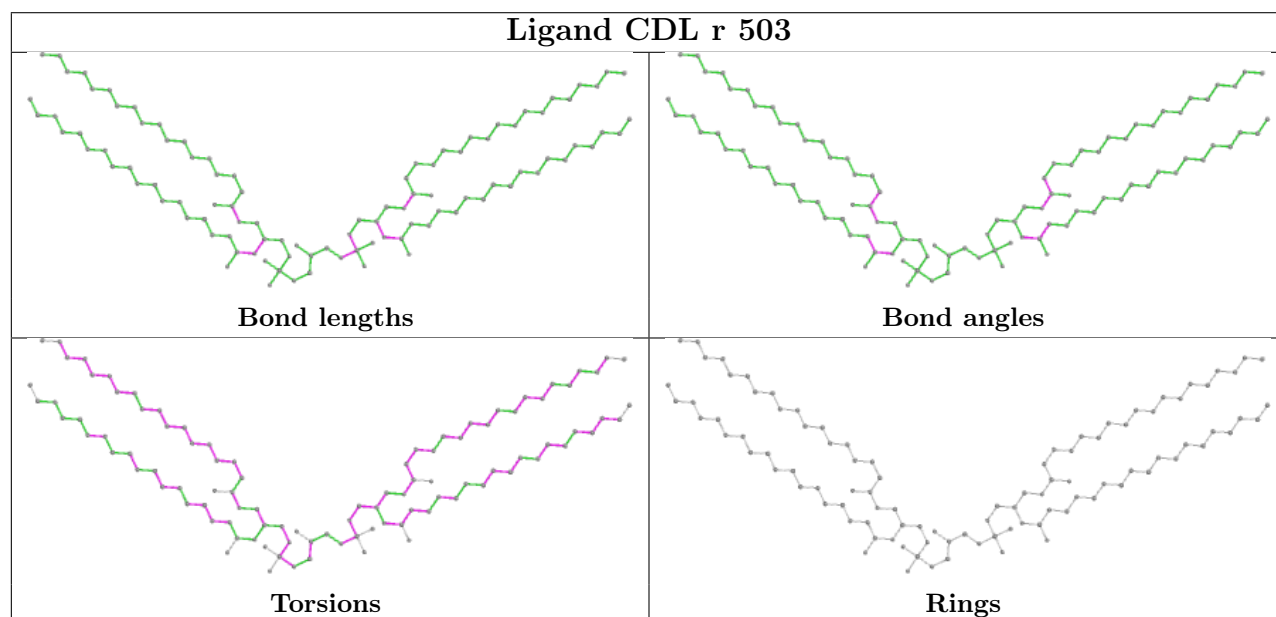
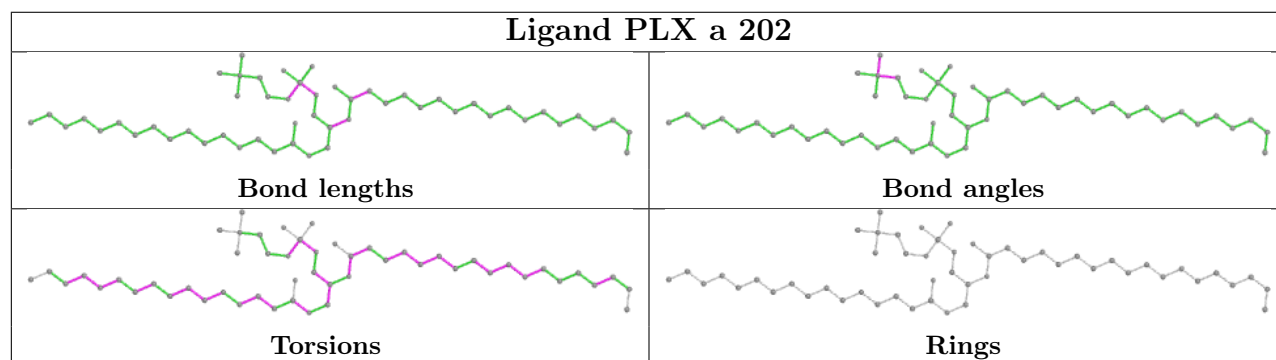
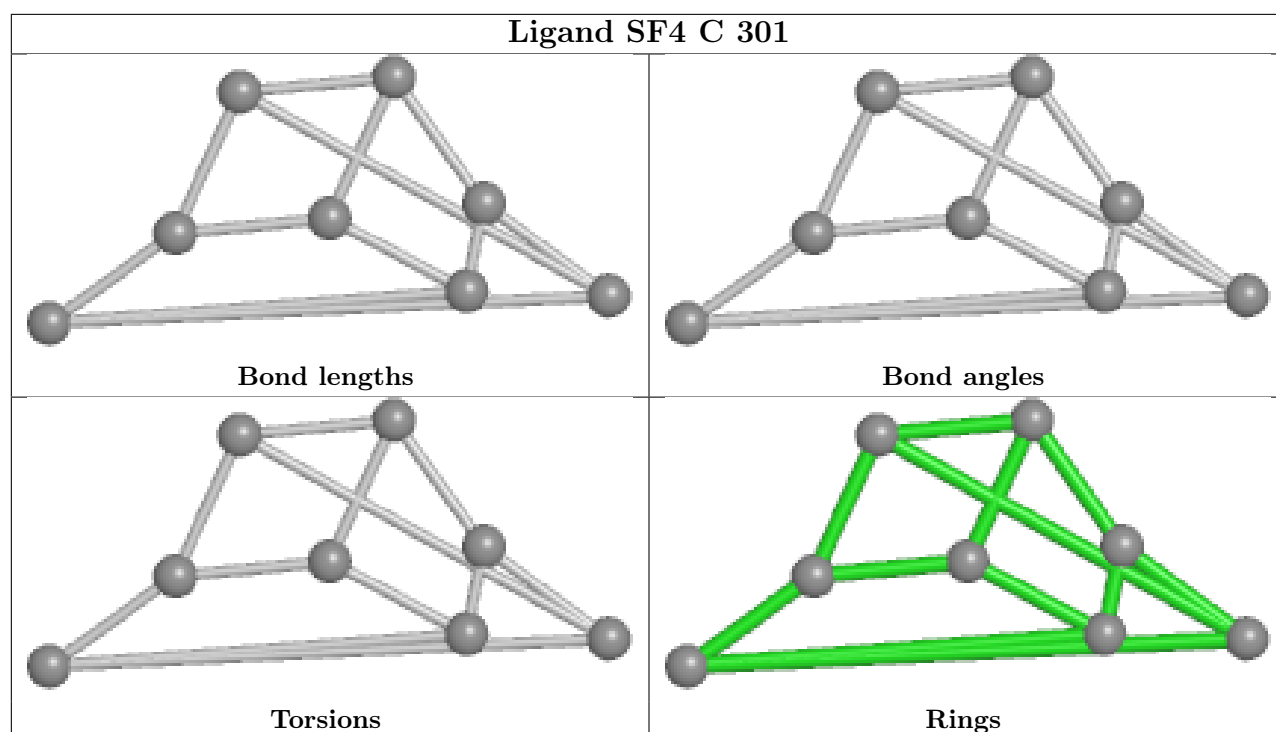


