



## Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 10:37 pm BST

PDB ID : 6YNY / pdb\_00006yny  
EMDB ID : EMD-10860  
Title : Cryo-EM structure of Tetrahymena thermophila mitochondrial ATP synthase  
- F1Fo composite dimer model  
Authors : Kock Flygaard, R.; Muhleip, A.; Amunts, A.  
Deposited on : 2020-04-14  
Resolution : 2.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

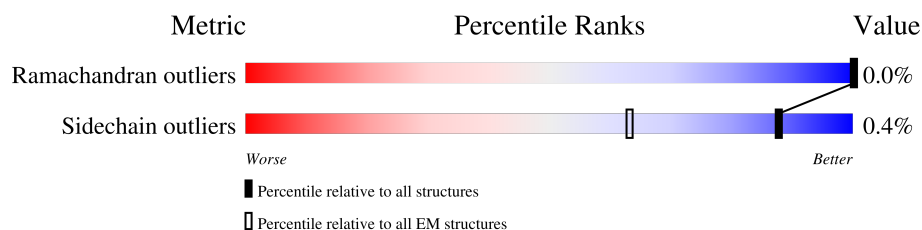
EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

# 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 2.70 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.




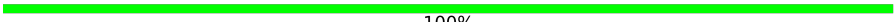
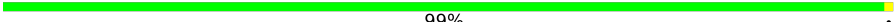
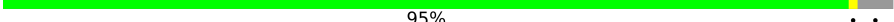
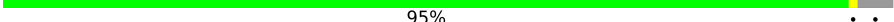




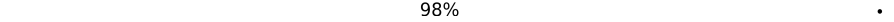
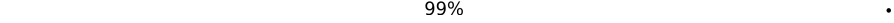
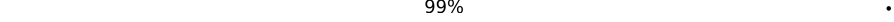
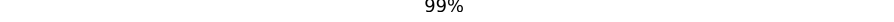
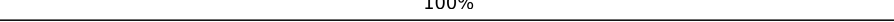
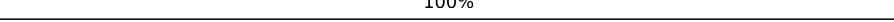










Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	446	97% .
1	a	446	97% .
2	B	381	34% 93% 7%
2	b	381	33% 93% 7%
3	D	234	17% 88% 12%
3	d	234	16% 88% 12%
4	F	204	98% .
4	f	204	98% .
5	I	209	99% .






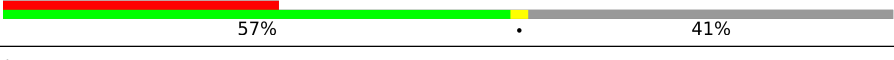



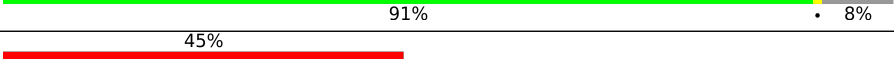

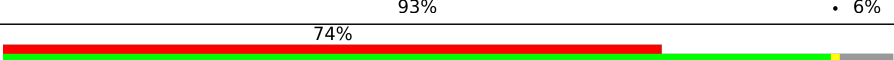
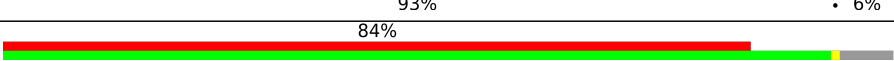
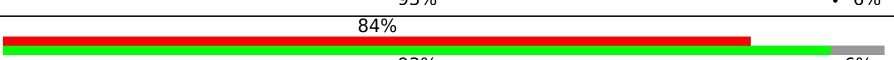
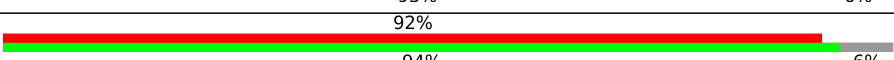
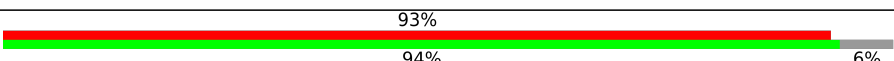
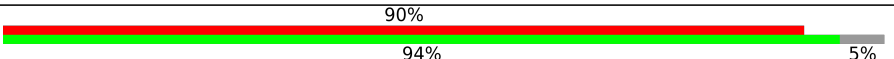
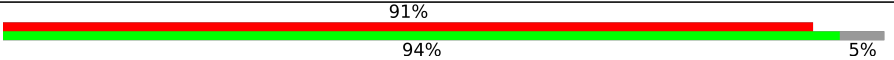
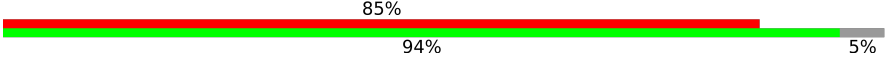
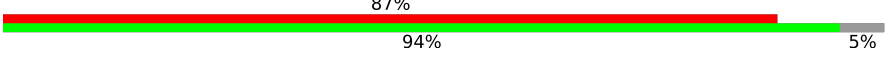
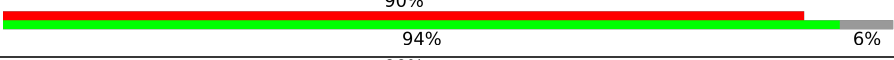
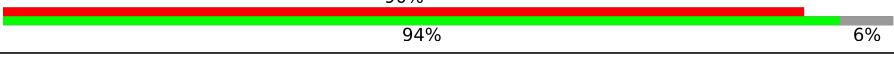
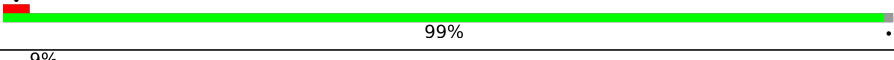
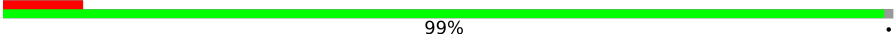

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Mol	Chain	Length	Quality of chain
5	i	209	 100%
6	K	179	 100%
6	k	179	 99%
7	C	100	 95%
7	c	100	 95%
8	G	286	 89% 10%
8	g	286	 89% 10%
9	H	268	 86% 14%
9	h	268	 86% 14%
10	J	273	 98%
10	j	273	 99%
11	L	247	 99%
11	l	247	 99%
12	M	221	 100%
12	m	221	 100%
13	N	179	 66% 34%
13	n	179	 66% 34%
14	O	154	 64% 36%
14	o	154	 64% 36%
15	P	152	 99%
15	p	152	 99%
16	Q	152	 71% 29%
16	q	152	 71% 29%
17	R	149	 93% 6%
17	r	149	 97%

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Mol	Chain	Length	Quality of chain
18	S	145	
18	s	145	
19	E	480	
19	e	480	
20	i1	108	
20	i2	108	
21	t	460	
22	G1	219	
22	G2	219	
23	g1	299	
23	g2	299	
24	A1	546	
24	A2	546	
24	B1	546	
24	B2	546	
24	C1	546	
24	C2	546	
25	D1	497	
25	D2	497	
25	E1	497	
25	E2	497	
25	F1	497	
25	F2	497	
26	H1	76	
26	H2	76	

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Mol	Chain	Length	Quality of chain
26	I1	76	
26	I2	76	
26	J1	76	
26	J2	76	
26	K1	76	
26	K2	76	
26	L1	76	
26	L2	76	
26	M1	76	
26	M2	76	
26	N1	76	
26	N2	76	
26	O1	76	
26	O2	76	
26	P1	76	
26	P2	76	
26	Q1	76	
26	Q2	76	
27	d1	158	
27	d2	158	
28	e1	71	
28	e2	71	

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 285933 atoms, of which 143905 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 subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	a	433	Total	C	H	N	O	S	0	0
			7155	2453	3527	526	633	16		
1	A	433	Total	C	H	N	O	S	0	0
			7157	2453	3529	526	633	16		

- Molecule 2 is a protein called subunit b.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	b	354	Total	C	H	N	O	S	0	0
			5726	1845	2851	487	531	12		
2	B	354	Total	C	H	N	O	S	0	0
			5724	1845	2849	487	531	12		

- Molecule 3 is a protein called subunit d.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	d	206	Total	C	H	N	O	S	0	0
			3274	1065	1598	274	332	5		
3	D	206	Total	C	H	N	O	S	0	0
			3274	1065	1598	274	332	5		

- Molecule 4 is a protein called subunit f.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	f	200	Total	C	H	N	O	S	0	0
			3373	1095	1691	299	278	10		
4	F	200	Total	C	H	N	O	S	0	0
			3374	1095	1692	299	278	10		

- Molecule 5 is a protein called subunit i/j.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	i	209	Total	C	H	N	O	S	0	0
			3462	1121	1742	304	285	10		
5	I	209	Total	C	H	N	O	S	0	0
			3460	1121	1740	304	285	10		

- Molecule 6 is a protein called subunit k.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	k	179	Total	C	H	N	O	S	0	0
			2902	939	1429	257	266	11		
6	K	179	Total	C	H	N	O	S	0	0
			2903	939	1430	257	266	11		

- Molecule 7 is a protein called subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	c	96	Total	C	H	N	O	S	0	0
			1671	565	830	131	143	2		
7	C	96	Total	C	H	N	O	S	0	0
			1671	565	830	131	143	2		

- Molecule 8 is a protein called ATPTT3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	g	256	Total	C	H	N	O	S	0	0
			4338	1474	2118	348	388	10		
8	G	256	Total	C	H	N	O	S	0	0
			4338	1474	2118	348	388	10		

- Molecule 9 is a protein called ATPTT4.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	h	231	Total	C	H	N	O	S	0	0
			3836	1236	1883	361	350	6		
9	H	231	Total	C	H	N	O	S	0	0
			3836	1236	1883	361	350	6		

- Molecule 10 is a protein called ATPTT5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	j	269	Total	C	H	N	O	S	0	0
			4346	1381	2147	406	404	8		

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	269	Total	C	H	N	O	S	0	0
			4346	1381	2147	406	404	8		

- Molecule 11 is a protein called ATPTT6.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	I	246	Total	C	H	N	O	S	0	0
			4070	1344	1999	360	361	6		
11	L	246	Total	C	H	N	O	S	0	0
			4070	1344	1999	360	361	6		

- Molecule 12 is a protein called ATPTT7.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	m	221	Total	C	H	N	O	S	0	0
			3696	1205	1835	313	336	7		
12	M	221	Total	C	H	N	O	S	0	0
			3696	1205	1835	313	336	7		

- Molecule 13 is a protein called ATPTT8.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	n	119	Total	C	H	N	O	S	0	0
			1960	655	962	164	173	6		
13	N	119	Total	C	H	N	O	S	0	0
			1960	655	962	164	173	6		

- Molecule 14 is a protein called ATPTT9.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	o	99	Total	C	H	N	O	S	0	0
			1599	507	794	145	147	6		
14	O	99	Total	C	H	N	O	S	0	0
			1599	507	794	145	147	6		

- Molecule 15 is a protein called ATPTT10.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	p	150	Total	C	H	N	O	S	0	0
			2413	788	1196	204	224	1		
15	P	150	Total	C	H	N	O	S	0	0
			2413	788	1196	204	224	1		



- Molecule 16 is a protein called ATPTT11.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	q	108	Total	C	H	N	O	S	0	0
			1749	556	874	149	169	1		
16	Q	108	Total	C	H	N	O	S	0	0
			1749	556	874	149	169	1		

- Molecule 17 is a protein called ATPTT12.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	r	145	Total	C	H	N	O	S	0	0
			2373	776	1180	201	212	4		
17	R	140	Total	C	H	N	O	S	0	0
			2288	750	1134	194	206	4		

- Molecule 18 is a protein called ATPTT13.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	s	124	Total	C	H	N	O	S	0	0
			2025	648	1009	174	189	5		
18	S	125	Total	C	H	N	O	S	0	0
			2039	652	1016	175	191	5		

- Molecule 19 is a protein called ATPTT1.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	e	417	Total	C	H	N	O	S	0	0
			6681	2171	3286	602	614	8		
19	E	417	Total	C	H	N	O	S	0	0
			6681	2171	3286	602	614	8		

- Molecule 20 is a protein called Inhibitor of F1 (IF1).

Mol	Chain	Residues	Atoms						AltConf	Trace
20	i2	64	Total	C	H	N	O	S	0	0
			1112	351	556	97	107	1		
20	i1	68	Total	C	H	N	O	S	0	0
			1167	368	582	103	113	1		

- Molecule 21 is a protein called ATPTT2.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	t	365	Total	C	H	N	O	S	0	0
			5889	1925	2876	533	544	11		

- Molecule 22 is a protein called Oligomycin sensitivity-conferring protein (OSCP).

Mol	Chain	Residues	Atoms						AltConf	Trace
22	G1	188	Total	C	H	N	O	S	0	0
			3000	942	1515	252	287	4		
22	G2	188	Total	C	H	N	O	S	0	0
			3000	942	1515	252	287	4		

- Molecule 23 is a protein called subunit gamma.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	g1	275	Total	C	H	N	O	S	0	0
			4332	1343	2206	373	400	10		
23	g2	275	Total	C	H	N	O	S	0	0
			4332	1343	2206	373	400	10		

- Molecule 24 is a protein called subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	C1	513	Total	C	H	N	O	S	0	0
			7980	2481	4058	685	739	17		
24	B1	511	Total	C	H	N	O	S	0	0
			7934	2469	4030	681	737	17		
24	A1	512	Total	C	H	N	O	S	0	0
			7946	2472	4037	682	738	17		
24	C2	513	Total	C	H	N	O	S	0	0
			7980	2481	4058	685	739	17		
24	B2	511	Total	C	H	N	O	S	0	0
			7934	2469	4030	681	737	17		
24	A2	512	Total	C	H	N	O	S	0	0
			7946	2472	4037	682	738	17		

- Molecule 25 is a protein called subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	D1	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
25	F1	469	Total	C	H	N	O	S	0	0
			7113	2237	3568	610	687	11		

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Mol	Chain	Residues	Atoms						AltConf	Trace
25	E1	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
25	D2	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
25	F2	469	Total	C	H	N	O	S	0	0
			7113	2237	3568	610	687	11		
25	E2	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		

- Molecule 26 is a protein called subunit c.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	P1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	O1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	N1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	M1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	L1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	K1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	J1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	I1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	H1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	Q1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	P2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	O2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	N2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	M2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	L2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
26	K2	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	J2	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	I2	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	H2	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	Q2	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		

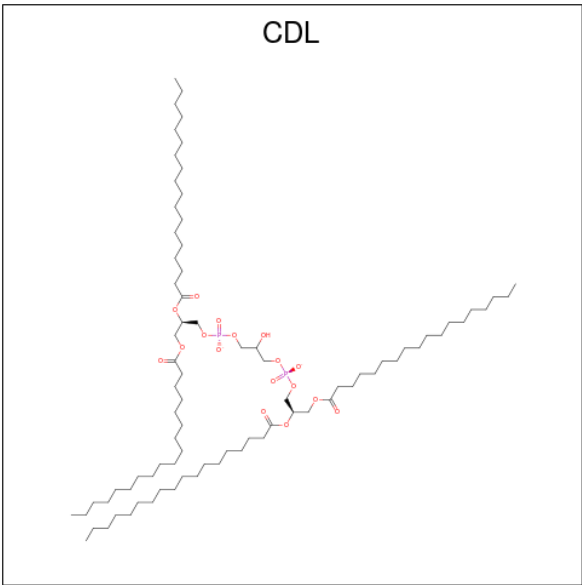
- Molecule 27 is a protein called subunit delta.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	d1	134	Total	C	H	N	O	S	0	0
			2144	674	1082	185	200	3		
27	d2	134	Total	C	H	N	O	S	0	0
			2144	674	1082	185	200	3		

- Molecule 28 is a protein called subunit epsilon.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	e1	68	Total	C	H	N	O	S	0	0
			1096	347	559	94	95	1		
28	e2	68	Total	C	H	N	O	S	0	0
			1096	347	559	94	95	1		

- Molecule 29 is CARDIOLIPIN (CCD ID: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



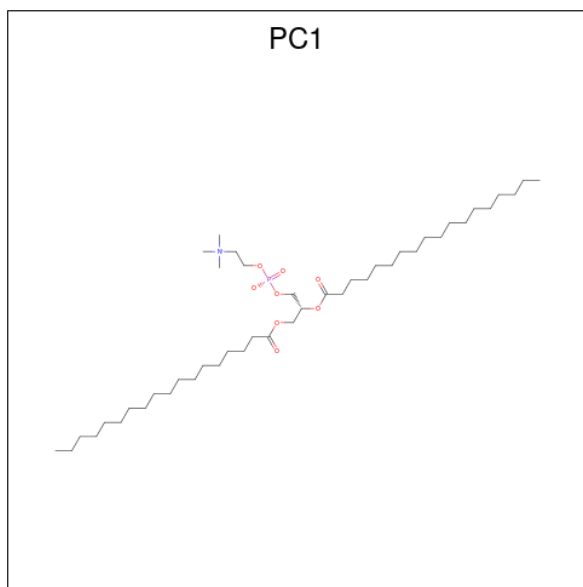
Mol	Chain	Residues	Atoms					AltConf
29	a	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	a	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	b	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	i	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	k	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	k	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	j	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	j	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	l	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	l	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	p	1	Total	C	H	O	P	0
			256	81	156	17	2	

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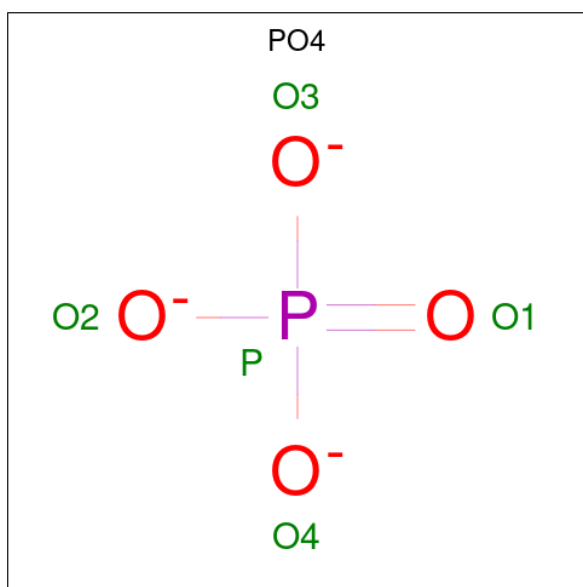
Mol	Chain	Residues	Atoms					AltConf
29	r	1	Total 256	C 81	H 156	O 17	P 2	0
29	A	1	Total 256	C 81	H 156	O 17	P 2	0
29	B	1	Total 256	C 81	H 156	O 17	P 2	0
29	B	1	Total 256	C 81	H 156	O 17	P 2	0
29	B	1	Total 256	C 81	H 156	O 17	P 2	0
29	B	1	Total 256	C 81	H 156	O 17	P 2	0
29	F	1	Total 256	C 81	H 156	O 17	P 2	0
29	I	1	Total 256	C 81	H 156	O 17	P 2	0
29	I	1	Total 256	C 81	H 156	O 17	P 2	0
29	K	1	Total 256	C 81	H 156	O 17	P 2	0
29	K	1	Total 256	C 81	H 156	O 17	P 2	0
29	J	1	Total 256	C 81	H 156	O 17	P 2	0
29	J	1	Total 256	C 81	H 156	O 17	P 2	0
29	L	1	Total 256	C 81	H 156	O 17	P 2	0
29	L	1	Total 256	C 81	H 156	O 17	P 2	0
29	P	1	Total 256	C 81	H 156	O 17	P 2	0

- Molecule 30 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C<sub>44</sub>H<sub>88</sub>NO<sub>8</sub>P).