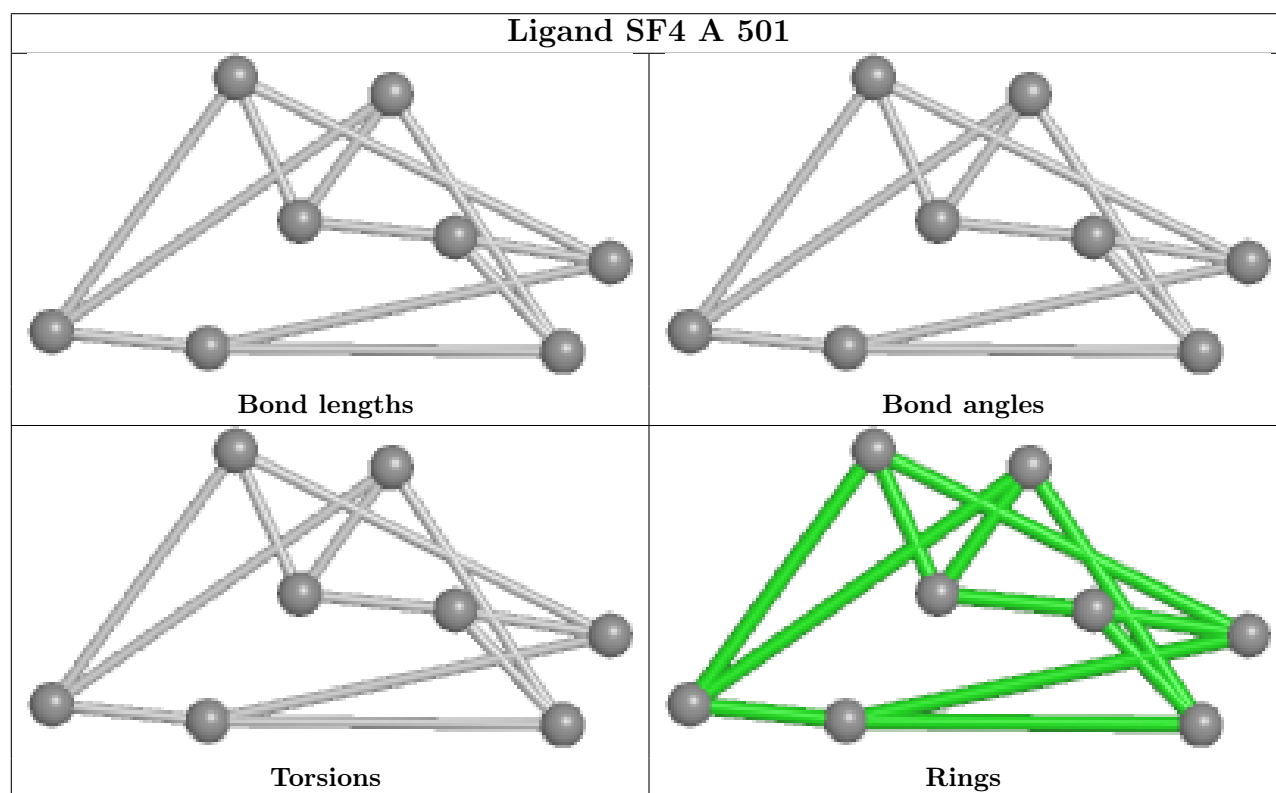
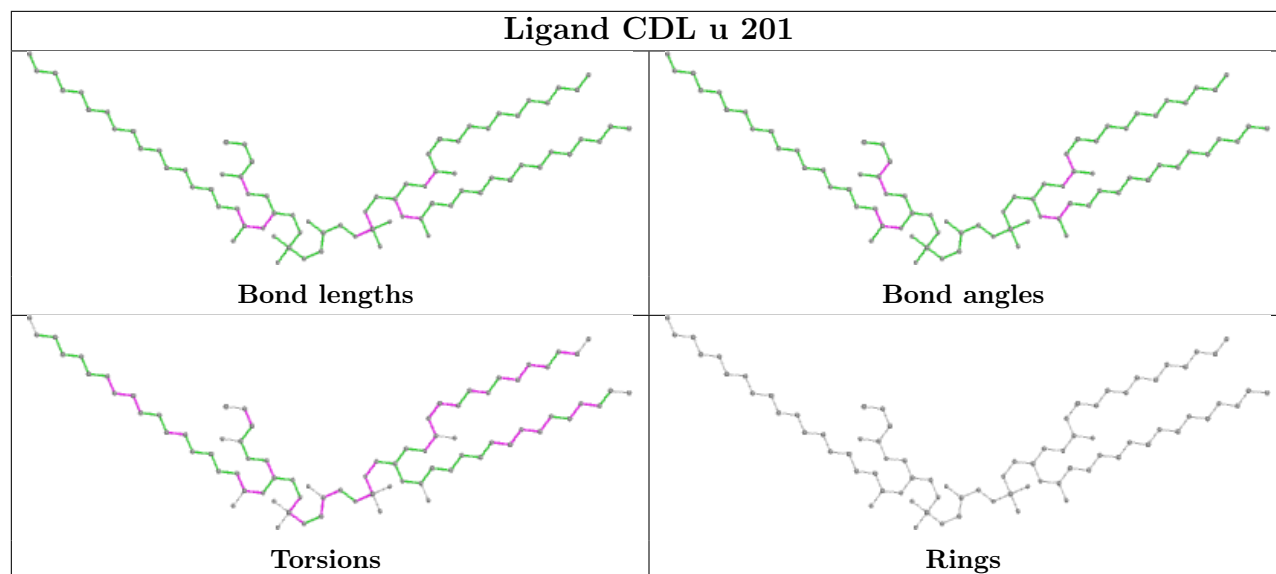


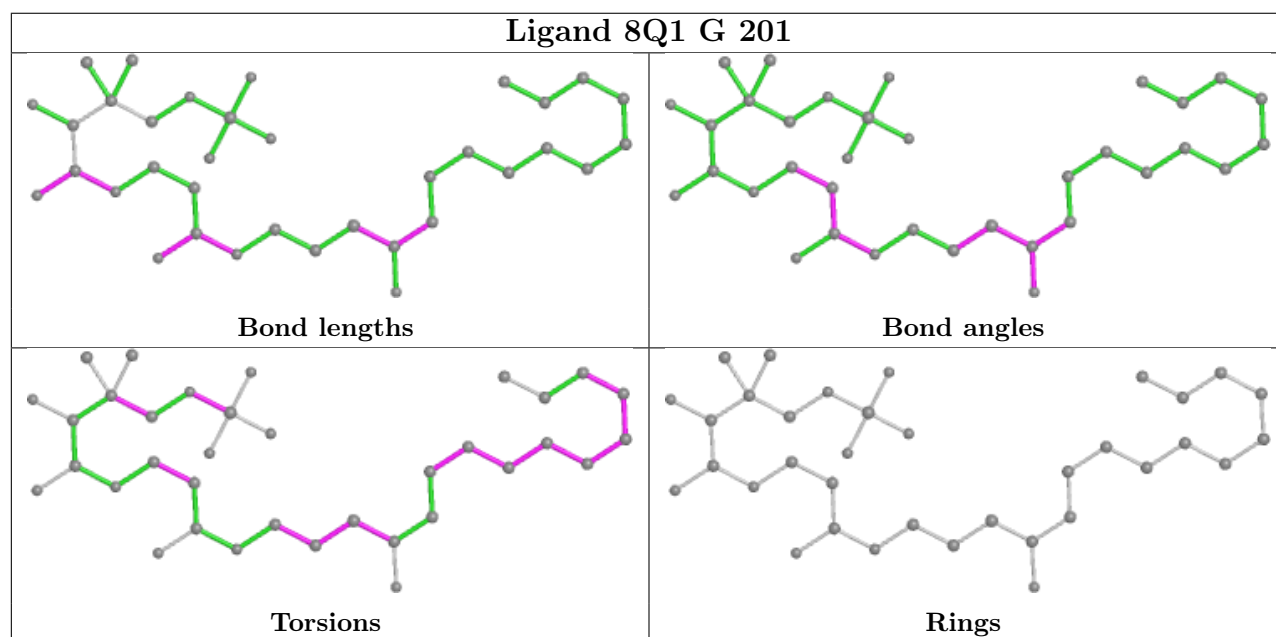
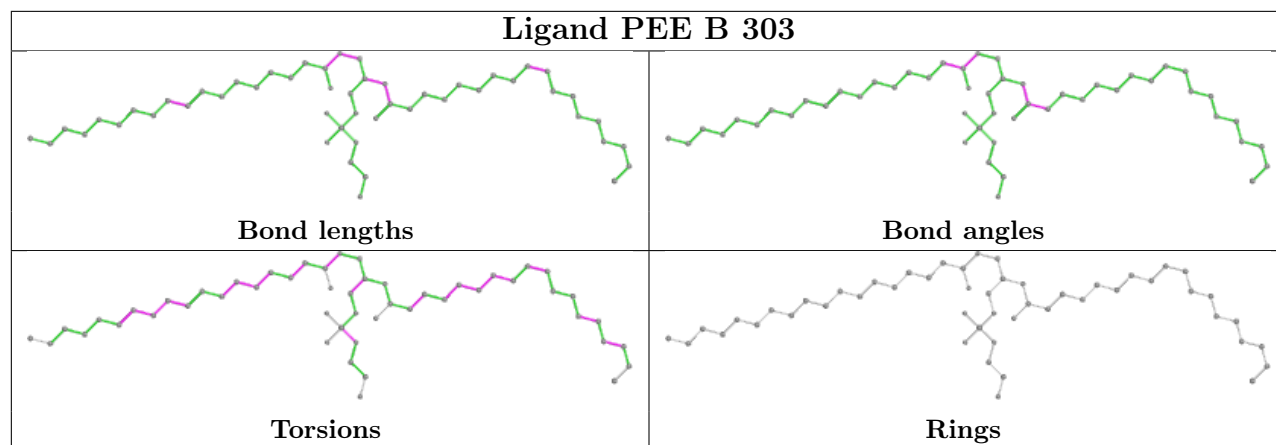