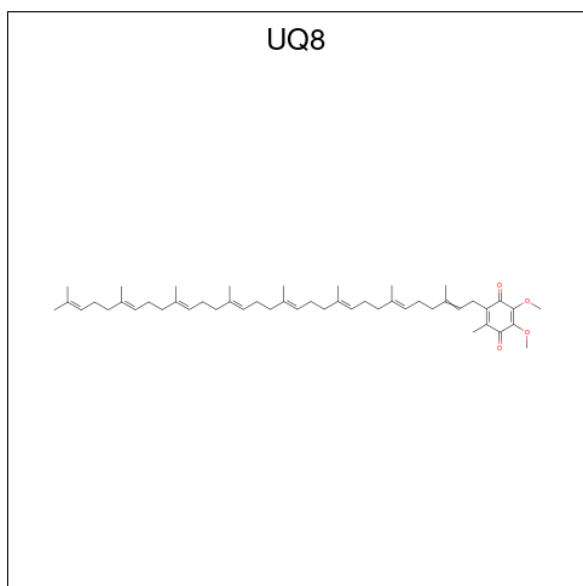
Mol	Chain	Residues	Atoms						AltConf
30	d	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	g	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	g	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	D	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	G	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	G	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

- Molecule 31 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			AltConf
31	f	1	Total	O	P	0
			5	4	1	
31	F	1	Total	O	P	0
			5	4	1	

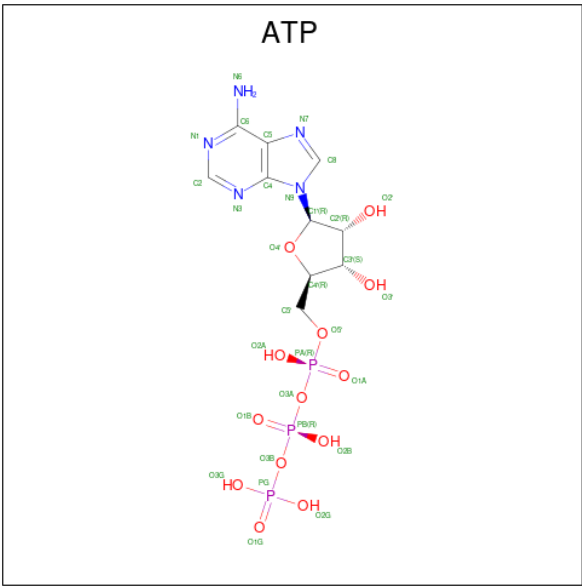
- Molecule 32 is Ubiquinone-8 (CCD ID: UQ8) (formula:  $C_{49}H_{74}O_4$ ).



Mol	Chain	Residues	Atoms				AltConf
32	i	1	Total	C	H	O	0
			127	49	74	4	
32	I	1	Total	C	H	O	0
			127	49	74	4	



- Molecule 33 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms						AltConf
33	g	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	G	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	C1	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	B1	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	A1	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	C2	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	B2	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	A2	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

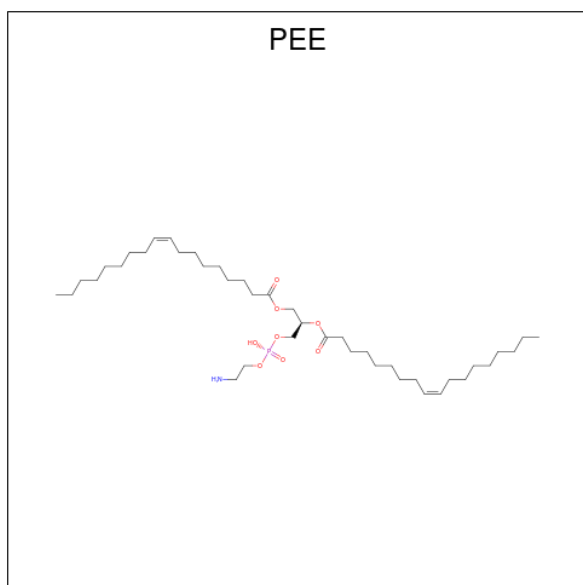
Mol	Chain	Residues	Atoms		AltConf
34	g	1	Total	Mg	0
			1	1	
34	G	1	Total	Mg	0
			1	1	
34	C1	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
34	D1	1	Total	Mg	0
			1	1	
34	B1	1	Total	Mg	0
			1	1	
34	A1	1	Total	Mg	0
			1	1	
34	E1	1	Total	Mg	0
			1	1	
34	C2	1	Total	Mg	0
			1	1	
34	D2	1	Total	Mg	0
			1	1	
34	B2	1	Total	Mg	0
			1	1	
34	A2	1	Total	Mg	0
			1	1	
34	E2	1	Total	Mg	0
			1	1	

- Molecule 35 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula:  $C_{41}H_{78}NO_8P$ ).



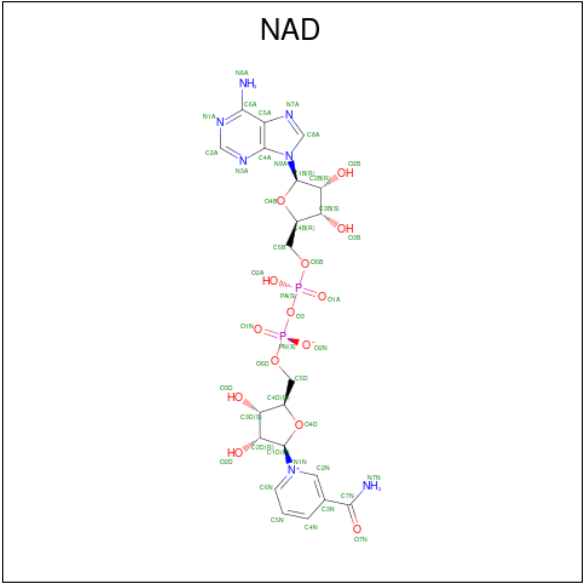
Mol	Chain	Residues	Atoms					AltConf	
35	m	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
35	A	1	Total 123	C 38	H 75	N 1	O 8	P 1	0

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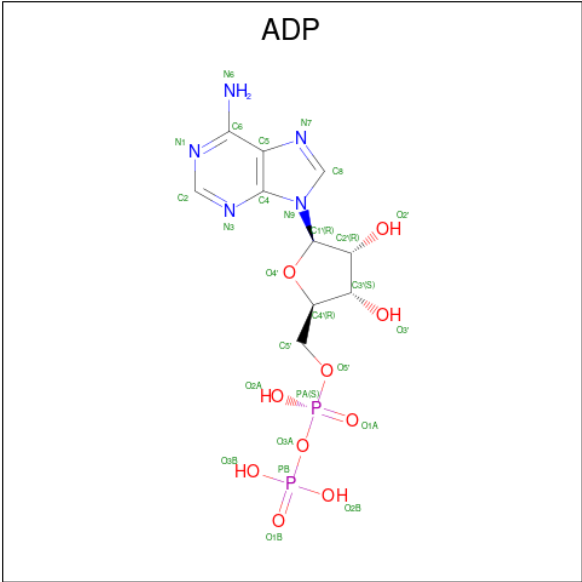
Mol	Chain	Residues	Atoms						AltConf
35	J	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
35	L	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	

- Molecule 36 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms						AltConf
36	e	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
36	E	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



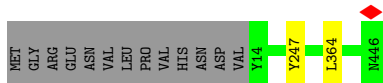
Mol	Chain	Residues	Atoms						AltConf
37	D1	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	
37	B1	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	
37	D2	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	
37	B2	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	

### 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.

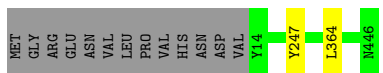
- Molecule 1: subunit a

Chain a:  97%



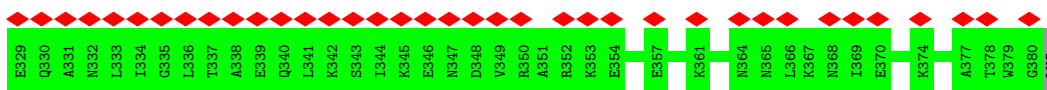
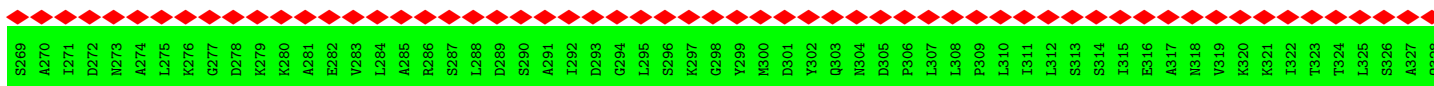
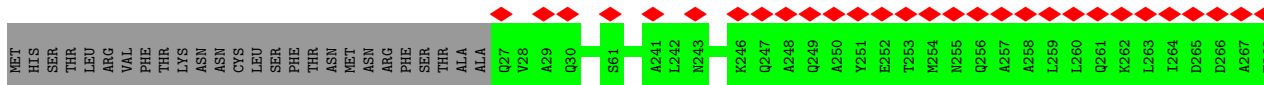
- Molecule 1: subunit a

Chain A:  97%

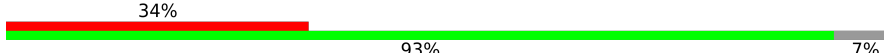


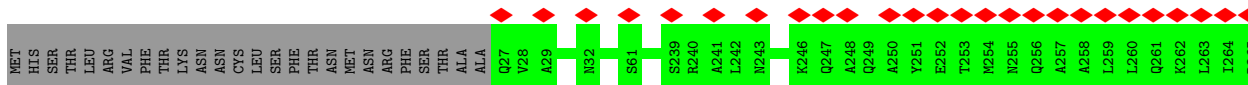
- Molecule 2: subunit b

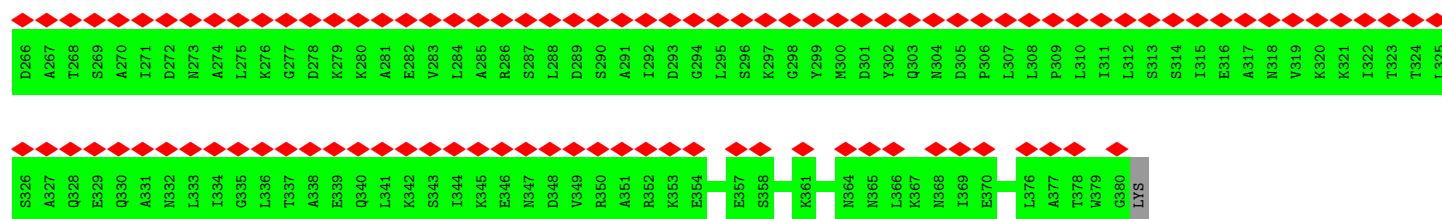
Chain b:  33% 93% 7%



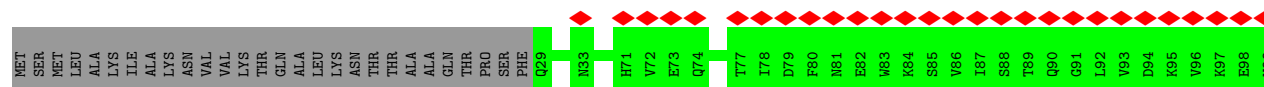
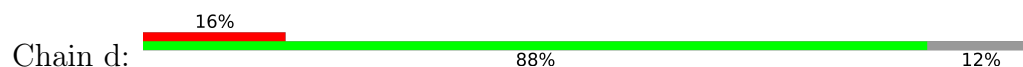
- Molecule 2: subunit b

Chain B:  34% 93% 7%

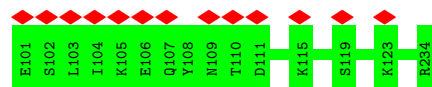
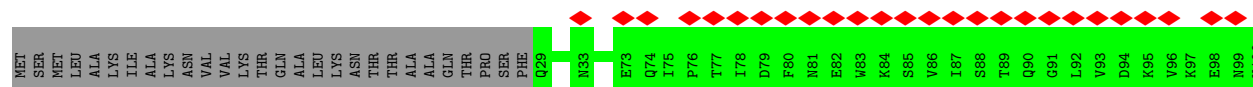
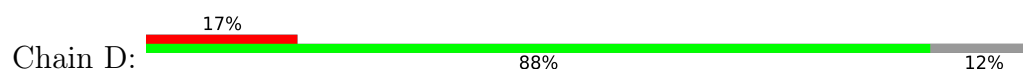




- Molecule 3: subunit d



- Molecule 3: subunit d



- Molecule 4: subunit f



- Molecule 4: subunit f



- Molecule 5: subunit i/j



- Molecule 5: subunit i/j

Chain I:  99%



- Molecule 6: subunit k

Chain k:  99%



- Molecule 6: subunit k

Chain K:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: subunit 8

Chain c:  95%





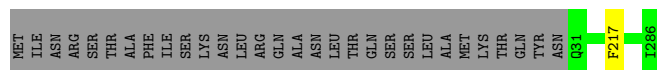
- Molecule 7: subunit 8

Chain C:  95%





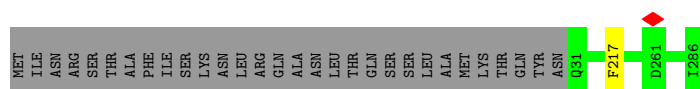
- Molecule 8: ATPPT3

Chain g:  89%  10%



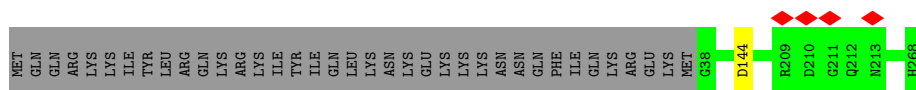
- Molecule 8: ATPPT3

Chain G:  89%  10%

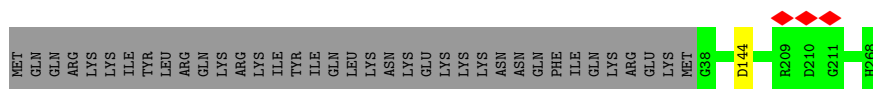
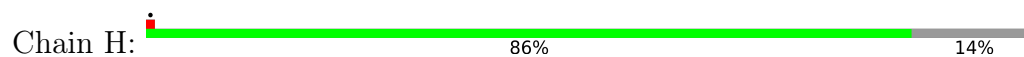


- Molecule 9: ATPPT4

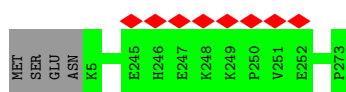
Chain h:  86%  14%



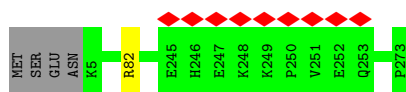
- Molecule 9: ATPTT4



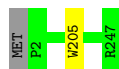
- Molecule 10: ATPTT5



- Molecule 10: ATPTT5



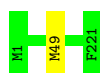
- Molecule 11: ATPTT6



- Molecule 11: ATPTT6



- Molecule 12: ATPTT7



- Molecule 12: ATPTT7





- Molecule 13: ATPTT8

MET	GLU	GLY	PHE	ILE	GLN	ASN	LYS	ARG	LYS	LYS	GLU	GLU	GLU	GLU	GLU	SER	LYS	LYS	GLU	GLU	GLU	GLU	GLN	LEU	ASN	LYS	GLN	GLN	GLN	LYS	LYS	ASP	GLN	LYS	ARG	LYS	LYS	TYR	TYR	LEU	GLN	GLN	ARG	LYS	LYS	GLU	MET
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- Molecule 13: ATPTT8

MET	GLU	GLY	PHE	ILE	GLN	ASN	LYS	ARG	LYS	LYS	GLU	GLU	GLU	GLU	SER	LYS	GLY	GLN	ASN	GLN	LEU	ASN	LYS	GLN	GLN	GLU	GLU	LYS	TYR	GLN	GLN	LYS	LYS	ASP	GLN	LYS	ARG	LYS	LYS	TYR	LEU	TYR	GLN	GLN	ARG	LYS	GLU	MET
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- Molecule 14: ATPTT9

MET	LYS	GLN	GLN	LYS	ILE	ASN	LYS	LEU	LYS	ASN	LYS	GLY	VAL	GLN	ASP	LYS	TYR	TYR	TYR	LEU	LEU	LEU	LEU	ASP	GLN	GLU	ILE	ILE	LYS	GLY	LYS	LYS	ARG	LYS	ASN	LYS	LYS	LYS	GLU	GLU	LYS	LYS	LEU	LEU	GLU	GLU	GLU	M55	K153
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- Molecule 14: ATPTT9

[illegible]

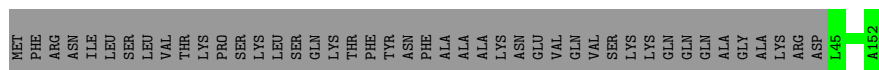
- Molecule 15: ATPTT10

- Molecule 15: ATPTT10

Diagram illustrating a protein segment with residues MET, S2, Q60, H151, and ASN. A red diamond is positioned above the Q60 residue.

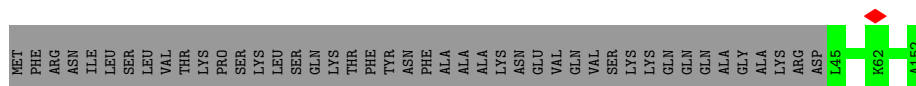
- Molecule 16: ATPTT11

Chain q:  71% 29%



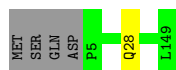
- Molecule 16: ATPTT11

Chain Q:  71% 29%



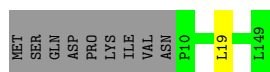
- Molecule 17: ATPTT12

Chain r:  97% ..