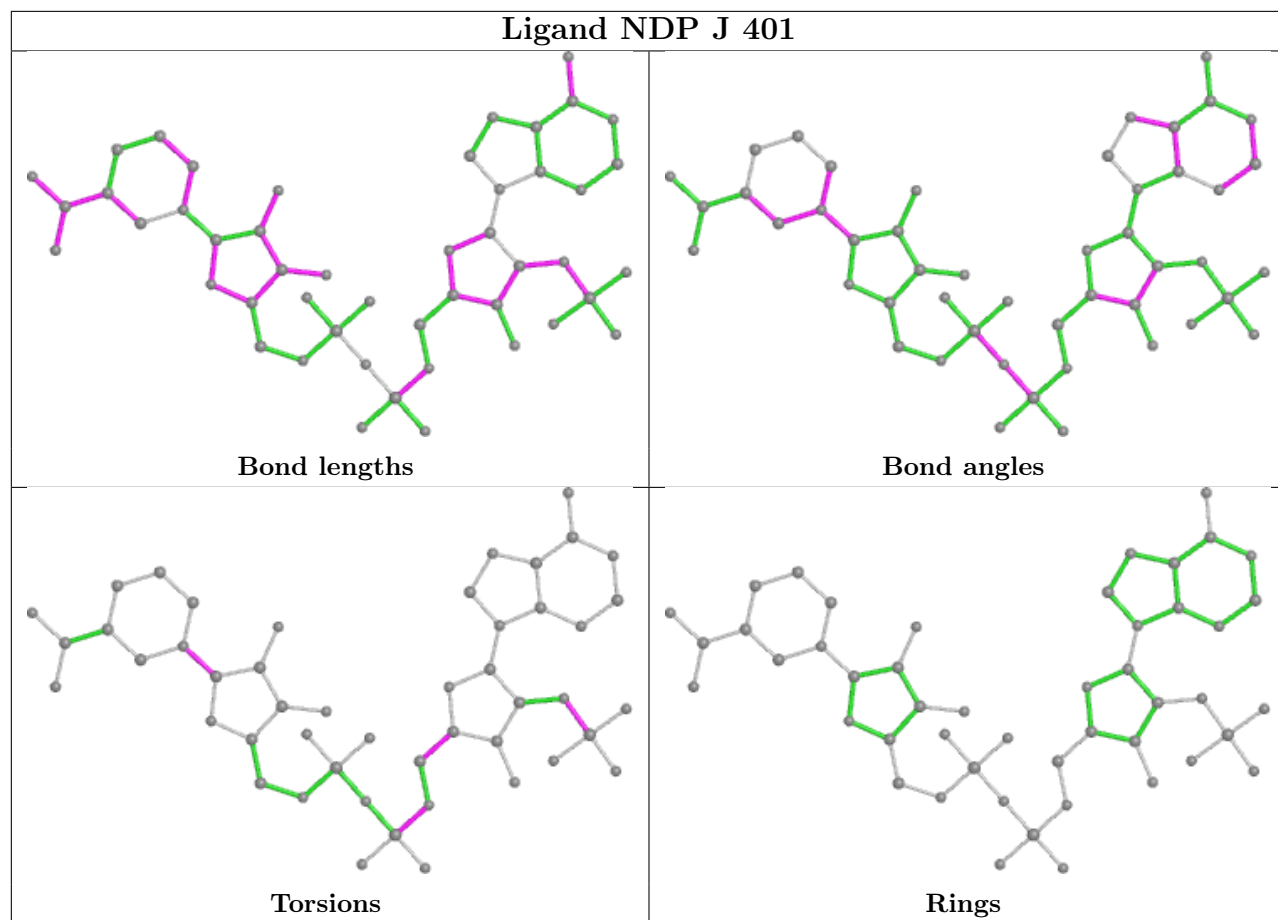


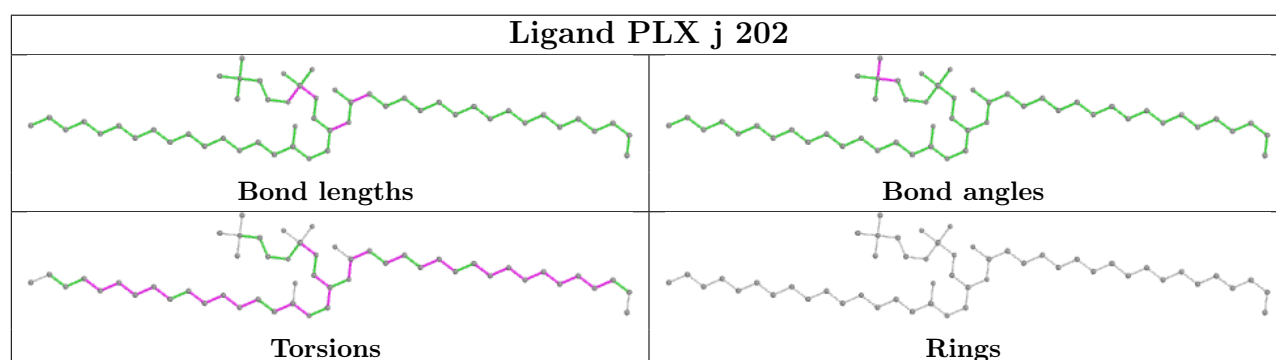
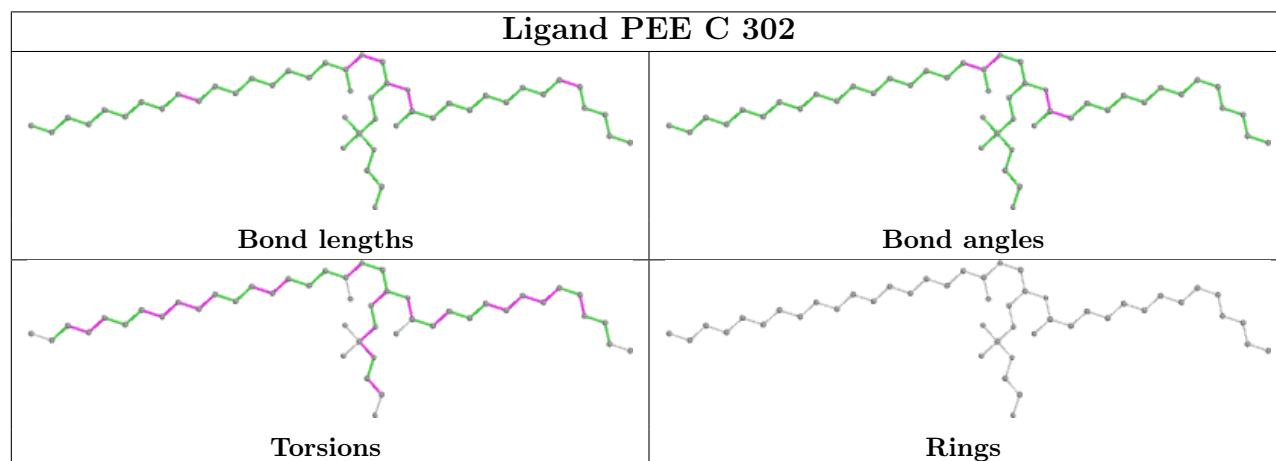
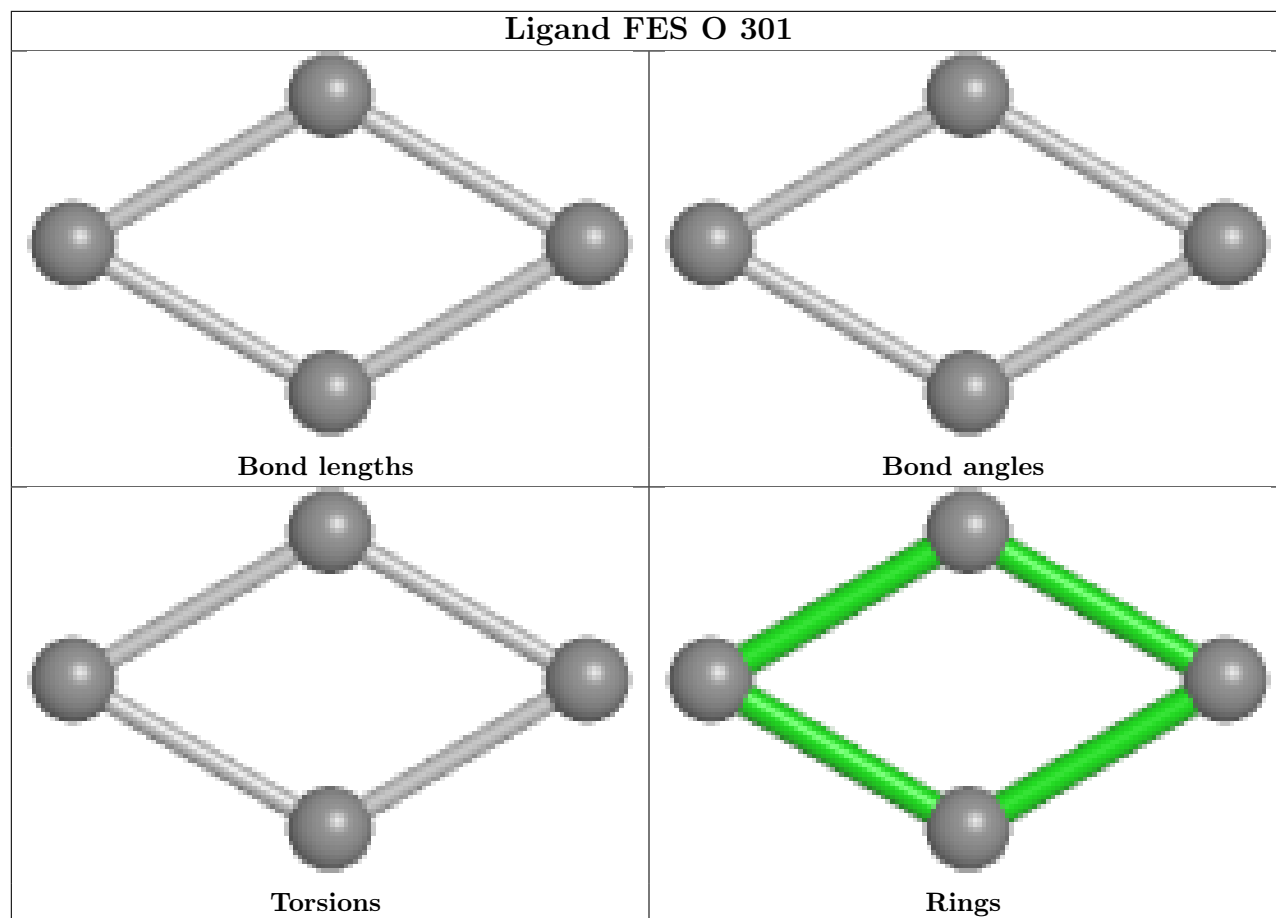












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

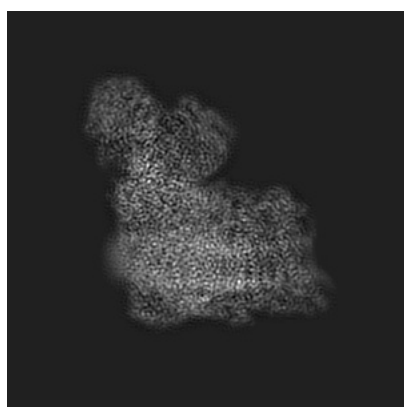
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32263. These allow visual inspection of the internal detail of the map and identification of artifacts.

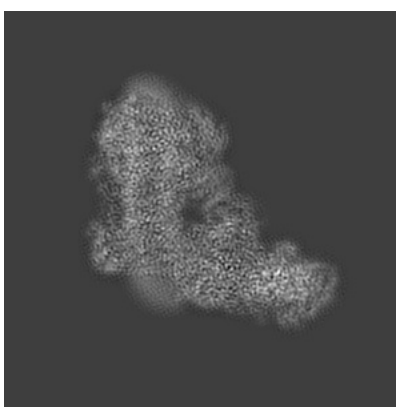
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

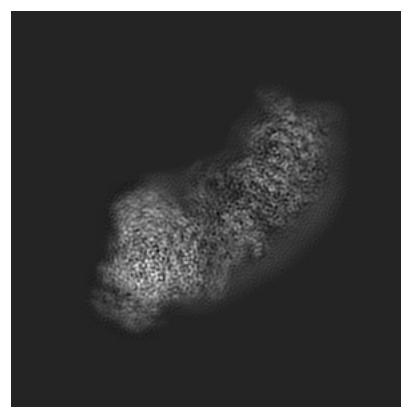
6.1.1 Primary map



X



Y

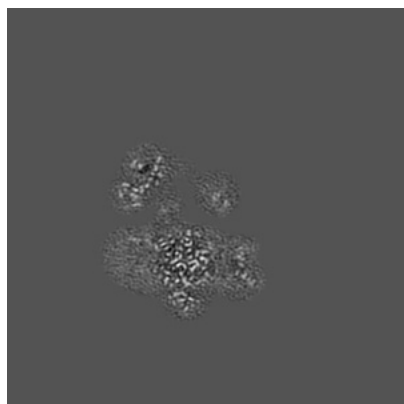


Z

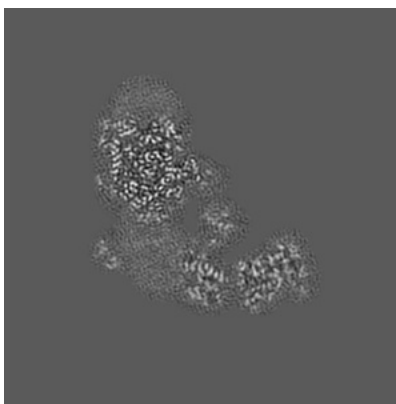
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

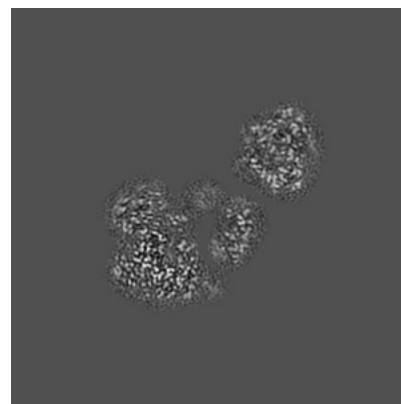
6.2.1 Primary map



X Index: 155



Y Index: 155



Z Index: 155

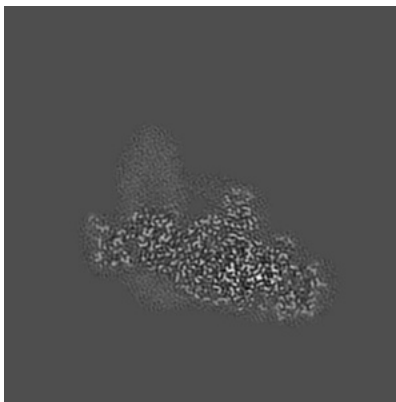
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

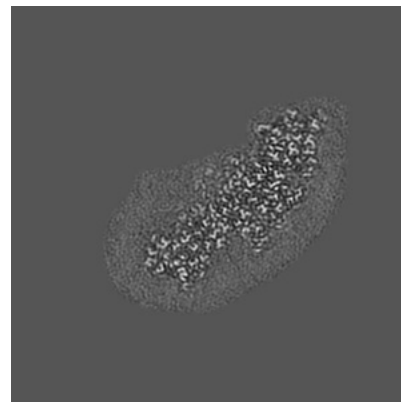
6.3.1 Primary map



X Index: 106



Y Index: 109

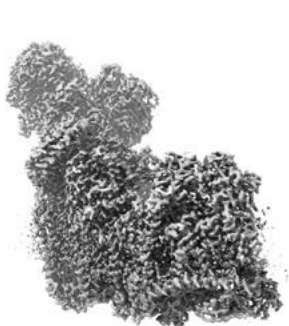


Z Index: 120

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

6.4 Orthogonal surface views [i](#)

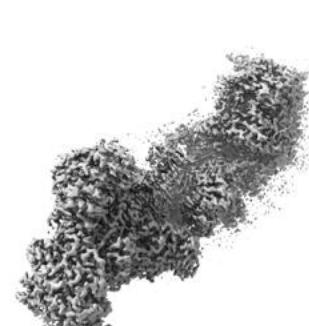
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0279. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