- Molecule 17: ATPTT12

Chain R:  93% • 6%




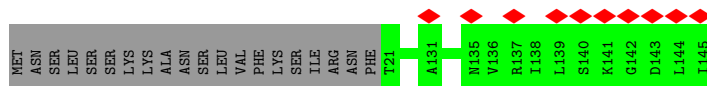
- Molecule 18: ATPTT13

Chain s:  6% 84% • 14%




- Molecule 18: ATPTT13

Chain S:  7% 86% 14%




- Molecule 19: ATPTT1

Chain e:  87% 13%



SER  
LYS  
TYR  
PHE  
PRO  
THR  
LYS  
THR  
GLU  
ASN  
LYS  
ALA  
HIS

• Molecule 19: ATPTT1

Chain E:  86% 13%

MET ILE HIS CYS ILE LEU LEU THR ASN ILE ARG THR THR VAL SER LEU GLN SER SER ILE ILE SER TYR ASN GLN GLY GLY ASN K27 D34 K57 E118 W350 L391 R439 F443 TYR HIS LYS VAL LEU LYS SER PHE PRO GLU LEU PRO GLY PRO GLU SER GLN GLN

SER  
SER  
GLY  
ILE  
SER  
LYS  
TYR  
PHE  
PRO  
THR  
LYS  
THR  
GLU  
ASN  
LYS  
ALA  
HIS

• Molecule 20: Inhibitor of F1 (IF1)

Chain i2:  31% 57% 41%

MET ASN ARG SER VAL ILE ALA LYS ASN THR ILE GLN THR TYR ARG ALA PHE PHE T28 R29 E30 E31 E32 D35 K36 R37 T38 K39 K43 V44 Y45 F46 D47 Q48 E49 D50 R51 K52 A53 M54 K55 R56 L57 L58 E59 K60 L61 N62 T63

THR SER LYS PHE VAL GLU ASP SER GLU TYR LEU ALA PRO GLN ASN L79 E82 N91 D102 G106 LYS ASN


• Molecule 20: Inhibitor of F1 (IF1)

Chain i1:  25% 63% 37%

MET ASN ARG SER VAL ILE ALA LYS ASN THR ILE GLN THR TYR ARG ALA PHE PHE T28 R29 E30 E31 E32 W33 L34 D35 K36 R37 Y45 F46 D47 Q48 E49 D50 R51 K52 A53 M54 K55 R56 L57 L58 E59 K60 N62 T63 THR SER LYS

PHE VAL GLU ASP SER GLU TYR LEU A75 H89 D102 G106 LYS ASN


• Molecule 21: ATPTT2

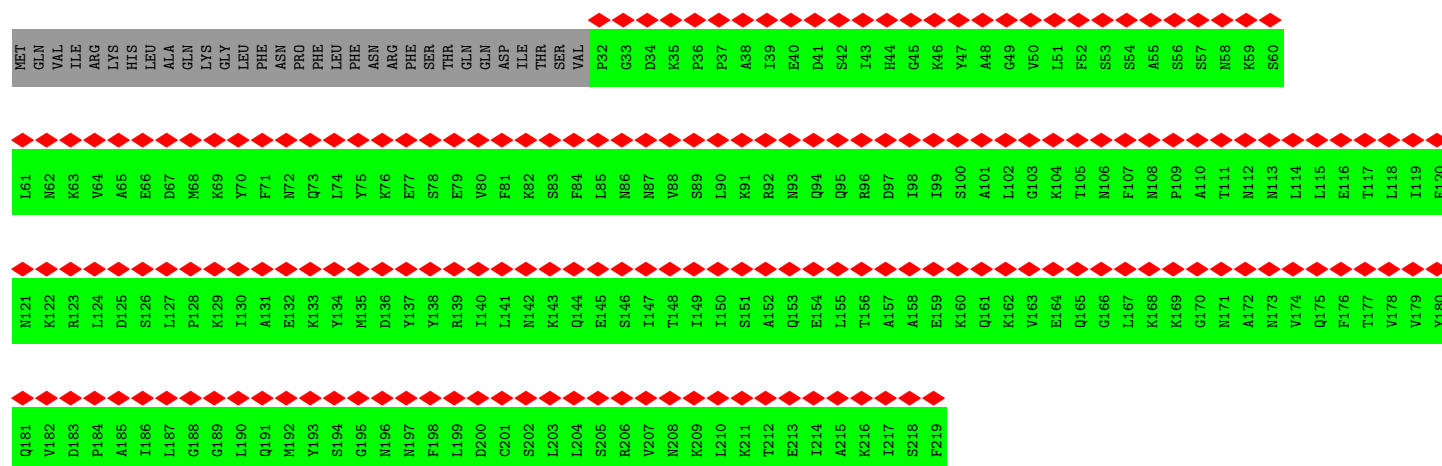
Chain t:  79% 21%

MET LYS MET GLU TYR LEU GLN SER GLU TYR GLU LYS ASP ALA ILE ASN GLN ILE HIS LYS GLU GLU GLU GLU GLN VAL PHE LYS CYS LEU TRP GLY ALA GLN PRO ALA TYR ASN PHE S94 E135 T140 R158 A288 K289 T290 Q291 M458 GLU GLN

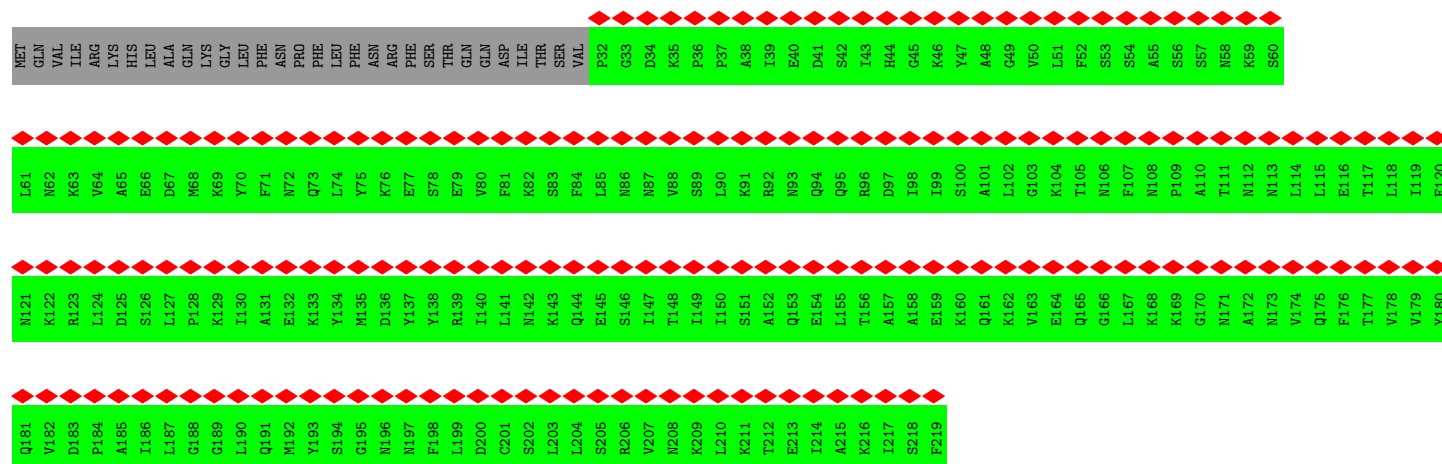
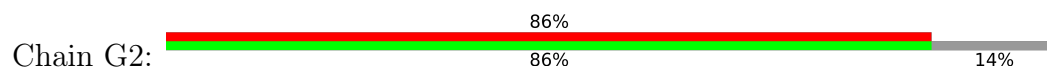
ILE GLN LYS LYS GLN ARG LYS TYR GLY ARG MET ILE ASN THR ARG LYS VAL PHE LYS CYS LEU TRP GLY ALA GLN PRO ALA TYR ASN PHE S94 E135 T140 R158 A288 K289 T290 Q291 M458 GLU GLN

• Molecule 22: Oligomycin sensitivity-conferring protein (OSCP)

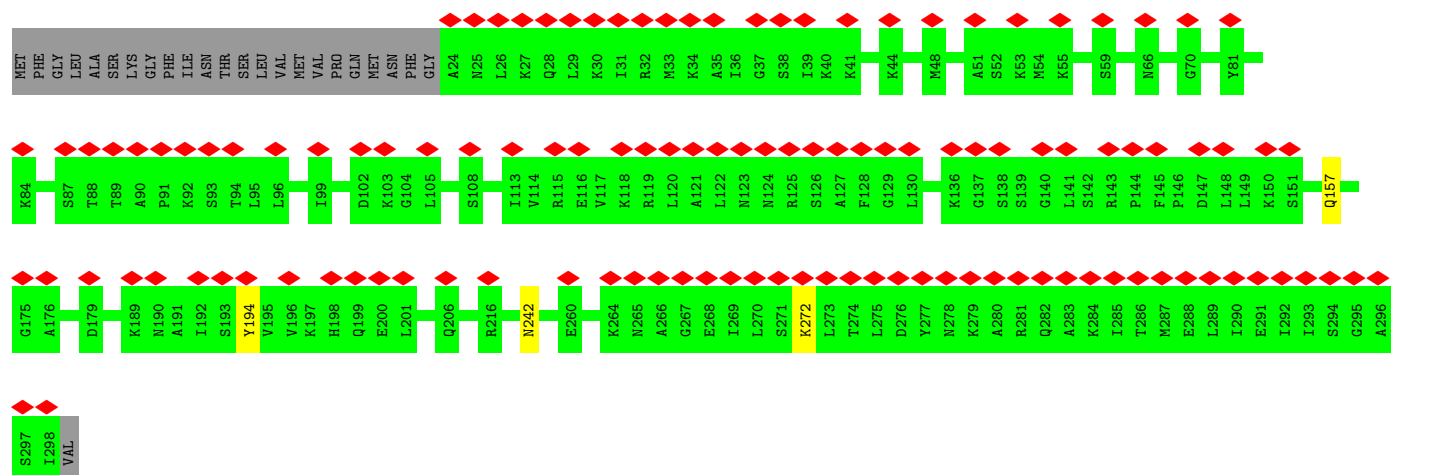
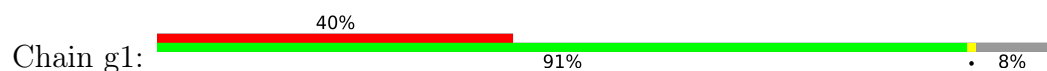
Chain G1:  86% 86% 14%



• Molecule 22: Oligomycin sensitivity-conferring protein (OSCP)

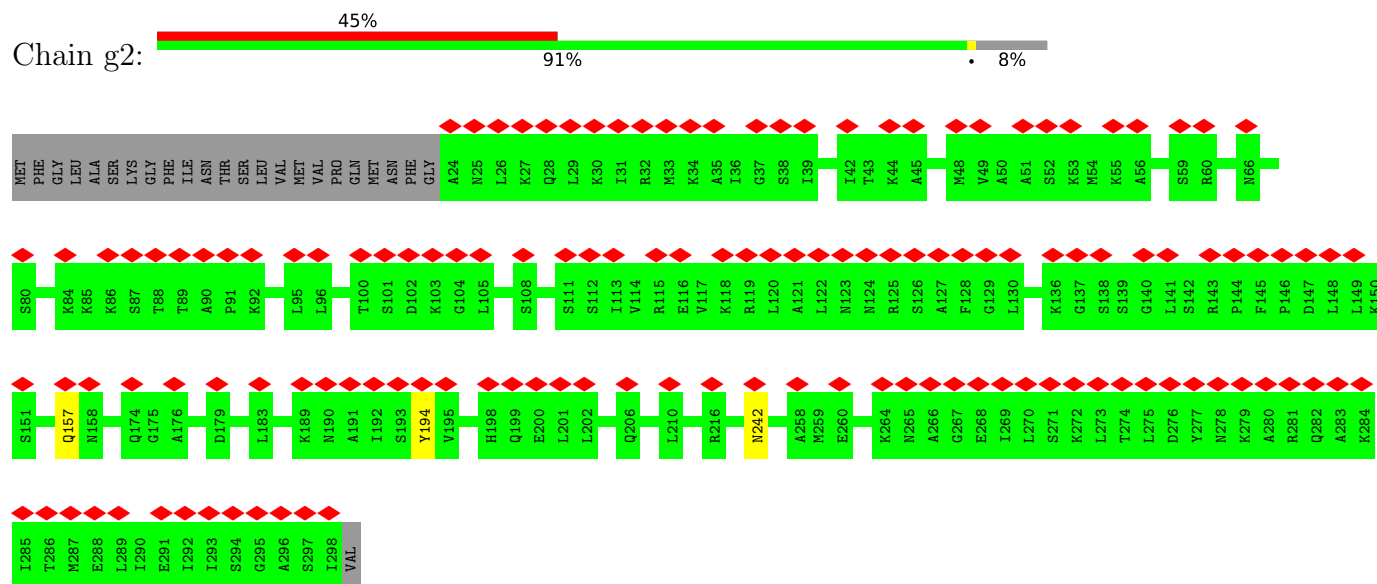


• Molecule 23: subunit gamma



- Molecule 23: subunit gamma

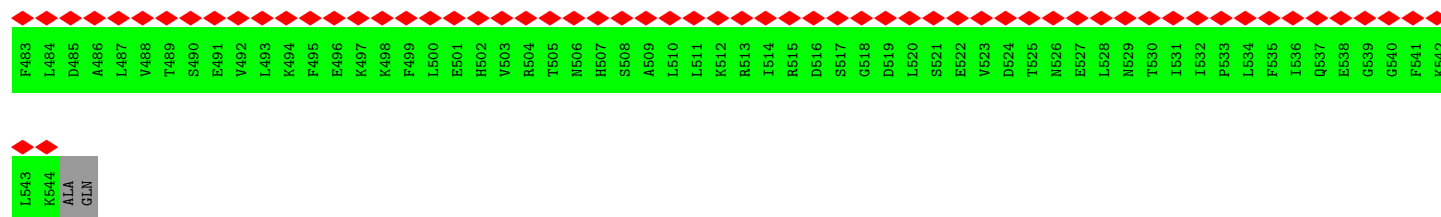
Chain g2:



- Molecule 24: subunit alpha

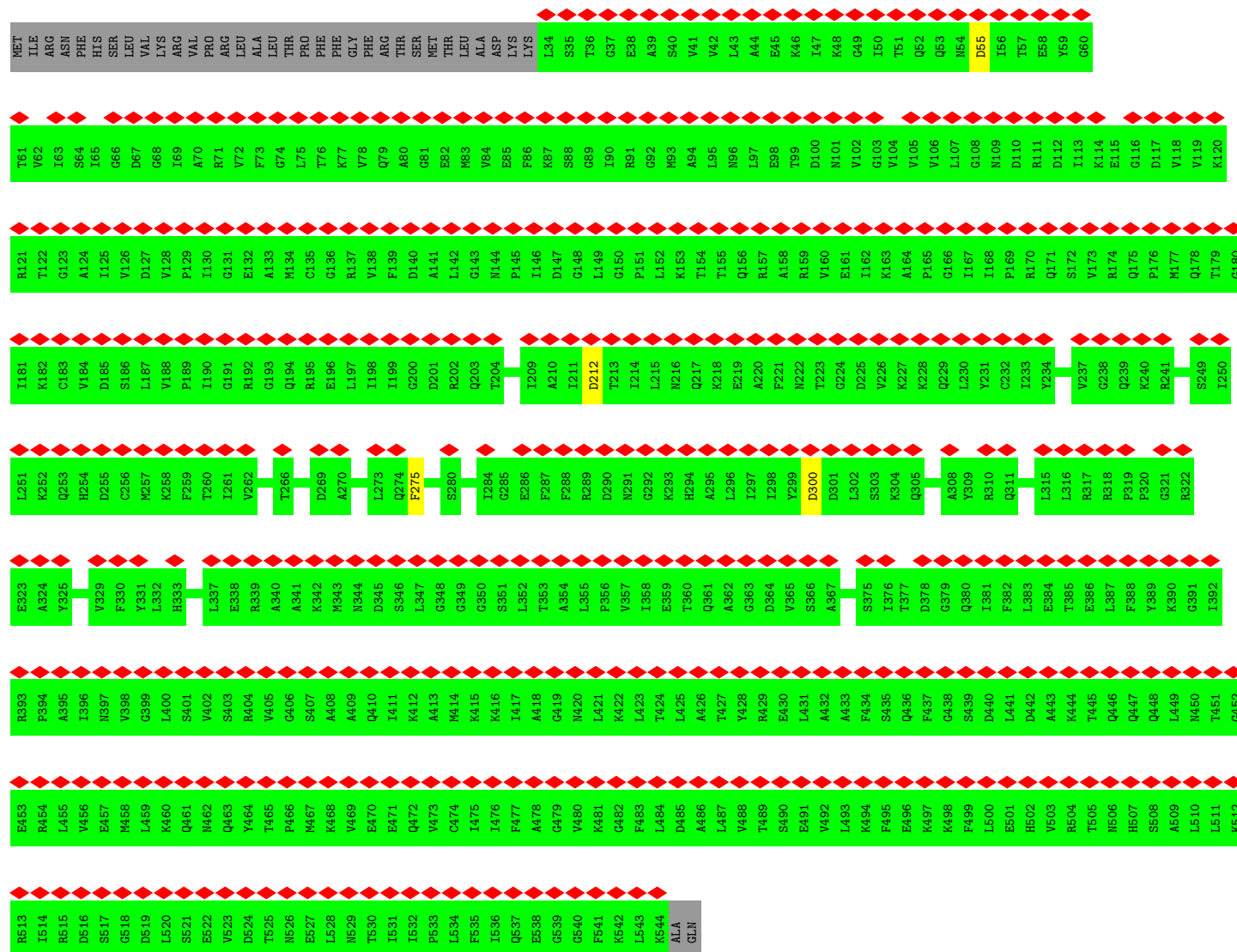
Chain C1:





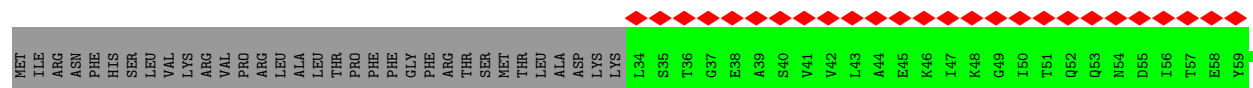
• Molecule 24: subunit alpha

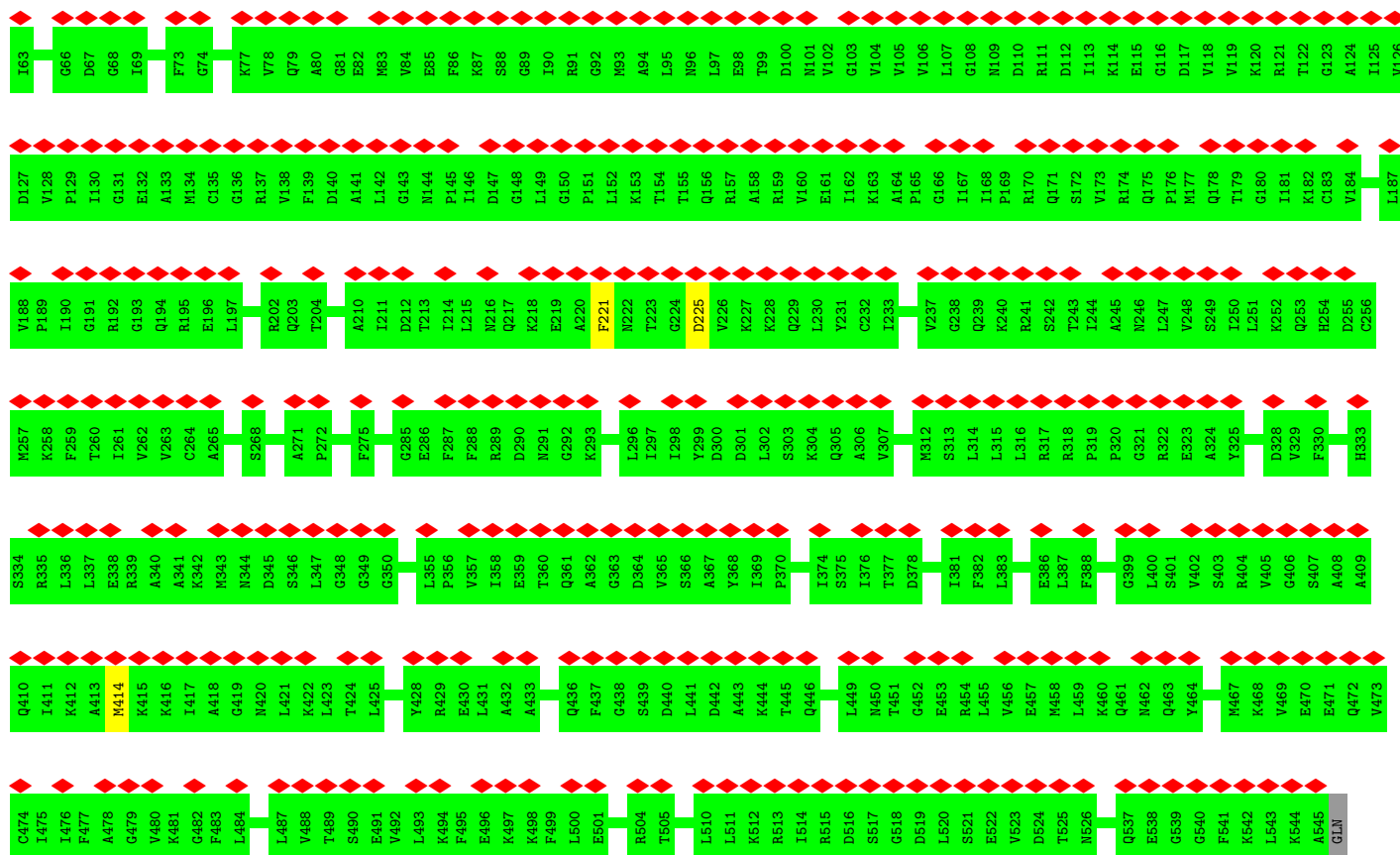
Chain B1: 84% 93% 6%



• Molecule 24: subunit alpha

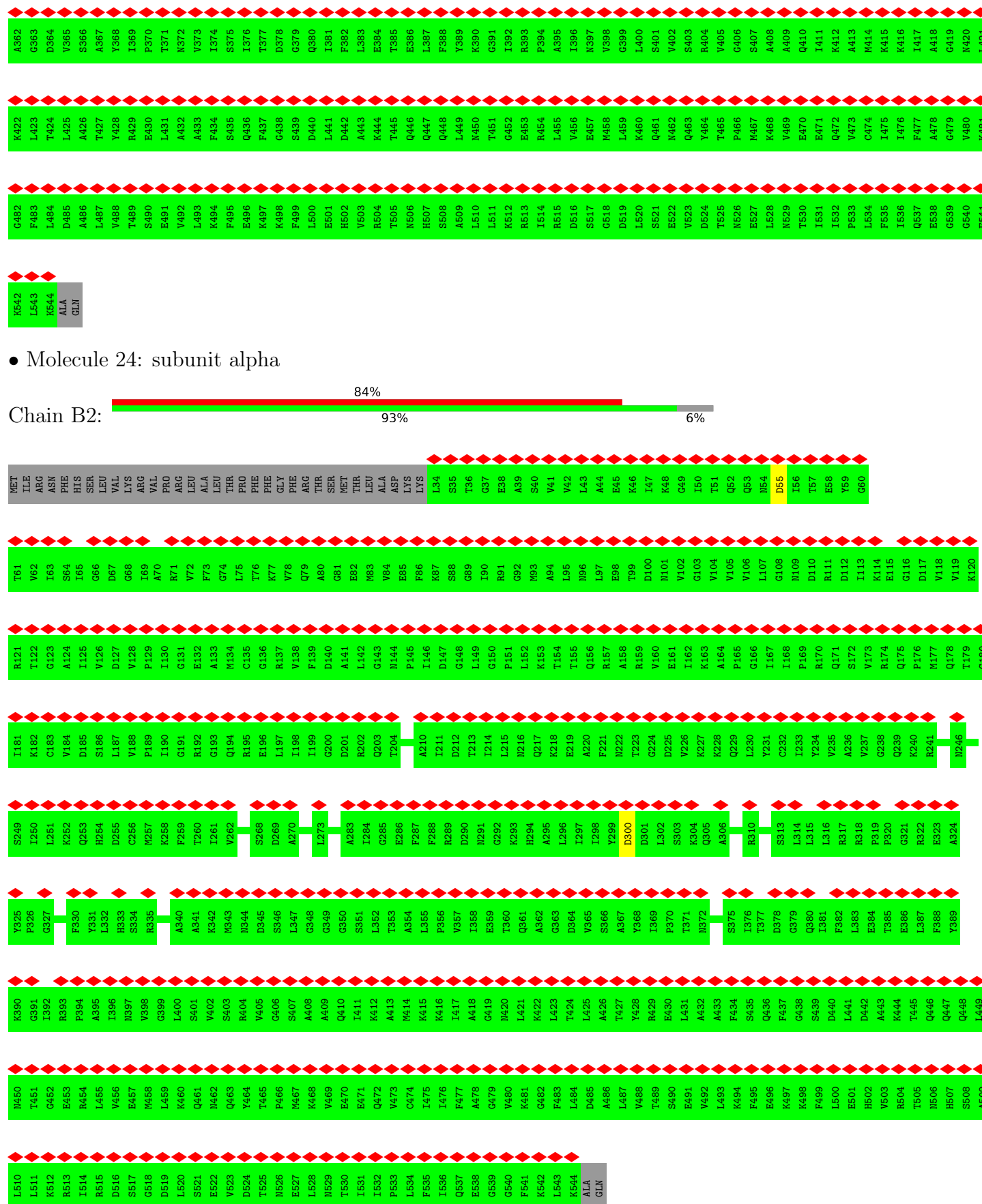
Chain A1: 69% 93% 6%





• Molecule 24: subunit alpha



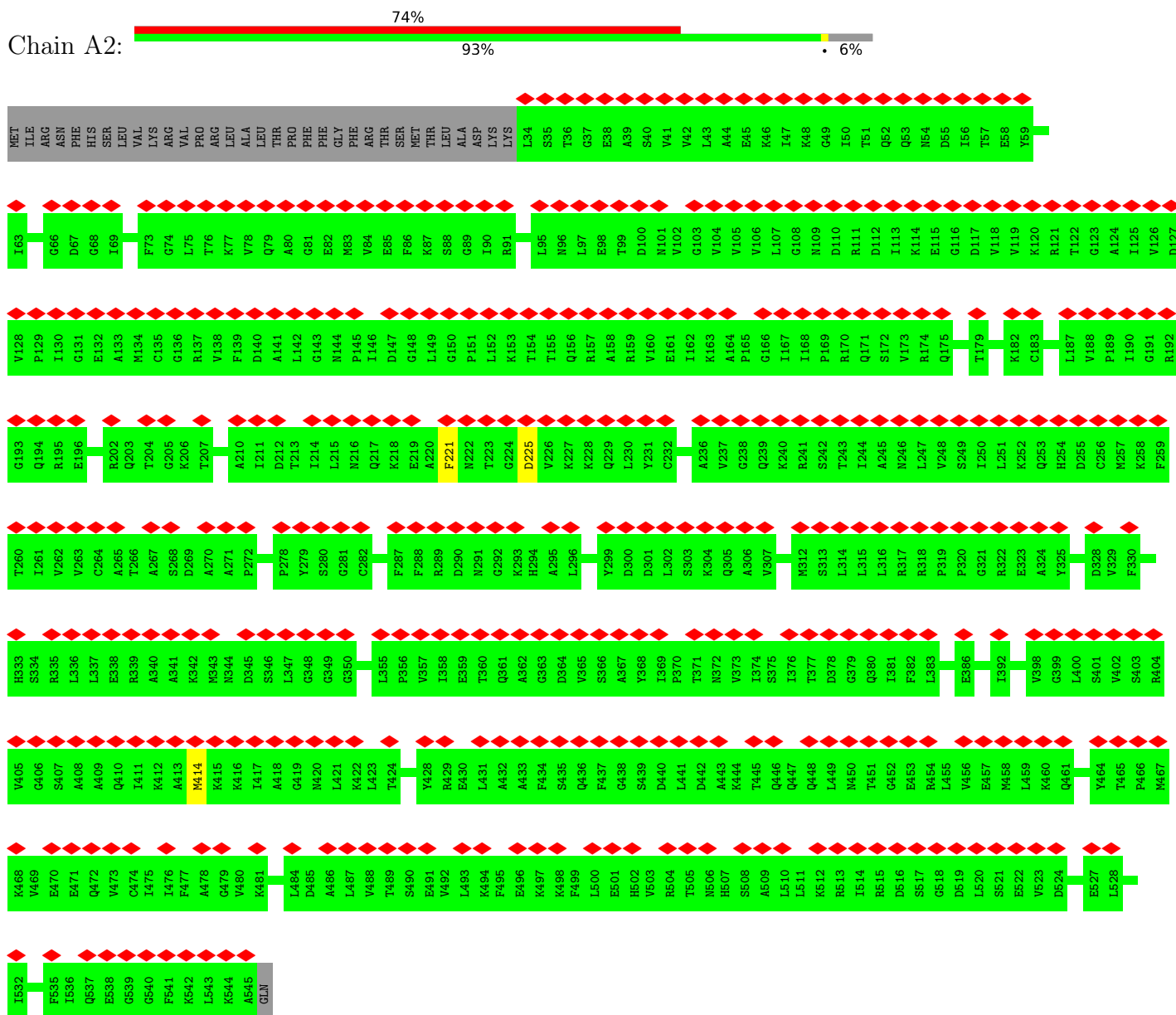


• Molecule 24: subunit alpha



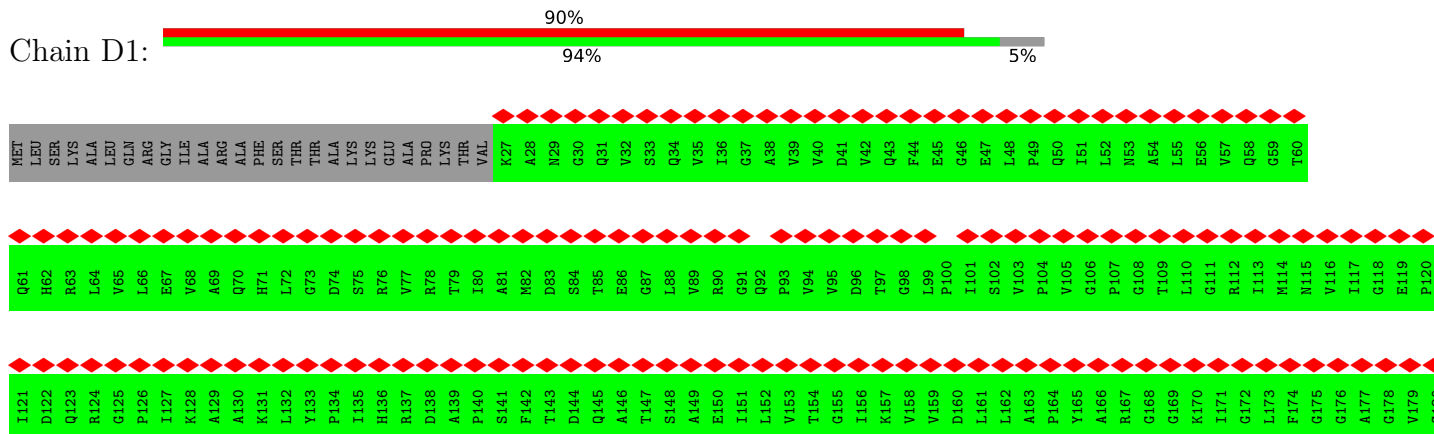
- Molecule 24: subunit alpha

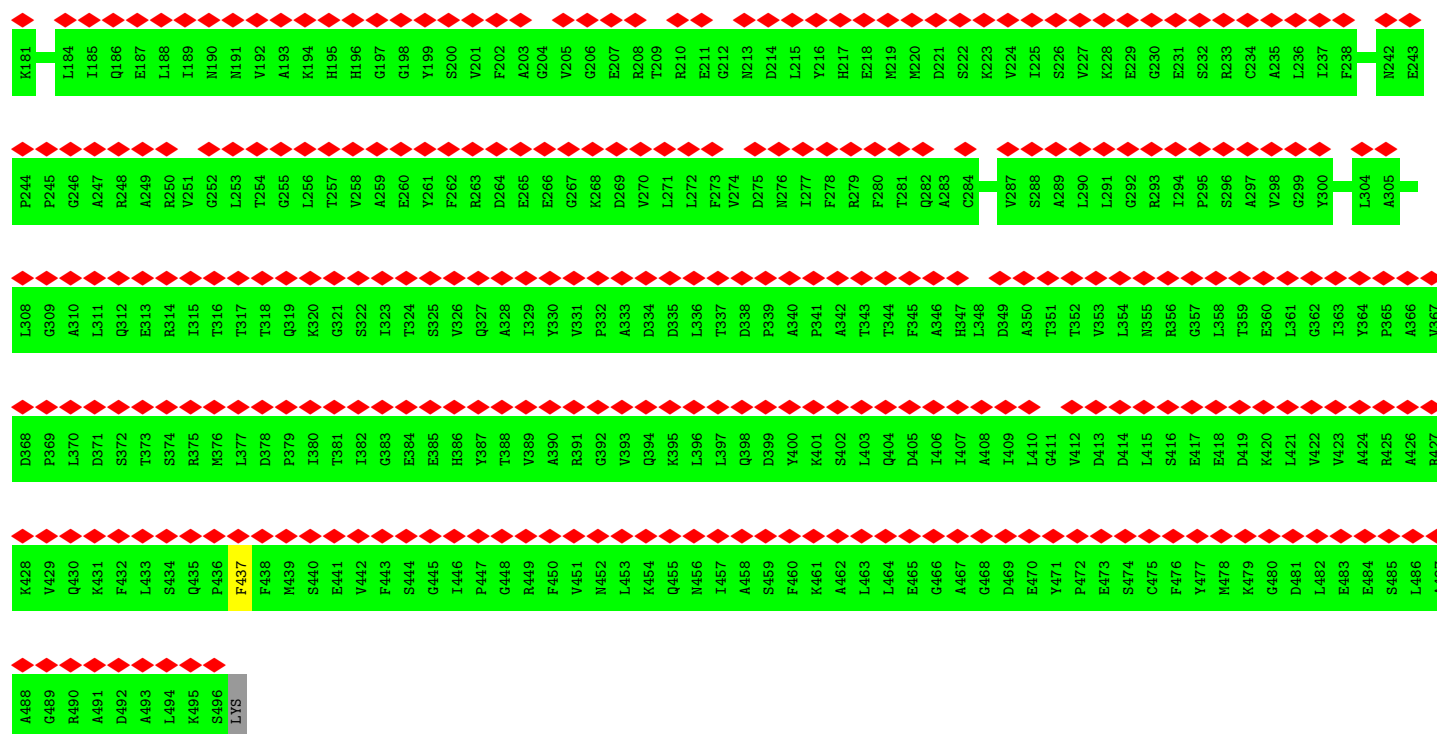
Chain A2:



- Molecule 25: subunit beta

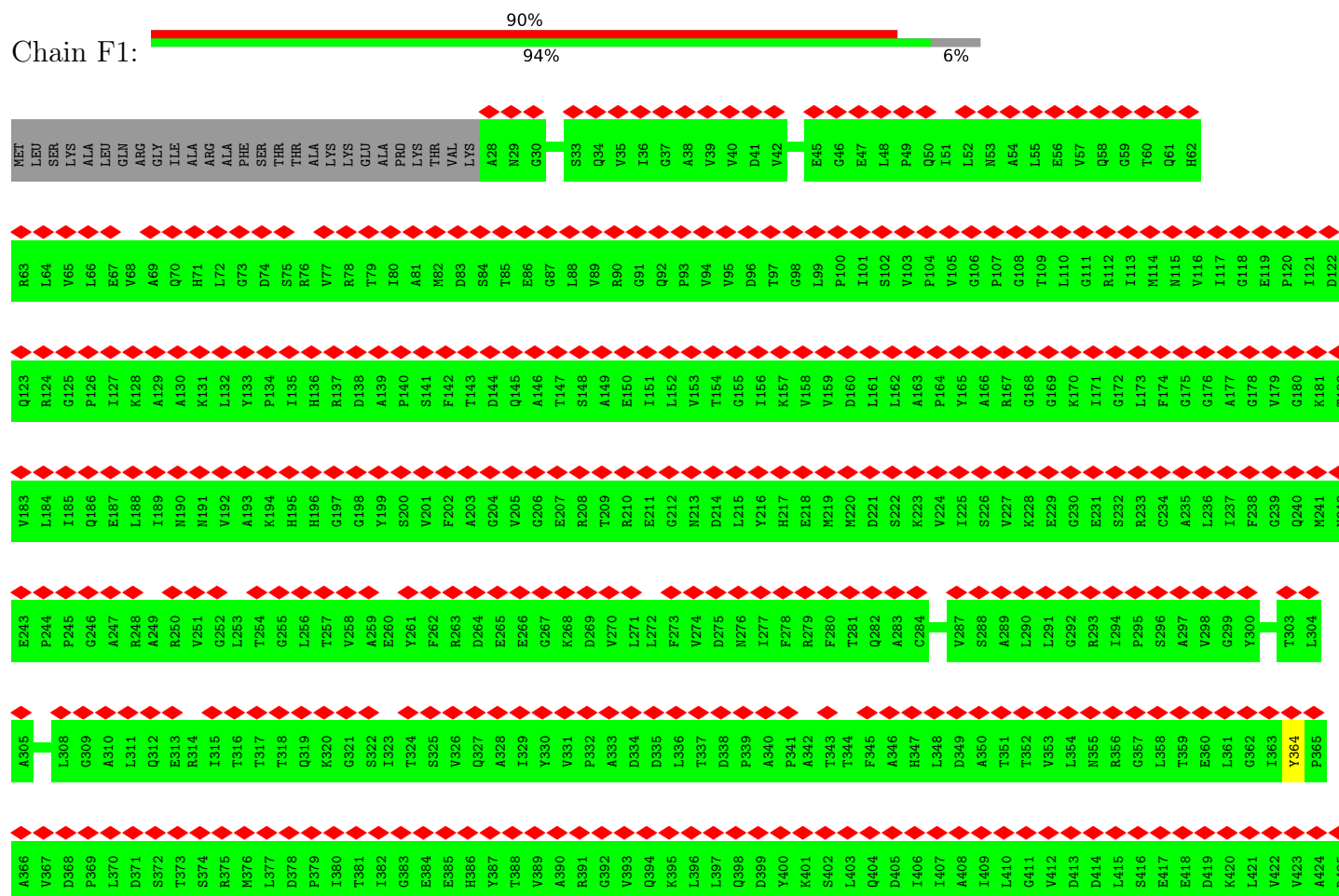
Chain D1:



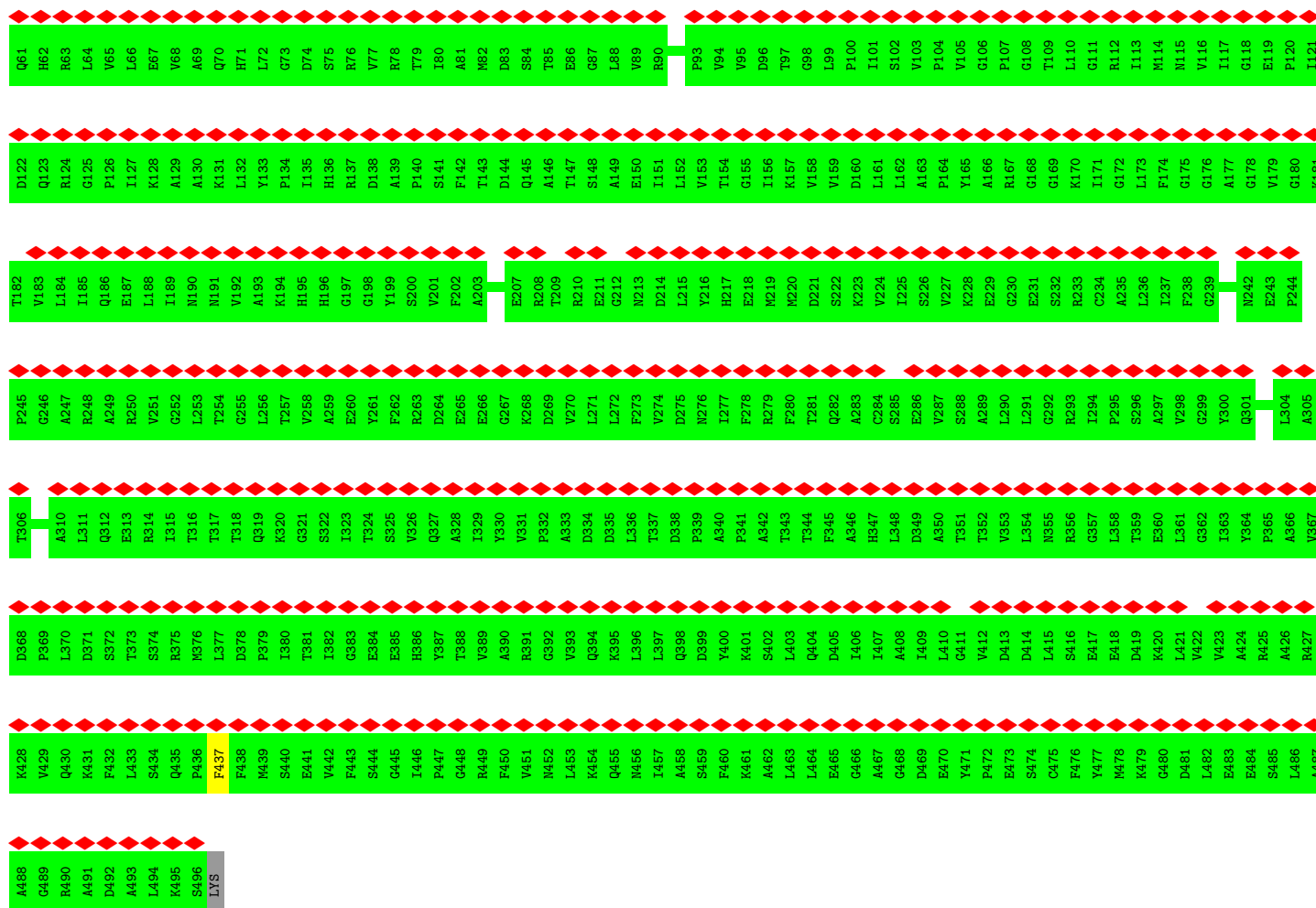


● Molecule 25: subunit beta

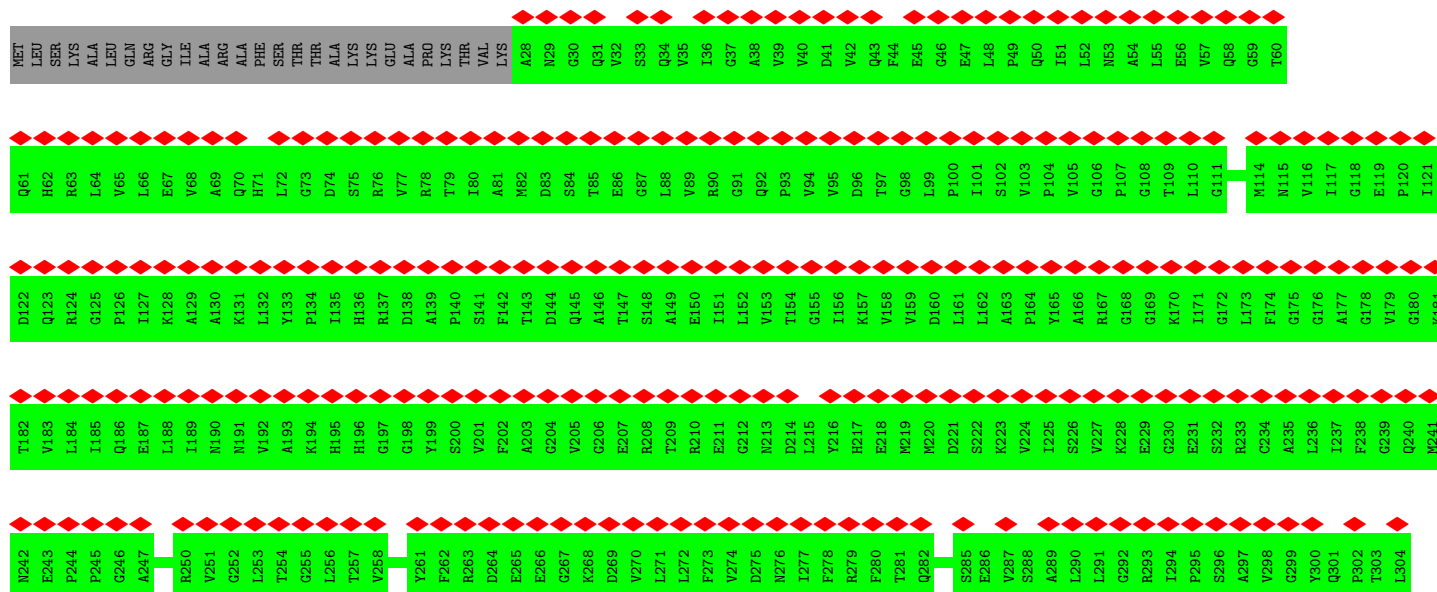
Chain F1:

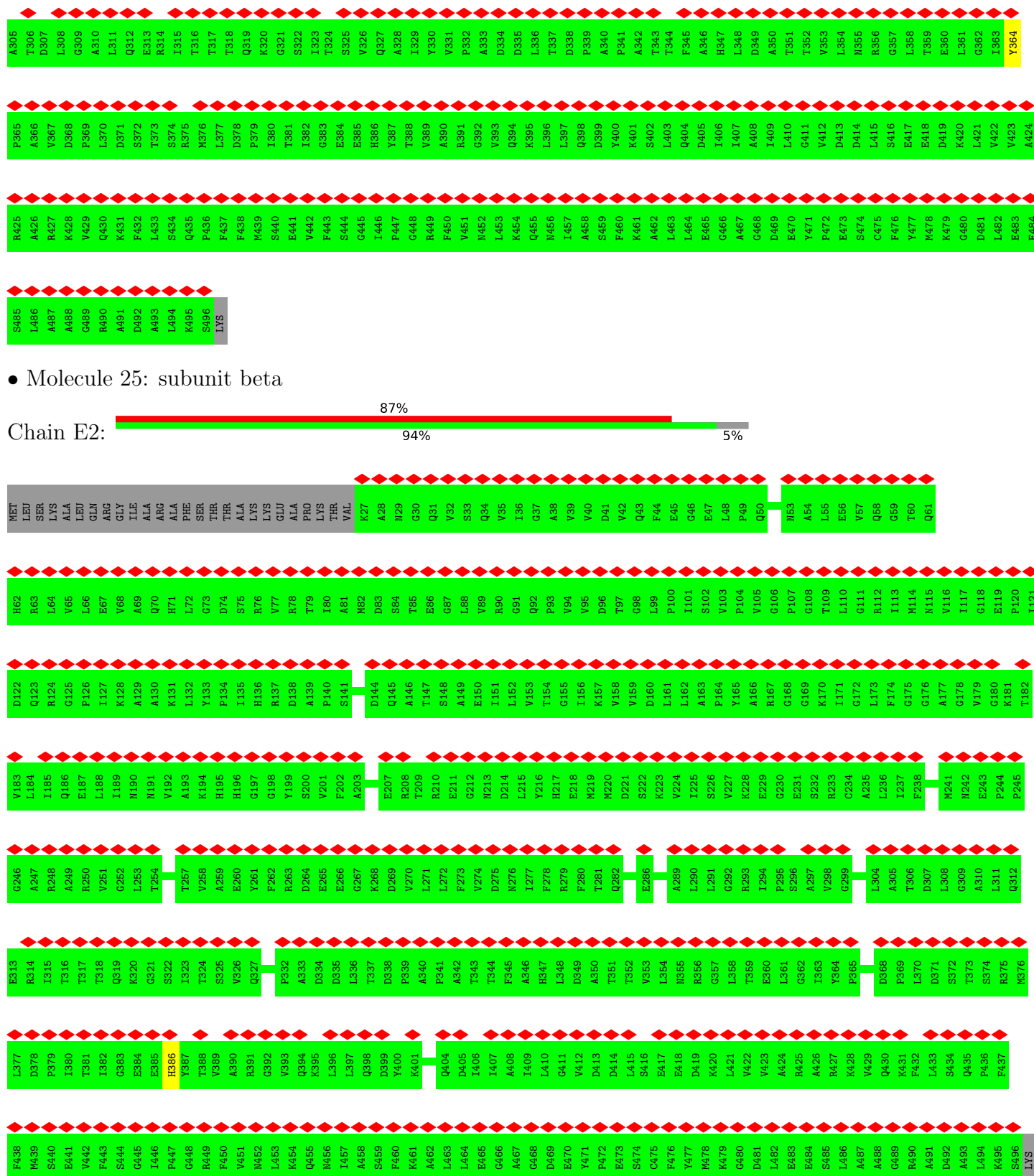


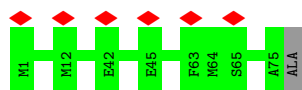




• Molecule 25: subunit beta



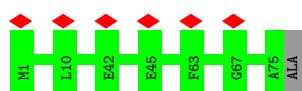




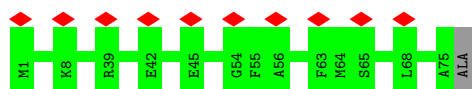
- Molecule 26: subunit c



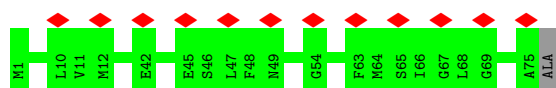
- Molecule 26: subunit c



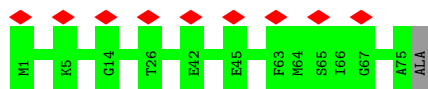
- Molecule 26: subunit c



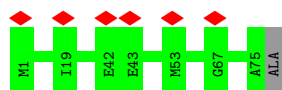
- Molecule 26: subunit c



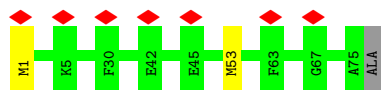
- Molecule 26: subunit c



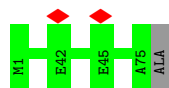
- Molecule 26: subunit c



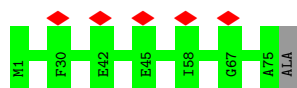
- Molecule 26: subunit c



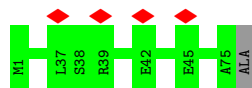
- Molecule 26: subunit c



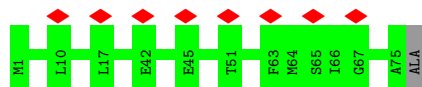
- Molecule 26: subunit c



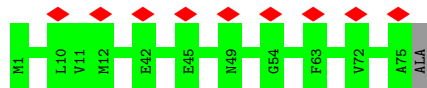
- Molecule 26: subunit c



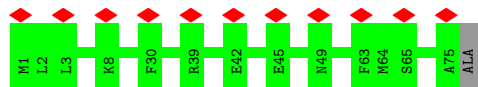
- Molecule 26: subunit c



- Molecule 26: subunit c

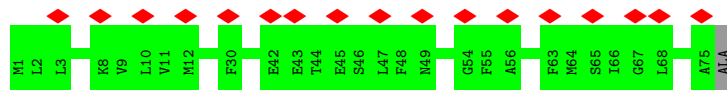


- Molecule 26: subunit c



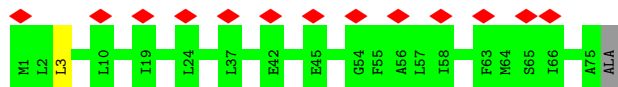
## ● Molecule 26: subunit c

Chain L2:  22% 99%



## ● Molecule 26: subunit c

Chain K2:  17% 97%



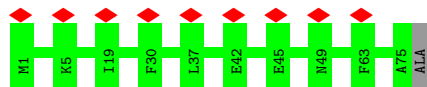
## ● Molecule 26: subunit c

Chain J2:  12% 99%



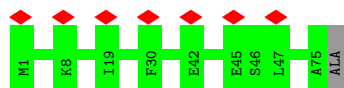
## ● Molecule 26: subunit c

Chain I2:  12% 99%



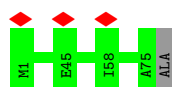
## ● Molecule 26: subunit c

Chain H2:  9% 99%




## ● Molecule 26: subunit c

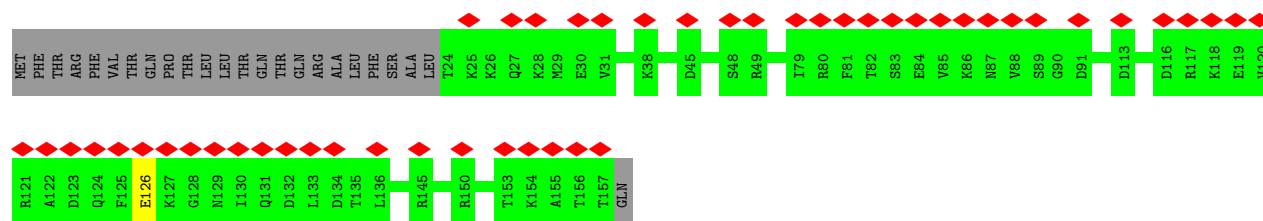
Chain Q2:  1% 99%



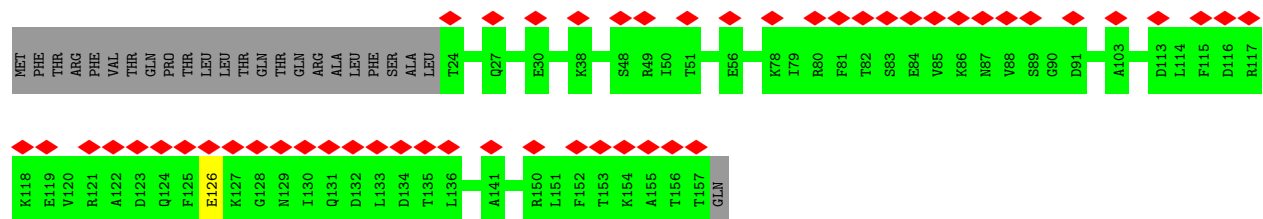
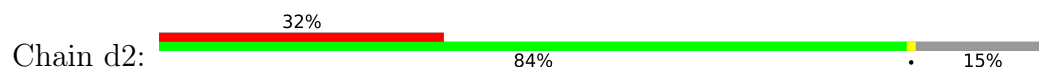
## ● Molecule 27: subunit delta