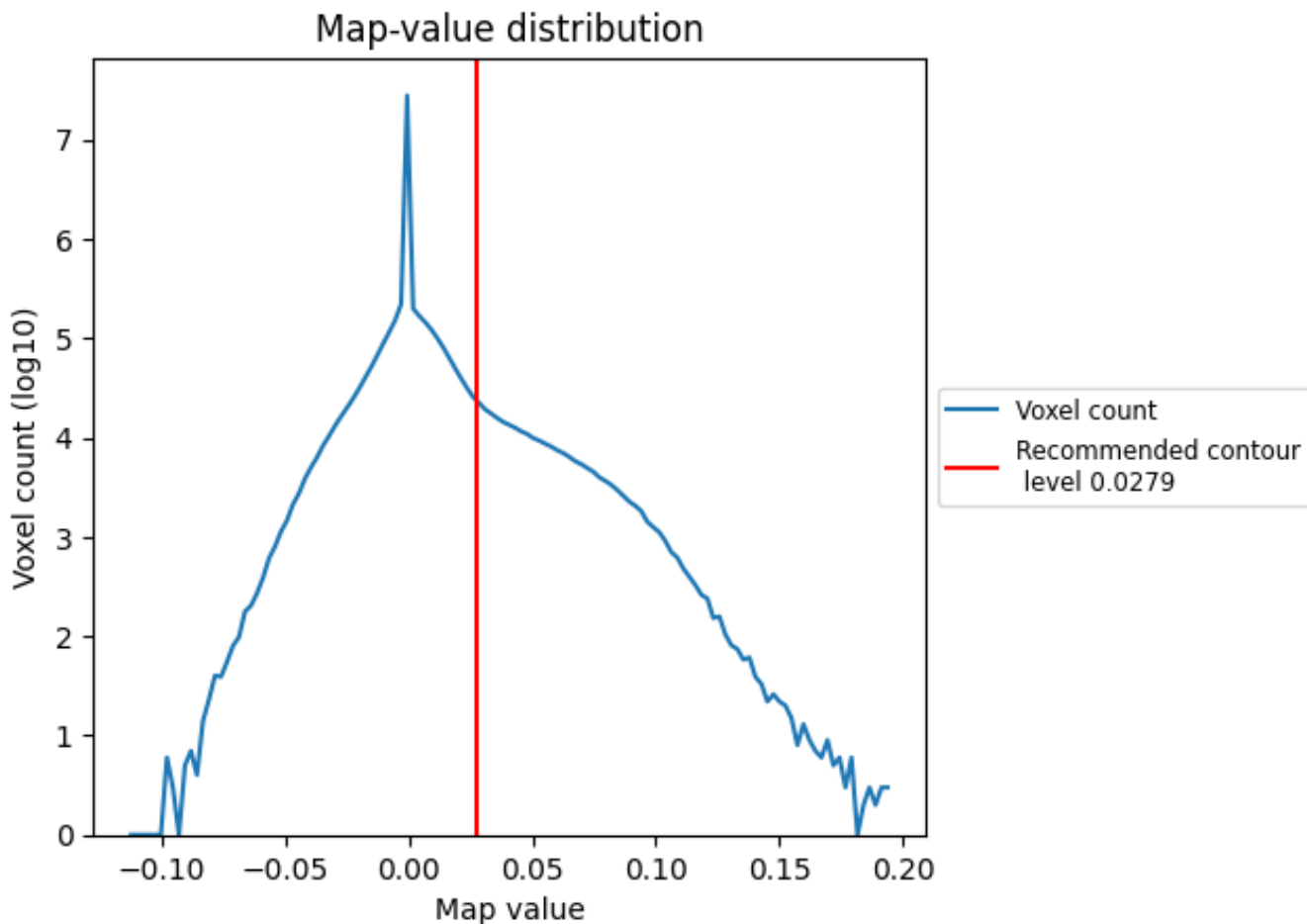
6.5 Mask visualisation

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

7 Map analysis [i](#)

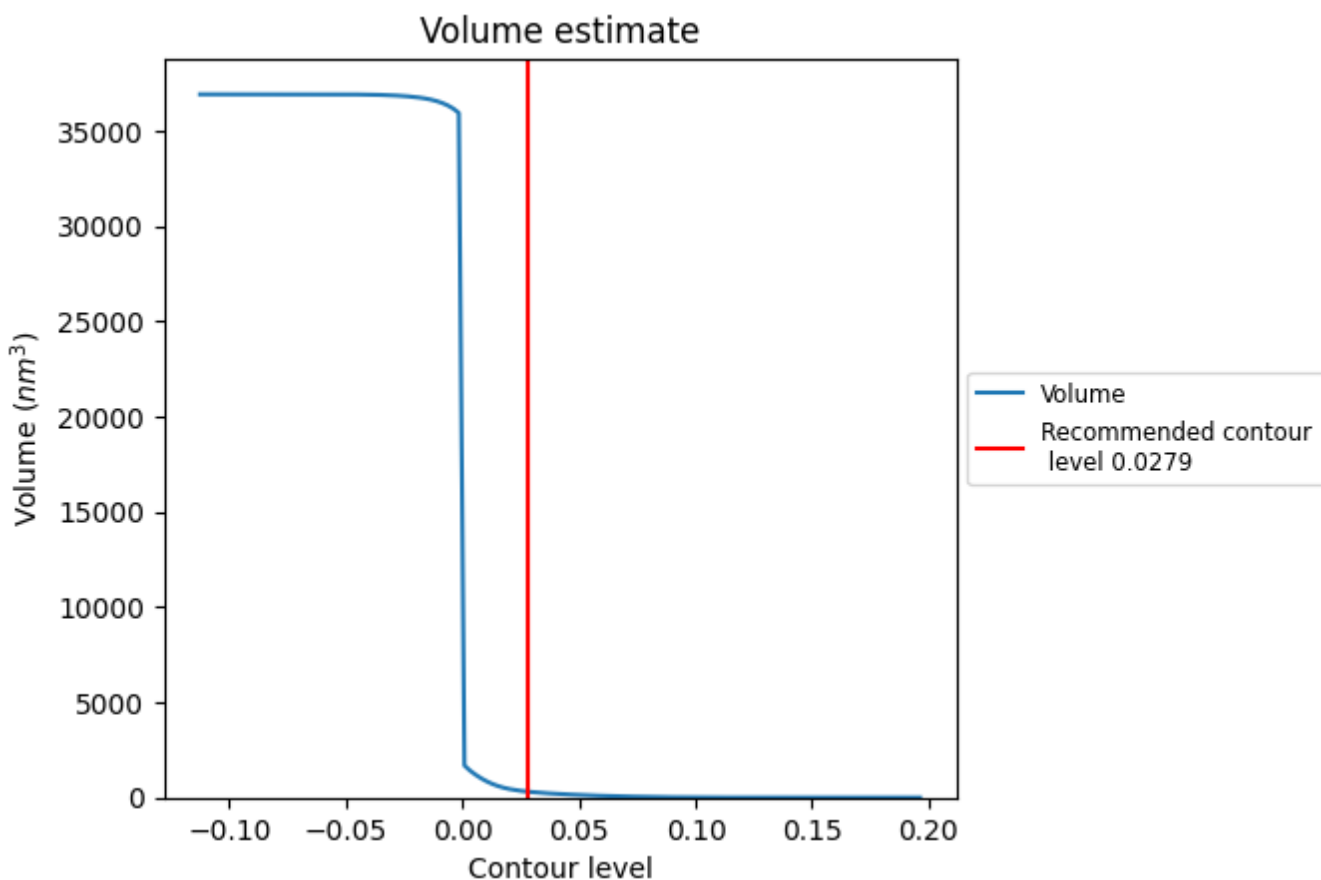
This section contains the results of statistical analysis of the map.

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.