Chain d1:  31% 84% 15%

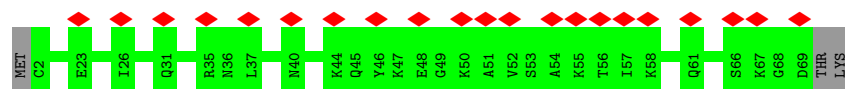




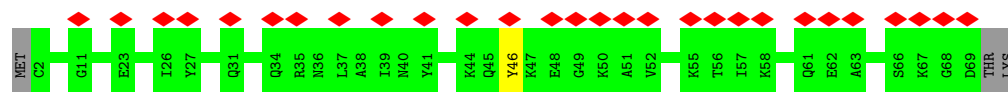
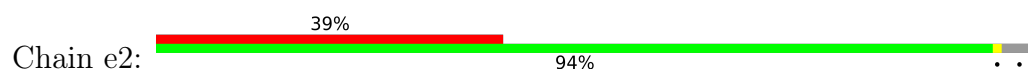
• Molecule 27: subunit delta



• Molecule 28: subunit epsilon



• Molecule 28: subunit epsilon



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	61157	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 ( $e^-/\text{\AA}^2$ )	30.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.155	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	498.0, 498.0, 498.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: UQ8, ADP, NAD, PO4, PEE, MG, PC1, CDL, ATP

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	0.36	0/3752	0.39	0/5109
1	a	0.36	0/3752	0.39	0/5109
2	B	0.30	0/2940	0.37	0/3969
2	b	0.30	0/2940	0.36	0/3969
3	D	0.30	0/1715	0.38	0/2321
3	d	0.30	0/1715	0.38	0/2321
4	F	0.36	0/1733	0.41	0/2327
4	f	0.35	0/1733	0.41	0/2327
5	I	0.35	0/1771	0.40	0/2394
5	i	0.35	0/1771	0.40	0/2394
6	K	0.31	0/1508	0.39	0/2024
6	k	0.31	0/1508	0.39	0/2024
7	C	0.35	0/866	0.40	0/1176
7	c	0.35	0/866	0.40	0/1176
8	G	0.36	0/2302	0.42	0/3115
8	g	0.36	0/2302	0.41	0/3115
9	H	0.33	0/2006	0.40	0/2704
9	h	0.33	0/2006	0.40	0/2704
10	J	0.34	0/2256	0.41	0/3069
10	j	0.34	0/2256	0.41	0/3069
11	L	0.35	0/2140	0.40	0/2903
11	l	0.35	0/2140	0.40	0/2903
12	M	0.36	0/1912	0.38	0/2598
12	m	0.35	0/1912	0.38	0/2598
13	N	0.37	0/1030	0.41	0/1393
13	n	0.37	0/1030	0.42	0/1393
14	O	0.31	0/821	0.40	0/1104
14	o	0.30	0/821	0.41	0/1104
15	P	0.29	0/1249	0.38	0/1695
15	p	0.29	0/1249	0.38	0/1695
16	Q	0.31	0/888	0.40	0/1200
16	q	0.32	0/888	0.40	0/1200

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	R	0.35	0/1185	0.39	0/1594
17	r	0.35	0/1225	0.39	0/1649
18	S	0.32	0/1044	0.42	0/1414
18	s	0.33	0/1037	0.42	0/1404
19	E	0.28	0/3492	0.41	0/4720
19	e	0.28	0/3492	0.40	0/4720
20	i1	0.23	0/593	0.34	0/795
20	i2	0.28	0/563	0.36	0/753
21	t	0.33	0/3103	0.40	0/4200
22	G1	0.24	0/1507	0.37	0/2027
22	G2	0.24	0/1507	0.37	0/2027
23	g1	0.24	0/2156	0.38	0/2900
23	g2	0.24	0/2156	0.38	0/2900
24	A1	0.24	0/3961	0.40	0/5346
24	A2	0.24	0/3961	0.40	0/5346
24	B1	0.24	0/3956	0.40	0/5339
24	B2	0.24	0/3956	0.40	0/5339
24	C1	0.24	0/3974	0.40	0/5361
24	C2	0.24	0/3974	0.40	0/5361
25	D1	0.24	0/3613	0.39	0/4900
25	D2	0.24	0/3613	0.39	0/4900
25	E1	0.24	0/3613	0.40	0/4900
25	E2	0.24	0/3613	0.40	0/4900
25	F1	0.24	0/3604	0.40	0/4889
25	F2	0.24	0/3604	0.40	0/4889
26	H1	0.28	0/572	0.36	0/771
26	H2	0.28	0/572	0.37	0/771
26	I1	0.27	0/572	0.36	0/771
26	I2	0.28	0/572	0.41	0/771
26	J1	0.27	0/572	0.36	0/771
26	J2	0.27	0/572	0.36	0/771
26	K1	0.27	0/572	0.36	0/771
26	K2	0.27	0/572	0.36	0/771
26	L1	0.27	0/572	0.36	0/771
26	L2	0.27	0/572	0.35	0/771
26	M1	0.27	0/572	0.35	0/771
26	M2	0.27	0/572	0.36	0/771
26	N1	0.27	0/572	0.35	0/771
26	N2	0.26	0/572	0.35	0/771
26	O1	0.27	0/572	0.35	0/771
26	O2	0.27	0/572	0.35	0/771
26	P1	0.27	0/572	0.35	0/771
26	P2	0.27	0/572	0.35	0/771

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
26	Q1	0.27	0/572	0.35	0/771
26	Q2	0.27	0/572	0.35	0/771
27	d1	0.25	0/1081	0.45	0/1459
27	d2	0.25	0/1081	0.45	0/1459
28	e1	0.25	0/547	0.41	0/735
28	e2	0.25	0/547	0.42	0/735
All	All	0.29	0/140976	0.39	0/190583

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
25	F1	0	1
25	F2	0	1
28	e2	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	F1	364	TYR	Peptide
25	F2	364	TYR	Peptide
28	e2	46	TYR	Peptide

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/446 (97%)	426 (99%)	5 (1%)	0	100	100
1	a	431/446 (97%)	422 (98%)	9 (2%)	0	100	100
2	B	352/381 (92%)	341 (97%)	11 (3%)	0	100	100
2	b	352/381 (92%)	339 (96%)	13 (4%)	0	100	100
3	D	204/234 (87%)	199 (98%)	5 (2%)	0	100	100
3	d	204/234 (87%)	198 (97%)	6 (3%)	0	100	100
4	F	198/204 (97%)	197 (100%)	1 (0%)	0	100	100
4	f	198/204 (97%)	196 (99%)	2 (1%)	0	100	100
5	I	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
5	i	207/209 (99%)	202 (98%)	5 (2%)	0	100	100
6	K	177/179 (99%)	166 (94%)	11 (6%)	0	100	100
6	k	177/179 (99%)	169 (96%)	8 (4%)	0	100	100
7	C	94/100 (94%)	90 (96%)	4 (4%)	0	100	100
7	c	94/100 (94%)	90 (96%)	4 (4%)	0	100	100
8	G	254/286 (89%)	246 (97%)	8 (3%)	0	100	100
8	g	254/286 (89%)	244 (96%)	10 (4%)	0	100	100
9	H	229/268 (85%)	225 (98%)	4 (2%)	0	100	100
9	h	229/268 (85%)	226 (99%)	3 (1%)	0	100	100
10	J	267/273 (98%)	261 (98%)	6 (2%)	0	100	100
10	j	267/273 (98%)	262 (98%)	5 (2%)	0	100	100
11	L	244/247 (99%)	239 (98%)	5 (2%)	0	100	100
11	l	244/247 (99%)	241 (99%)	3 (1%)	0	100	100
12	M	219/221 (99%)	219 (100%)	0	0	100	100
12	m	219/221 (99%)	217 (99%)	2 (1%)	0	100	100
13	N	117/179 (65%)	114 (97%)	3 (3%)	0	100	100
13	n	117/179 (65%)	115 (98%)	2 (2%)	0	100	100
14	O	97/154 (63%)	95 (98%)	2 (2%)	0	100	100
14	o	97/154 (63%)	96 (99%)	1 (1%)	0	100	100
15	P	148/152 (97%)	140 (95%)	8 (5%)	0	100	100
15	p	148/152 (97%)	138 (93%)	10 (7%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Q	106/152 (70%)	105 (99%)	1 (1%)	0	100	100
16	q	106/152 (70%)	105 (99%)	1 (1%)	0	100	100
17	R	138/149 (93%)	136 (99%)	2 (1%)	0	100	100
17	r	143/149 (96%)	142 (99%)	1 (1%)	0	100	100
18	S	123/145 (85%)	119 (97%)	4 (3%)	0	100	100
18	s	122/145 (84%)	122 (100%)	0	0	100	100
19	E	415/480 (86%)	406 (98%)	9 (2%)	0	100	100
19	e	415/480 (86%)	405 (98%)	10 (2%)	0	100	100
20	i1	64/108 (59%)	64 (100%)	0	0	100	100
20	i2	60/108 (56%)	60 (100%)	0	0	100	100
21	t	363/460 (79%)	360 (99%)	3 (1%)	0	100	100
22	G1	186/219 (85%)	176 (95%)	10 (5%)	0	100	100
22	G2	186/219 (85%)	176 (95%)	10 (5%)	0	100	100
23	g1	273/299 (91%)	265 (97%)	8 (3%)	0	100	100
23	g2	273/299 (91%)	265 (97%)	8 (3%)	0	100	100
24	A1	510/546 (93%)	503 (99%)	7 (1%)	0	100	100
24	A2	510/546 (93%)	503 (99%)	7 (1%)	0	100	100
24	B1	509/546 (93%)	498 (98%)	10 (2%)	1 (0%)	44	68
24	B2	509/546 (93%)	500 (98%)	8 (2%)	1 (0%)	44	68
24	C1	511/546 (94%)	509 (100%)	2 (0%)	0	100	100
24	C2	511/546 (94%)	507 (99%)	4 (1%)	0	100	100
25	D1	468/497 (94%)	461 (98%)	7 (2%)	0	100	100
25	D2	468/497 (94%)	463 (99%)	5 (1%)	0	100	100
25	E1	468/497 (94%)	459 (98%)	9 (2%)	0	100	100
25	E2	468/497 (94%)	459 (98%)	9 (2%)	0	100	100
25	F1	467/497 (94%)	454 (97%)	13 (3%)	0	100	100
25	F2	467/497 (94%)	455 (97%)	12 (3%)	0	100	100
26	H1	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	H2	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	I1	73/76 (96%)	73 (100%)	0	0	100	100
26	I2	73/76 (96%)	71 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	J1	73/76 (96%)	73 (100%)	0	0	100	100
26	J2	73/76 (96%)	73 (100%)	0	0	100	100
26	K1	73/76 (96%)	73 (100%)	0	0	100	100
26	K2	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	L1	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	L2	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	M1	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	M2	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	N1	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	N2	73/76 (96%)	73 (100%)	0	0	100	100
26	O1	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	O2	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	P1	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	P2	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	Q1	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	Q2	73/76 (96%)	70 (96%)	3 (4%)	0	100	100
27	d1	132/158 (84%)	126 (96%)	6 (4%)	0	100	100
27	d2	132/158 (84%)	127 (96%)	5 (4%)	0	100	100
28	e1	66/71 (93%)	60 (91%)	6 (9%)	0	100	100
28	e2	66/71 (93%)	60 (91%)	6 (9%)	0	100	100
All	All	17171/18866 (91%)	16800 (98%)	369 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	B1	55	ASP
24	B2	55	ASP

### 5.3.2 Protein sidechains ⓘ

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

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



analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	397/409 (97%)	395 (100%)	2 (0%)	86	95
1	a	397/409 (97%)	395 (100%)	2 (0%)	86	95
2	B	306/331 (92%)	306 (100%)	0	100	100
2	b	306/331 (92%)	306 (100%)	0	100	100
3	D	183/206 (89%)	183 (100%)	0	100	100
3	d	183/206 (89%)	183 (100%)	0	100	100
4	F	175/178 (98%)	174 (99%)	1 (1%)	84	94
4	f	175/178 (98%)	174 (99%)	1 (1%)	84	94
5	I	182/182 (100%)	180 (99%)	2 (1%)	70	87
5	i	182/182 (100%)	181 (100%)	1 (0%)	86	95
6	K	152/152 (100%)	152 (100%)	0	100	100
6	k	152/152 (100%)	151 (99%)	1 (1%)	81	93
7	C	93/97 (96%)	92 (99%)	1 (1%)	70	87
7	c	93/97 (96%)	92 (99%)	1 (1%)	70	87
8	G	235/262 (90%)	234 (100%)	1 (0%)	89	96
8	g	235/262 (90%)	234 (100%)	1 (0%)	89	96
9	H	208/245 (85%)	207 (100%)	1 (0%)	86	95
9	h	208/245 (85%)	207 (100%)	1 (0%)	86	95
10	J	235/239 (98%)	234 (100%)	1 (0%)	89	96
10	j	235/239 (98%)	235 (100%)	0	100	100
11	L	219/220 (100%)	217 (99%)	2 (1%)	75	90
11	l	219/220 (100%)	218 (100%)	1 (0%)	86	95
12	M	202/202 (100%)	202 (100%)	0	100	100
12	m	202/202 (100%)	201 (100%)	1 (0%)	86	95
13	N	104/162 (64%)	104 (100%)	0	100	100
13	n	104/162 (64%)	103 (99%)	1 (1%)	73	89
14	O	89/142 (63%)	89 (100%)	0	100	100
14	o	89/142 (63%)	89 (100%)	0	100	100
15	P	131/133 (98%)	131 (100%)	0	100	100
15	p	131/133 (98%)	131 (100%)	0	100	100
16	Q	97/135 (72%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	q	97/135 (72%)	97 (100%)	0	100	100
17	R	120/129 (93%)	119 (99%)	1 (1%)	79	91
17	r	125/129 (97%)	124 (99%)	1 (1%)	79	91
18	S	112/131 (86%)	112 (100%)	0	100	100
18	s	111/131 (85%)	109 (98%)	2 (2%)	54	80
19	E	359/414 (87%)	357 (99%)	2 (1%)	84	94
19	e	359/414 (87%)	358 (100%)	1 (0%)	91	97
20	i1	64/101 (63%)	64 (100%)	0	100	100
20	i2	61/101 (60%)	59 (97%)	2 (3%)	33	62
21	t	325/414 (78%)	322 (99%)	3 (1%)	75	90
22	G1	166/195 (85%)	166 (100%)	0	100	100
22	G2	166/195 (85%)	166 (100%)	0	100	100
23	g1	234/254 (92%)	230 (98%)	4 (2%)	56	81
23	g2	234/254 (92%)	231 (99%)	3 (1%)	65	85
24	A1	422/453 (93%)	419 (99%)	3 (1%)	81	93
24	A2	422/453 (93%)	419 (99%)	3 (1%)	81	93
24	B1	422/453 (93%)	419 (99%)	3 (1%)	81	93
24	B2	422/453 (93%)	421 (100%)	1 (0%)	92	98
24	C1	424/453 (94%)	423 (100%)	1 (0%)	92	98
24	C2	424/453 (94%)	423 (100%)	1 (0%)	92	98
25	D1	381/402 (95%)	380 (100%)	1 (0%)	91	97
25	D2	381/402 (95%)	380 (100%)	1 (0%)	91	97
25	E1	381/402 (95%)	380 (100%)	1 (0%)	91	97
25	E2	381/402 (95%)	380 (100%)	1 (0%)	91	97
25	F1	380/402 (94%)	380 (100%)	0	100	100
25	F2	380/402 (94%)	380 (100%)	0	100	100
26	H1	59/59 (100%)	59 (100%)	0	100	100
26	H2	59/59 (100%)	59 (100%)	0	100	100
26	I1	59/59 (100%)	57 (97%)	2 (3%)	32	61
26	I2	59/59 (100%)	59 (100%)	0	100	100
26	J1	59/59 (100%)	59 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	J2	59/59 (100%)	59 (100%)	0	100	100
26	K1	59/59 (100%)	59 (100%)	0	100	100
26	K2	59/59 (100%)	58 (98%)	1 (2%)	56	81
26	L1	59/59 (100%)	59 (100%)	0	100	100
26	L2	59/59 (100%)	59 (100%)	0	100	100
26	M1	59/59 (100%)	59 (100%)	0	100	100
26	M2	59/59 (100%)	59 (100%)	0	100	100
26	N1	59/59 (100%)	59 (100%)	0	100	100
26	N2	59/59 (100%)	59 (100%)	0	100	100
26	O1	59/59 (100%)	59 (100%)	0	100	100
26	O2	59/59 (100%)	59 (100%)	0	100	100
26	P1	59/59 (100%)	59 (100%)	0	100	100
26	P2	59/59 (100%)	59 (100%)	0	100	100
26	Q1	59/59 (100%)	59 (100%)	0	100	100
26	Q2	59/59 (100%)	59 (100%)	0	100	100
27	d1	117/139 (84%)	116 (99%)	1 (1%)	75	90
27	d2	117/139 (84%)	116 (99%)	1 (1%)	75	90
28	e1	57/60 (95%)	57 (100%)	0	100	100
28	e2	57/60 (95%)	57 (100%)	0	100	100
All	All	14800/16160 (92%)	14738 (100%)	62 (0%)	88	96

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	247	TYR
1	a	364	LEU
4	f	37	THR
5	i	44	TYR
6	k	148	ASP
7	c	19	ARG
8	g	217	PHE
9	h	144	ASP
11	l	205	TRP
12	m	49	MET
13	n	87	HIS

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Mol	Chain	Res	Type
17	r	28	GLN
18	s	44	VAL
18	s	67	LEU
19	e	391	LEU
1	A	247	TYR
1	A	364	LEU
4	F	31	TYR
5	I	44	TYR
5	I	90	HIS
7	C	19	ARG
8	G	217	PHE
9	H	144	ASP
10	J	82	ARG
11	L	118	ARG
11	L	205	TRP
17	R	19	LEU
19	E	350	TRP
19	E	391	LEU
20	i2	79	LEU
20	i2	82	GLU
21	t	135	GLU
21	t	140	THR
21	t	158	ARG
23	g1	157	GLN
23	g1	194	TYR
23	g1	242	ASN
23	g1	272	LYS
24	C1	247	LEU
25	D1	437	PHE
24	B1	212	ASP
24	B1	275	PHE
24	B1	300	ASP
24	A1	221	PHE
24	A1	225	ASP
24	A1	414	MET
25	E1	386	HIS
26	I1	1	MET
26	I1	53	MET
27	d1	126	GLU
23	g2	157	GLN
23	g2	194	TYR
23	g2	242	ASN