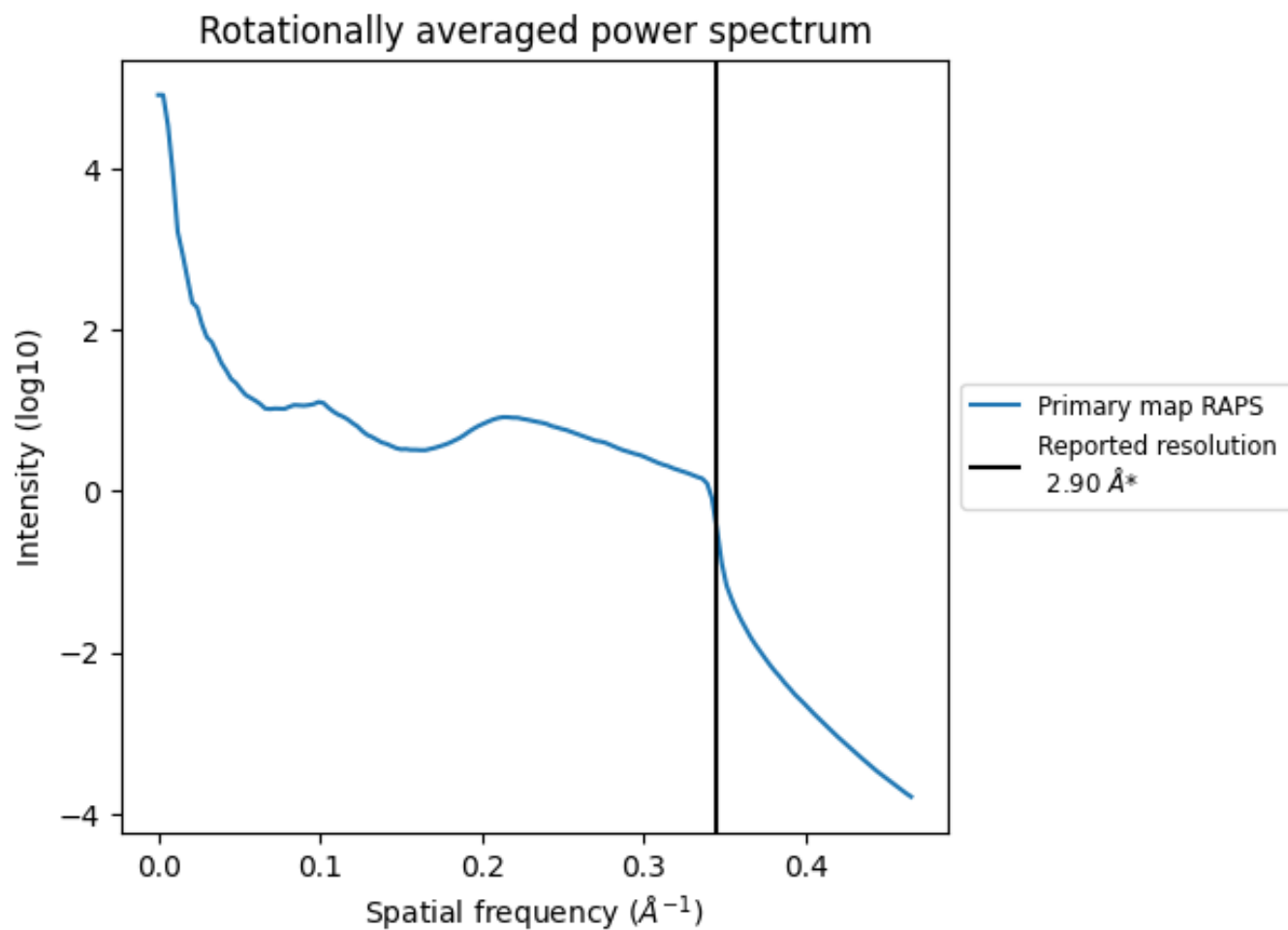
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 312 nm³; this corresponds to an approximate mass of 282 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 0.345\AA^{-1}

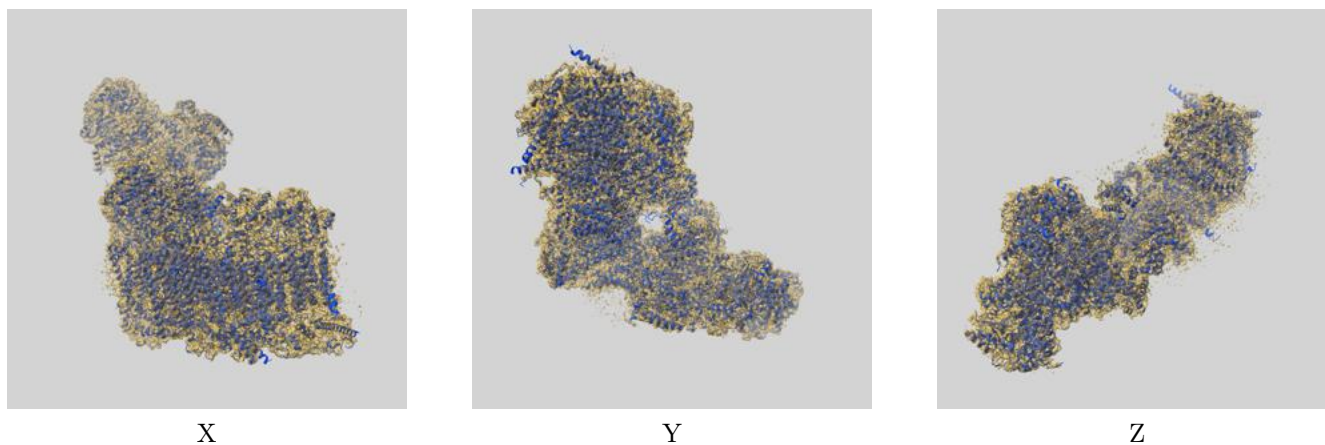
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

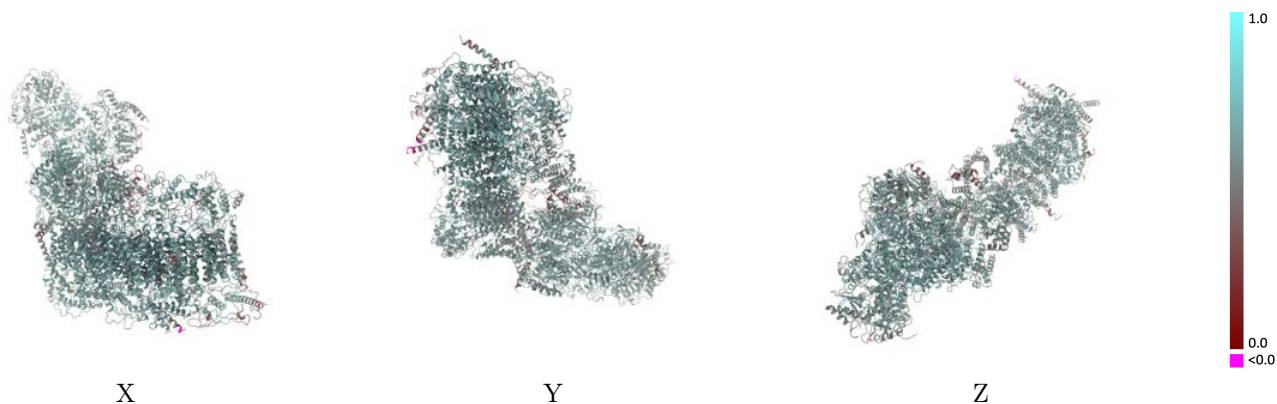
This section contains information regarding the fit between EMDB map EMD-32263 and PDB model 7W2K. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