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Mol	Chain	Res	Type
24	C2	247	LEU
25	D2	437	PHE
24	B2	300	ASP
24	A2	221	PHE
24	A2	225	ASP
24	A2	414	MET
25	E2	386	HIS
26	K2	3	LEU
27	d2	126	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	124	HIS
10	j	130	GLN
11	l	50	GLN
11	l	217	HIS
19	e	165	ASN
19	e	361	ASN
1	A	391	HIS
2	B	255	ASN
3	D	29	GLN
5	I	20	ASN
5	I	201	ASN
5	I	209	GLN
9	H	101	GLN
10	J	130	GLN
12	M	3	ASN
15	P	150	GLN
16	Q	69	GLN
19	E	165	ASN
19	E	361	ASN
22	G1	161	GLN
22	G1	165	GLN
23	g1	242	ASN
25	D1	145	GLN
24	A1	171	GLN
25	E1	92	GLN
26	P1	40	ASN
26	K1	50	ASN
27	d1	62	GLN
27	d1	63	ASN

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Mol	Chain	Res	Type
22	G2	161	GLN
22	G2	165	GLN
24	A2	171	GLN
25	E2	92	GLN
27	d2	63	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 70 ligands modelled in this entry, 12 are monoatomic - leaving 58 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	$\# Z  > 2$
29	CDL	i	301	-	99,99,99	0.88	8 (8%)	105,111,111	1.07	4 (3%)
30	PC1	d	301	3	53,53,53	0.93	4 (7%)	59,61,61	1.07	2 (3%)
37	ADP	D1	501	34	24,29,29	3.65	9 (37%)	29,45,45	3.77	7 (24%)
37	ADP	B2	603	34,24	24,29,29	3.71	9 (37%)	29,45,45	3.57	7 (24%)
33	ATP	C2	601	34	26,33,33	4.79	8 (30%)	31,52,52	2.43	7 (22%)
33	ATP	B1	601	25,34,24	26,33,33	4.80	9 (34%)	31,52,52	2.45	8 (25%)
29	CDL	b	401	2,4	99,99,99	0.87	8 (8%)	105,111,111	1.11	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	PEE	A	501	-	47,47,50	1.18	6 (12%)	50,52,55	1.16	2 (4%)
33	ATP	B2	601	25,34,24	26,33,33	4.80	8 (30%)	31,52,52	2.45	8 (25%)
29	CDL	k	201	6	99,99,99	0.89	8 (8%)	105,111,111	1.02	4 (3%)
29	CDL	K	201	-	99,99,99	0.88	8 (8%)	105,111,111	1.03	4 (3%)
29	CDL	B	401	-	99,99,99	0.87	8 (8%)	105,111,111	0.99	4 (3%)
29	CDL	J	302	-	99,99,99	0.87	8 (8%)	105,111,111	1.00	4 (3%)
29	CDL	B	402	2	99,99,99	0.87	7 (7%)	105,111,111	1.13	5 (4%)
33	ATP	G	301	34	26,33,33	4.77	7 (26%)	31,52,52	2.44	7 (22%)
29	CDL	a	502	-	99,99,99	0.88	8 (8%)	105,111,111	1.09	6 (5%)
33	ATP	g	301	34	26,33,33	4.78	7 (26%)	31,52,52	2.42	7 (22%)
35	PEE	L	303	-	47,47,50	1.17	6 (12%)	50,52,55	1.16	3 (6%)
29	CDL	P	201	-	99,99,99	0.88	7 (7%)	105,111,111	1.03	5 (4%)
30	PC1	G	303	-	53,53,53	0.96	4 (7%)	59,61,61	0.98	2 (3%)
31	PO4	F	301	-	4,4,4	1.04	0	6,6,6	0.44	0
33	ATP	C1	601	34	26,33,33	4.79	8 (30%)	31,52,52	2.40	7 (22%)
29	CDL	f	303	-	99,99,99	0.88	8 (8%)	105,111,111	1.09	5 (4%)
29	CDL	l	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.05	4 (3%)
29	CDL	B	403	-	99,99,99	0.88	7 (7%)	105,111,111	1.05	4 (3%)
35	PEE	m	301	-	50,50,50	1.15	6 (12%)	53,55,55	1.08	4 (7%)
29	CDL	j	302	-	99,99,99	0.88	7 (7%)	105,111,111	1.01	4 (3%)
32	UQ8	I	303	-	53,53,53	1.79	7 (13%)	64,67,67	1.68	17 (26%)
29	CDL	a	501	-	99,99,99	0.89	7 (7%)	105,111,111	1.05	5 (4%)
36	NAD	E	900	-	42,48,48	3.82	19 (45%)	50,73,73	2.13	7 (14%)
30	PC1	G	304	8	53,53,53	0.95	4 (7%)	59,61,61	1.00	2 (3%)
30	PC1	g	304	8	53,53,53	0.96	4 (7%)	59,61,61	0.93	2 (3%)
29	CDL	r	201	-	99,99,99	0.87	8 (8%)	105,111,111	1.03	4 (3%)
29	CDL	f	302	-	99,99,99	0.87	7 (7%)	105,111,111	1.04	4 (3%)
29	CDL	k	202	-	99,99,99	0.88	7 (7%)	105,111,111	1.12	5 (4%)
29	CDL	B	404	2	99,99,99	0.88	8 (8%)	105,111,111	1.09	5 (4%)
29	CDL	l	301	-	99,99,99	0.88	6 (6%)	105,111,111	1.05	5 (4%)
29	CDL	K	202	-	99,99,99	0.88	7 (7%)	105,111,111	1.10	5 (4%)
31	PO4	f	301	-	4,4,4	1.04	0	6,6,6	0.44	0
29	CDL	L	302	-	99,99,99	0.88	7 (7%)	105,111,111	1.03	3 (2%)
29	CDL	J	301	-	99,99,99	0.89	6 (6%)	105,111,111	1.08	4 (3%)
29	CDL	j	301	-	99,99,99	0.88	7 (7%)	105,111,111	1.09	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	UQ8	i	302	-	53,53,53	1.79	7 (13%)	64,67,67	1.65	16 (25%)
29	CDL	I	301	5	99,99,99	0.87	7 (7%)	105,111,111	0.99	4 (3%)
29	CDL	p	201	-	99,99,99	0.88	8 (8%)	105,111,111	1.04	4 (3%)
33	ATP	A1	601	34	26,33,33	4.82	8 (30%)	31,52,52	2.41	7 (22%)
29	CDL	L	301	-	99,99,99	0.89	7 (7%)	105,111,111	1.01	4 (3%)
30	PC1	D	301	3	53,53,53	0.94	4 (7%)	59,61,61	1.10	2 (3%)
29	CDL	I	302	-	99,99,99	0.88	8 (8%)	105,111,111	1.04	4 (3%)
37	ADP	D2	501	34	24,29,29	3.68	9 (37%)	29,45,45	3.54	7 (24%)
30	PC1	g	303	-	53,53,53	0.96	4 (7%)	59,61,61	0.97	2 (3%)
35	PEE	J	303	-	50,50,50	1.15	6 (12%)	53,55,55	1.16	3 (5%)
37	ADP	B1	603	34,24	24,29,29	3.70	9 (37%)	29,45,45	3.58	7 (24%)
29	CDL	A	502	-	99,99,99	0.88	7 (7%)	105,111,111	1.08	4 (3%)
36	NAD	e	900	-	42,48,48	3.83	19 (45%)	50,73,73	2.14	7 (14%)
33	ATP	A2	601	34	26,33,33	4.83	8 (30%)	31,52,52	2.40	7 (22%)
29	CDL	f	304	-	99,99,99	0.89	7 (7%)	105,111,111	1.05	4 (3%)
29	CDL	F	302	-	99,99,99	0.88	8 (8%)	105,111,111	1.07	4 (3%)

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
29	CDL	i	301	-	-	38/110/110/110	-
30	PC1	d	301	3	-	23/57/57/57	-
37	ADP	D1	501	34	-	2/12/32/32	0/3/3/3
37	ADP	B2	603	34,24	-	2/12/32/32	0/3/3/3
33	ATP	C2	601	34	-	4/18/38/38	0/3/3/3
33	ATP	B1	601	25,34,24	-	2/18/38/38	0/3/3/3
29	CDL	b	401	2,4	-	44/110/110/110	-
35	PEE	A	501	-	-	21/51/51/54	-
33	ATP	B2	601	25,34,24	-	2/18/38/38	0/3/3/3
29	CDL	k	201	6	-	37/110/110/110	-
29	CDL	K	201	-	-	27/110/110/110	-
29	CDL	B	401	-	-	43/110/110/110	-
29	CDL	J	302	-	-	41/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CDL	B	402	2	-	40/110/110/110	-
33	ATP	G	301	34	-	0/18/38/38	0/3/3/3
29	CDL	a	502	-	-	39/110/110/110	-
33	ATP	g	301	34	-	0/18/38/38	0/3/3/3
35	PEE	L	303	-	-	22/51/51/54	-
29	CDL	P	201	-	-	36/110/110/110	-
30	PC1	G	303	-	-	29/57/57/57	-
33	ATP	C1	601	34	-	5/18/38/38	0/3/3/3
35	PEE	m	301	-	-	24/54/54/54	-
29	CDL	f	303	-	-	41/110/110/110	-
29	CDL	l	302	-	-	40/110/110/110	-
29	CDL	B	403	-	-	33/110/110/110	-
29	CDL	j	302	-	-	41/110/110/110	-
32	UQ8	I	303	-	-	9/51/75/75	0/1/1/1
29	CDL	a	501	-	-	33/110/110/110	-
36	NAD	E	900	-	-	7/26/62/62	0/5/5/5
30	PC1	G	304	8	-	19/57/57/57	-
30	PC1	g	304	8	-	19/57/57/57	-
29	CDL	r	201	-	-	36/110/110/110	-
29	CDL	f	302	-	-	54/110/110/110	-
29	CDL	k	202	-	-	35/110/110/110	-
29	CDL	B	404	2	-	46/110/110/110	-
29	CDL	l	301	-	-	39/110/110/110	-
29	CDL	K	202	-	-	36/110/110/110	-
29	CDL	L	302	-	-	45/110/110/110	-
29	CDL	J	301	-	-	42/110/110/110	-
29	CDL	j	301	-	-	40/110/110/110	-
32	UQ8	i	302	-	-	8/51/75/75	0/1/1/1
29	CDL	I	301	5	-	42/110/110/110	-
29	CDL	p	201	-	-	44/110/110/110	-
33	ATP	A1	601	34	-	5/18/38/38	0/3/3/3
29	CDL	L	301	-	-	38/110/110/110	-
30	PC1	D	301	3	-	21/57/57/57	-
29	CDL	I	302	-	-	38/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	ADP	D2	501	34	-	2/12/32/32	0/3/3/3
30	PC1	g	303	-	-	22/57/57/57	-
35	PEE	J	303	-	-	29/54/54/54	-
37	ADP	B1	603	34,24	-	1/12/32/32	0/3/3/3
29	CDL	A	502	-	-	46/110/110/110	-
36	NAD	e	900	-	-	6/26/62/62	0/5/5/5
33	ATP	A2	601	34	-	5/18/38/38	0/3/3/3
29	CDL	f	304	-	-	49/110/110/110	-
29	CDL	F	302	-	-	47/110/110/110	-