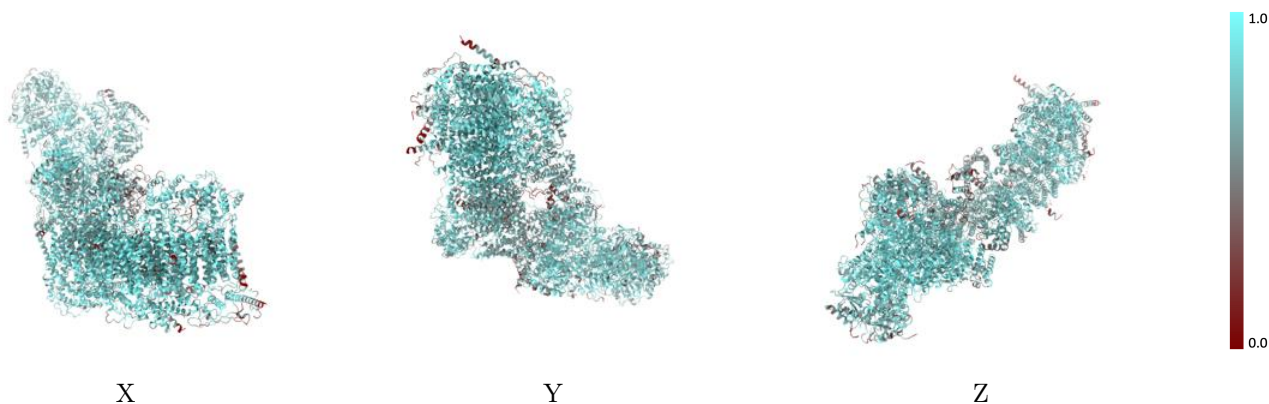
The images above show the 3D surface view of the map at the recommended contour level 0.0279 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



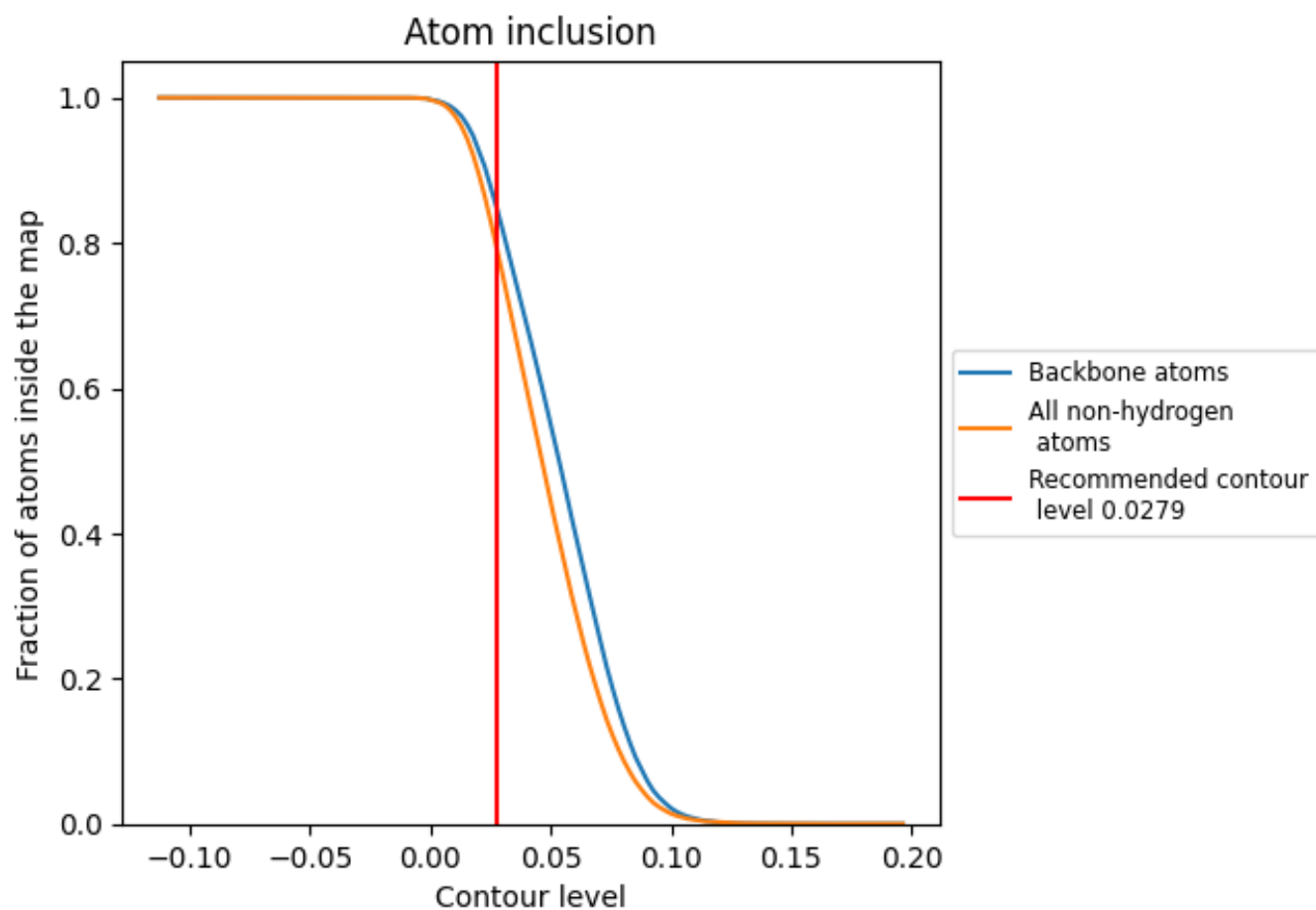
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0279).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary























The table lists the average atom inclusion at the recommended contour level (0.0279) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7888	 0.5830
A	 0.7719	 0.5670
B	 0.9181	 0.6290
C	 0.8490	 0.6110
E	 0.7431	 0.5680
F	 0.6398	 0.5080
G	 0.4404	 0.4210
H	 0.7531	 0.5670
I	 0.7466	 0.5830
J	 0.7203	 0.5600
K	 0.6890	 0.5540
L	 0.8300	 0.6020
M	 0.8201	 0.5880
N	 0.7648	 0.5930
O	 0.7330	 0.5490
P	 0.8995	 0.6210
Q	 0.8787	 0.6190
S	 0.8788	 0.6060
T	 0.8006	 0.5970
U	 0.7886	 0.5740
V	 0.5864	 0.5290
W	 0.8146	 0.5890
X	 0.7448	 0.5670
Y	 0.7025	 0.5440
Z	 0.5866	 0.4990
a	 0.8106	 0.6030
b	 0.6745	 0.5370
c	 0.7725	 0.5710
d	 0.7647	 0.5680
e	 0.7188	 0.5630
f	 0.6916	 0.5520
g	 0.8325	 0.6010
h	 0.8109	 0.5930
i	 0.8664	 0.6180
j	 0.6570	 0.5630



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Chain	Atom inclusion	Q-score
k	 0.7561	 0.5920
l	 0.8265	 0.6020
m	 0.7321	 0.5680
n	 0.6840	 0.5620
o	 0.7805	 0.5840
p	 0.7847	 0.5700
r	 0.8742	 0.6180
s	 0.8282	 0.5970
u	 0.8144	 0.5980
v	 0.6876	 0.5220
w	 0.7358	 0.5630