All (421) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A2	601	ATP	C2'-C1'	-17.27	1.27	1.53
33	B2	601	ATP	C2'-C1'	-17.23	1.27	1.53
33	A1	601	ATP	C2'-C1'	-17.22	1.27	1.53
33	B1	601	ATP	C2'-C1'	-17.21	1.27	1.53
33	g	301	ATP	C2'-C1'	-17.19	1.27	1.53
33	C2	601	ATP	C2'-C1'	-17.15	1.27	1.53
33	G	301	ATP	C2'-C1'	-17.07	1.27	1.53
33	C1	601	ATP	C2'-C1'	-17.06	1.27	1.53
33	A2	601	ATP	O4'-C1'	11.45	1.57	1.41
33	C1	601	ATP	O4'-C1'	11.42	1.57	1.41
33	A1	601	ATP	O4'-C1'	11.38	1.57	1.41
33	B1	601	ATP	O4'-C1'	11.31	1.56	1.41
33	C2	601	ATP	O4'-C1'	11.30	1.56	1.41
33	B2	601	ATP	O4'-C1'	11.28	1.56	1.41
33	g	301	ATP	O4'-C1'	11.15	1.56	1.41
33	G	301	ATP	O4'-C1'	11.13	1.56	1.41
37	D2	501	ADP	C2'-C3'	-10.47	1.24	1.53
37	B1	603	ADP	C2'-C3'	-10.44	1.24	1.53
37	B2	603	ADP	C2'-C3'	-10.44	1.24	1.53
37	D1	501	ADP	C2'-C3'	-10.42	1.24	1.53
36	e	900	NAD	O4D-C1D	-9.92	1.27	1.41
36	E	900	NAD	O4D-C1D	-9.81	1.27	1.41
32	i	302	UQ8	C6-C1	9.76	1.53	1.35
32	I	303	UQ8	C6-C1	9.68	1.52	1.35
33	g	301	ATP	C3'-C4'	-9.62	1.28	1.53
33	G	301	ATP	C3'-C4'	-9.57	1.28	1.53
33	A1	601	ATP	C3'-C4'	-9.49	1.28	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A2	601	ATP	C3'-C4'	-9.47	1.28	1.53
33	C1	601	ATP	C3'-C4'	-9.41	1.28	1.53
33	C2	601	ATP	C3'-C4'	-9.39	1.29	1.53
33	B2	601	ATP	C3'-C4'	-9.35	1.29	1.53
33	B1	601	ATP	C3'-C4'	-9.34	1.29	1.53
36	E	900	NAD	C3B-C4B	-9.21	1.29	1.53
36	e	900	NAD	C3B-C4B	-9.20	1.29	1.53
36	E	900	NAD	C3D-C4D	-8.45	1.31	1.53
36	e	900	NAD	C7N-N7N	8.45	1.49	1.33
36	E	900	NAD	C7N-N7N	8.43	1.49	1.33
36	e	900	NAD	C3D-C4D	-8.42	1.31	1.53
37	B2	603	ADP	O4'-C1'	7.93	1.52	1.41
37	B1	603	ADP	O4'-C1'	7.92	1.52	1.41
37	D2	501	ADP	O4'-C1'	7.85	1.52	1.41
37	D1	501	ADP	O4'-C1'	7.62	1.51	1.41
36	e	900	NAD	O4B-C4B	7.59	1.62	1.45
36	E	900	NAD	O4B-C4B	7.55	1.61	1.45
36	E	900	NAD	O4D-C4D	7.42	1.61	1.45
36	e	900	NAD	O4D-C4D	7.35	1.61	1.45
37	B2	603	ADP	O4'-C4'	-6.47	1.30	1.45
37	B1	603	ADP	O4'-C4'	-6.45	1.30	1.45
37	D1	501	ADP	O4'-C4'	-6.41	1.30	1.45
36	E	900	NAD	O4B-C1B	-6.40	1.32	1.41
36	e	900	NAD	O4B-C1B	-6.39	1.32	1.41
37	D2	501	ADP	O4'-C4'	-6.29	1.30	1.45
37	D2	501	ADP	C3'-C4'	5.95	1.68	1.53
37	D1	501	ADP	C3'-C4'	5.90	1.68	1.53
37	B1	603	ADP	C3'-C4'	5.81	1.67	1.53
37	B2	603	ADP	C3'-C4'	5.79	1.67	1.53
37	B2	603	ADP	C2'-C1'	5.37	1.61	1.53
37	B1	603	ADP	C2'-C1'	5.31	1.61	1.53
37	D2	501	ADP	C2'-C1'	4.93	1.61	1.53
37	D1	501	ADP	C2'-C1'	4.83	1.61	1.53
33	B1	601	ATP	C2'-C3'	4.80	1.66	1.53
33	B2	601	ATP	C2'-C3'	4.80	1.66	1.53
33	C1	601	ATP	C2'-C3'	4.77	1.66	1.53
33	C2	601	ATP	C2'-C3'	4.77	1.66	1.53
33	A2	601	ATP	C2'-C3'	4.73	1.66	1.53
33	B2	601	ATP	O4'-C4'	4.71	1.55	1.45
33	C1	601	ATP	O4'-C4'	4.71	1.55	1.45
33	A2	601	ATP	O4'-C4'	4.71	1.55	1.45
33	C2	601	ATP	O4'-C4'	4.70	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A1	601	ATP	O4'-C4'	4.70	1.55	1.45
33	A1	601	ATP	C2'-C3'	4.70	1.66	1.53
33	B1	601	ATP	O4'-C4'	4.69	1.55	1.45
33	G	301	ATP	C2'-C3'	4.68	1.66	1.53
36	E	900	NAD	C3N-C7N	4.67	1.57	1.50
36	e	900	NAD	C3N-C7N	4.66	1.57	1.50
33	g	301	ATP	C2'-C3'	4.60	1.65	1.53
36	e	900	NAD	O3D-C3D	4.51	1.53	1.43
36	E	900	NAD	O3D-C3D	4.50	1.53	1.43
33	G	301	ATP	O4'-C4'	4.47	1.55	1.45
33	g	301	ATP	O4'-C4'	4.40	1.54	1.45
36	e	900	NAD	C6A-N6A	4.21	1.49	1.34
36	E	900	NAD	C6A-N6A	4.18	1.49	1.34
32	i	302	UQ8	C4-C3	4.08	1.52	1.36
32	I	303	UQ8	C4-C3	4.06	1.52	1.36
37	D2	501	ADP	O2'-C2'	3.83	1.52	1.43
37	D1	501	ADP	O2'-C2'	3.82	1.52	1.43
37	B1	603	ADP	O2'-C2'	3.81	1.52	1.43
37	B2	603	ADP	O2'-C2'	3.81	1.52	1.43
35	m	301	PEE	C39-C38	3.71	1.53	1.31
35	A	501	PEE	C39-C38	3.71	1.53	1.31
35	m	301	PEE	C18-C19	3.71	1.53	1.31
35	J	303	PEE	C39-C38	3.70	1.53	1.31
35	L	303	PEE	C39-C38	3.69	1.53	1.31
35	J	303	PEE	C18-C19	3.69	1.53	1.31
35	A	501	PEE	C18-C19	3.66	1.53	1.31
35	L	303	PEE	C18-C19	3.65	1.52	1.31
33	C1	601	ATP	C6-N6	3.30	1.46	1.34
37	D2	501	ADP	C5-C4	-3.30	1.32	1.40
33	A2	601	ATP	C6-N6	3.30	1.46	1.34
33	B1	601	ATP	C6-N6	3.29	1.46	1.34
33	C2	601	ATP	C6-N6	3.28	1.46	1.34
33	A1	601	ATP	C6-N6	3.28	1.46	1.34
33	B2	601	ATP	C6-N6	3.27	1.46	1.34
37	B2	603	ADP	C5-C4	-3.25	1.32	1.40
37	D1	501	ADP	C5-C4	-3.24	1.32	1.40
37	B1	603	ADP	C5-C4	-3.21	1.32	1.40
36	E	900	NAD	O3B-C3B	3.18	1.50	1.43
37	B1	603	ADP	C6-N6	3.18	1.45	1.34
37	B2	603	ADP	C6-N6	3.18	1.45	1.34
37	D1	501	ADP	C6-N6	3.16	1.45	1.34
33	G	301	ATP	C6-N6	3.15	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	D2	501	ADP	C6-N6	3.14	1.45	1.34
36	e	900	NAD	O3B-C3B	3.13	1.50	1.43
33	g	301	ATP	C6-N6	3.10	1.45	1.34
29	L	302	CDL	OA6-CA4	-2.89	1.39	1.46
29	A	502	CDL	OA6-CA4	-2.88	1.39	1.46
29	a	501	CDL	OA6-CA4	-2.83	1.39	1.46
29	a	501	CDL	OB6-CB4	-2.80	1.39	1.46
29	l	301	CDL	OA6-CA4	-2.80	1.39	1.46
29	K	202	CDL	OA6-CA4	-2.79	1.39	1.46
36	E	900	NAD	O2B-C2B	-2.79	1.36	1.43
36	e	900	NAD	O2B-C2B	-2.77	1.36	1.43
29	J	301	CDL	OA6-CA4	-2.77	1.39	1.46
33	g	301	ATP	C5-C4	-2.75	1.33	1.40
33	G	301	ATP	C5-C4	-2.73	1.33	1.40
29	f	302	CDL	OB6-CB4	-2.73	1.39	1.46
29	b	401	CDL	OA6-CA4	-2.72	1.39	1.46
29	l	301	CDL	OB6-CB4	-2.70	1.39	1.46
29	f	304	CDL	OB6-CB4	-2.69	1.39	1.46
29	a	502	CDL	OB6-CB4	-2.69	1.39	1.46
29	I	301	CDL	OB6-CB4	-2.69	1.39	1.46
29	L	301	CDL	OB8-CB7	2.69	1.41	1.33
29	r	201	CDL	OB6-CB4	-2.67	1.39	1.46
29	K	202	CDL	OB6-CB4	-2.67	1.39	1.46
29	L	302	CDL	OB6-CB4	-2.67	1.39	1.46
29	b	401	CDL	OB6-CB4	-2.66	1.39	1.46
29	B	402	CDL	OA6-CA4	-2.66	1.39	1.46
29	k	202	CDL	OA6-CA4	-2.66	1.39	1.46
29	I	302	CDL	OA6-CA4	-2.66	1.39	1.46
35	m	301	PEE	O2-C2	-2.64	1.40	1.46
29	f	303	CDL	OB6-CB4	-2.64	1.40	1.46
30	g	303	PC1	O21-C2	-2.63	1.40	1.46
29	j	301	CDL	OA6-CA4	-2.63	1.40	1.46
30	g	304	PC1	O21-C2	-2.62	1.40	1.46
29	a	502	CDL	OA8-CA6	-2.62	1.39	1.45
29	B	403	CDL	OB6-CB4	-2.62	1.40	1.46
33	A2	601	ATP	C5-C4	-2.62	1.34	1.40
29	A	502	CDL	OB6-CB4	-2.61	1.40	1.46
33	B2	601	ATP	C5-C4	-2.61	1.34	1.40
29	B	402	CDL	OB6-CB4	-2.60	1.40	1.46
33	A1	601	ATP	C5-C4	-2.60	1.34	1.40
29	i	301	CDL	OA6-CA4	-2.60	1.40	1.46
29	f	304	CDL	OB8-CB7	2.60	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	p	201	CDL	OB6-CB4	-2.60	1.40	1.46
29	J	302	CDL	OB6-CB4	-2.59	1.40	1.46
30	G	303	PC1	O21-C2	-2.59	1.40	1.46
33	C2	601	ATP	C5-C4	-2.58	1.34	1.40
29	P	201	CDL	OA6-CA4	-2.58	1.40	1.46
33	C1	601	ATP	C5-C4	-2.57	1.34	1.40
33	B1	601	ATP	C5-C4	-2.57	1.34	1.40
29	F	302	CDL	OA6-CA4	-2.57	1.40	1.46
29	j	302	CDL	OB6-CB4	-2.56	1.40	1.46
36	e	900	NAD	C2A-N1A	2.55	1.38	1.33
29	J	301	CDL	OB8-CB7	2.55	1.40	1.33
29	f	304	CDL	OA6-CA4	-2.54	1.40	1.46
29	f	303	CDL	OA6-CA4	-2.54	1.40	1.46
29	J	301	CDL	OB6-CB4	-2.54	1.40	1.46
29	k	202	CDL	OB6-CB4	-2.54	1.40	1.46
30	D	301	PC1	O21-C2	-2.54	1.40	1.46
29	B	404	CDL	OB8-CB7	2.54	1.40	1.33
29	f	303	CDL	OB8-CB7	2.53	1.40	1.33
35	J	303	PEE	O2-C2	-2.53	1.40	1.46
29	j	301	CDL	OB6-CB4	-2.53	1.40	1.46
29	j	301	CDL	OB8-CB7	2.53	1.40	1.33
29	J	301	CDL	OA8-CA7	2.53	1.40	1.33
29	i	301	CDL	OB6-CB4	-2.52	1.40	1.46
29	K	202	CDL	OA8-CA7	2.52	1.40	1.33
29	I	302	CDL	OA8-CA7	2.51	1.40	1.33
29	b	401	CDL	OA8-CA7	2.51	1.40	1.33
29	I	301	CDL	OA8-CA7	2.51	1.40	1.33
29	j	302	CDL	OA8-CA7	2.51	1.40	1.33
29	B	401	CDL	OB6-CB4	-2.51	1.40	1.46
29	k	202	CDL	OA8-CA7	2.51	1.40	1.33
29	l	302	CDL	OA8-CA7	2.50	1.40	1.33
29	k	201	CDL	OA6-CA4	-2.50	1.40	1.46
29	k	201	CDL	OB6-CB4	-2.50	1.40	1.46
30	G	304	PC1	O21-C2	-2.50	1.40	1.46
29	P	201	CDL	OB8-CB7	2.50	1.40	1.33
29	p	201	CDL	OA6-CA4	-2.49	1.40	1.46
36	e	900	NAD	C5A-C4A	-2.49	1.34	1.40
29	B	402	CDL	OA8-CA7	2.49	1.40	1.33
29	k	201	CDL	OA8-CA7	2.49	1.40	1.33
36	E	900	NAD	C2N-N1N	2.49	1.38	1.35
29	I	301	CDL	OA6-CA4	-2.49	1.40	1.46
29	k	201	CDL	OB8-CB7	2.48	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	E	900	NAD	C5A-C4A	-2.48	1.34	1.40
29	J	302	CDL	OB8-CB7	2.48	1.40	1.33
29	f	302	CDL	OA8-CA7	2.48	1.40	1.33
29	K	201	CDL	OA6-CA4	-2.48	1.40	1.46
29	L	301	CDL	OB6-CB4	-2.48	1.40	1.46
29	K	201	CDL	OB8-CB7	2.47	1.40	1.33
35	L	303	PEE	O2-C2	-2.47	1.40	1.46
29	j	301	CDL	OA8-CA7	2.47	1.40	1.33
29	P	201	CDL	OB6-CB4	-2.47	1.40	1.46
36	e	900	NAD	C2N-N1N	2.46	1.38	1.35
29	i	301	CDL	OA8-CA7	2.46	1.40	1.33
29	B	404	CDL	OB6-CB4	-2.46	1.40	1.46
29	r	201	CDL	OA8-CA7	2.46	1.40	1.33
29	J	302	CDL	OA8-CA7	2.46	1.40	1.33
29	L	301	CDL	OA8-CA7	2.46	1.40	1.33
29	B	401	CDL	OA8-CA7	2.46	1.40	1.33
29	L	301	CDL	OA6-CA4	-2.45	1.40	1.46
35	A	501	PEE	O2-C2	-2.45	1.40	1.46
36	E	900	NAD	C2A-N1A	2.45	1.38	1.33
30	g	304	PC1	O31-C31	2.45	1.40	1.33
29	I	302	CDL	OB6-CB4	-2.45	1.40	1.46
29	a	501	CDL	OA8-CA7	2.45	1.40	1.33
29	r	201	CDL	OA6-CA4	-2.45	1.40	1.46
29	F	302	CDL	OA8-CA7	2.45	1.40	1.33
29	I	301	CDL	OB8-CB7	2.45	1.40	1.33
29	L	302	CDL	OB8-CB7	2.45	1.40	1.33
29	K	201	CDL	OB6-CB4	-2.45	1.40	1.46
29	J	302	CDL	OA6-CA4	-2.44	1.40	1.46
30	d	301	PC1	O21-C2	-2.44	1.40	1.46
29	j	302	CDL	OB8-CB7	2.43	1.40	1.33
29	l	302	CDL	OA6-CA4	-2.43	1.40	1.46
29	i	301	CDL	OB8-CB7	2.43	1.40	1.33
29	a	502	CDL	OB8-CB7	2.43	1.40	1.33
29	L	302	CDL	OA8-CA7	2.43	1.40	1.33
29	B	404	CDL	OA6-CA4	-2.43	1.40	1.46
29	F	302	CDL	OB8-CB7	2.42	1.40	1.33
30	g	303	PC1	O31-C31	2.42	1.40	1.33
29	p	201	CDL	OA8-CA7	2.42	1.40	1.33
36	E	900	NAD	C2D-C1D	2.42	1.57	1.53
29	K	202	CDL	OB8-CB7	2.42	1.40	1.33
29	f	302	CDL	OB8-CB7	2.41	1.40	1.33
29	l	302	CDL	OB8-CB7	2.41	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	K	201	CDL	OA8-CA7	2.41	1.40	1.33
35	J	303	PEE	O3-C30	2.41	1.40	1.33
29	A	502	CDL	OA8-CA7	2.41	1.40	1.33
36	e	900	NAD	C2D-C1D	2.41	1.57	1.53
30	G	304	PC1	O31-C31	2.41	1.40	1.33
29	a	501	CDL	OB8-CB7	2.40	1.40	1.33
29	k	202	CDL	OB8-CB7	2.40	1.40	1.33
29	l	301	CDL	OA8-CA7	2.40	1.40	1.33
29	P	201	CDL	OA8-CA7	2.40	1.40	1.33
29	B	403	CDL	OA6-CA4	-2.40	1.40	1.46
29	F	302	CDL	OB6-CB4	-2.39	1.40	1.46
29	l	302	CDL	OB6-CB4	-2.38	1.40	1.46
29	p	201	CDL	OB8-CB7	2.37	1.40	1.33
29	I	302	CDL	OB8-CB7	2.37	1.40	1.33
35	A	501	PEE	O3-C30	2.36	1.40	1.33
32	i	302	UQ8	O4-C4M	-2.36	1.39	1.45
29	f	302	CDL	OA6-CA4	-2.36	1.40	1.46
30	G	303	PC1	O31-C3	-2.35	1.39	1.45
36	E	900	NAD	O7N-C7N	-2.35	1.19	1.24
30	G	303	PC1	O31-C31	2.35	1.40	1.33
29	B	403	CDL	OA8-CA7	2.35	1.40	1.33
29	b	401	CDL	OB8-CB7	2.35	1.40	1.33
29	A	502	CDL	OB8-CB7	2.35	1.40	1.33
36	e	900	NAD	O7N-C7N	-2.34	1.19	1.24
29	B	403	CDL	OB8-CB7	2.34	1.40	1.33
30	d	301	PC1	O31-C31	2.34	1.40	1.33
29	l	301	CDL	OB8-CB7	2.34	1.40	1.33
29	r	201	CDL	OB8-CB7	2.34	1.40	1.33
29	B	401	CDL	OB8-CB7	2.34	1.40	1.33
29	B	404	CDL	OA8-CA7	2.33	1.40	1.33
35	m	301	PEE	O3-C30	2.33	1.40	1.33
32	i	302	UQ8	O3-C3M	-2.32	1.39	1.45
29	L	302	CDL	OA8-CA6	-2.32	1.39	1.45
32	I	303	UQ8	O3-C3M	-2.32	1.39	1.45
29	F	302	CDL	OB6-CB5	2.32	1.40	1.34
30	D	301	PC1	O31-C3	-2.31	1.39	1.45
29	f	303	CDL	OA8-CA7	2.31	1.40	1.33
29	B	404	CDL	OB6-CB5	2.31	1.40	1.34
29	f	304	CDL	OA8-CA7	2.31	1.40	1.33
29	B	402	CDL	OB8-CB7	2.31	1.40	1.33
29	f	304	CDL	OA8-CA6	-2.31	1.39	1.45
29	B	403	CDL	OA8-CA6	-2.30	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	502	CDL	OA6-CA4	-2.30	1.40	1.46
35	L	303	PEE	O3-C30	2.29	1.40	1.33
32	I	303	UQ8	O4-C4M	-2.28	1.39	1.45
29	B	403	CDL	OB8-CB6	-2.28	1.39	1.45
29	l	302	CDL	OB8-CB6	-2.28	1.40	1.45
30	D	301	PC1	O31-C31	2.28	1.40	1.33
29	B	401	CDL	OA6-CA4	-2.28	1.40	1.46
29	j	302	CDL	OA6-CA4	-2.27	1.40	1.46
29	I	302	CDL	OB8-CB6	-2.27	1.40	1.45
29	B	402	CDL	OB8-CB6	-2.27	1.40	1.45
29	B	401	CDL	OB8-CB6	-2.27	1.40	1.45
29	A	502	CDL	OB8-CB6	-2.27	1.40	1.45
35	L	303	PEE	O2-C10	2.26	1.40	1.34
29	B	404	CDL	OA6-CA5	2.26	1.40	1.34
29	f	303	CDL	OB6-CB5	2.25	1.40	1.34
29	f	303	CDL	OA8-CA6	-2.25	1.40	1.45
29	K	201	CDL	OB6-CB5	2.25	1.40	1.34
35	A	501	PEE	O2-C10	2.25	1.40	1.34
29	f	302	CDL	OB8-CB6	-2.24	1.40	1.45
29	l	302	CDL	OB6-CB5	2.24	1.40	1.34
29	L	301	CDL	OA6-CA5	2.24	1.40	1.34
29	j	301	CDL	OB6-CB5	2.23	1.40	1.34
29	K	201	CDL	OA6-CA5	2.23	1.40	1.34
29	B	401	CDL	OA6-CA5	2.22	1.40	1.34
29	k	201	CDL	OA6-CA5	2.21	1.40	1.34
29	l	302	CDL	OA6-CA5	2.21	1.40	1.34
29	I	302	CDL	OB6-CB5	2.21	1.40	1.34
29	f	304	CDL	OA6-CA5	2.21	1.40	1.34
30	d	301	PC1	O31-C3	-2.21	1.40	1.45
29	P	201	CDL	OB6-CB5	2.21	1.40	1.34
32	i	302	UQ8	O2-C2	-2.21	1.18	1.23
35	L	303	PEE	O3-C3	-2.20	1.40	1.45
29	k	201	CDL	OB6-CB5	2.20	1.40	1.34
29	l	301	CDL	OB8-CB6	-2.20	1.40	1.45
29	L	301	CDL	OB6-CB5	2.19	1.40	1.34
30	G	304	PC1	O21-C21	2.19	1.40	1.34
29	a	502	CDL	OB8-CB6	-2.19	1.40	1.45
29	b	401	CDL	OB8-CB6	-2.19	1.40	1.45
29	B	403	CDL	OA6-CA5	2.19	1.40	1.34
35	A	501	PEE	O3-C3	-2.18	1.40	1.45
29	a	502	CDL	OA6-CA5	2.18	1.40	1.34
32	i	302	UQ8	O5-C5	-2.18	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	r	201	CDL	OA8-CA6	-2.18	1.40	1.45
35	m	301	PEE	O3-C3	-2.18	1.40	1.45
29	J	301	CDL	OB6-CB5	2.17	1.40	1.34
29	j	302	CDL	OB8-CB6	-2.17	1.40	1.45
32	I	303	UQ8	C6-C5	2.17	1.52	1.46
29	i	301	CDL	OB6-CB5	2.17	1.40	1.34
29	a	502	CDL	OA8-CA7	2.16	1.39	1.33
29	p	201	CDL	OA6-CA5	2.16	1.40	1.34
32	i	302	UQ8	C6-C5	2.16	1.52	1.46
29	l	301	CDL	OA8-CA6	-2.16	1.40	1.45
35	J	303	PEE	O3-C3	-2.16	1.40	1.45
29	f	302	CDL	OA6-CA5	2.15	1.40	1.34
29	B	401	CDL	OB6-CB5	2.15	1.40	1.34
29	F	302	CDL	OA8-CA6	-2.15	1.40	1.45
29	k	202	CDL	OB6-CB5	2.15	1.40	1.34
29	F	302	CDL	OA6-CA5	2.15	1.40	1.34
29	k	202	CDL	OB8-CB6	-2.15	1.40	1.45
29	B	401	CDL	OA8-CA6	-2.14	1.40	1.45
32	I	303	UQ8	O5-C5	-2.14	1.18	1.23
29	j	302	CDL	OB6-CB5	2.14	1.40	1.34
30	g	303	PC1	O31-C3	-2.14	1.40	1.45
30	D	301	PC1	O21-C21	2.14	1.40	1.34
29	a	501	CDL	OA8-CA6	-2.14	1.40	1.45
29	J	302	CDL	OB6-CB5	2.13	1.40	1.34
29	A	502	CDL	OA8-CA6	-2.13	1.40	1.45
29	j	302	CDL	OA6-CA5	2.13	1.40	1.34
29	i	301	CDL	OA6-CA5	2.13	1.40	1.34
29	f	303	CDL	OA6-CA5	2.13	1.40	1.34
30	g	304	PC1	O21-C21	2.13	1.40	1.34
29	K	202	CDL	OB8-CB6	-2.12	1.40	1.45
30	d	301	PC1	O21-C21	2.12	1.40	1.34
29	A	502	CDL	OB6-CB5	2.12	1.40	1.34
29	K	202	CDL	OA8-CA6	-2.12	1.40	1.45
29	B	402	CDL	OB6-CB5	2.12	1.40	1.34
35	m	301	PEE	O2-C10	2.12	1.40	1.34
29	i	301	CDL	OB8-CB6	-2.12	1.40	1.45
29	l	302	CDL	OA8-CA6	-2.12	1.40	1.45
29	p	201	CDL	OB6-CB5	2.12	1.40	1.34
29	P	201	CDL	OA8-CA6	-2.12	1.40	1.45
36	E	900	NAD	C2A-N3A	2.11	1.35	1.32
32	I	303	UQ8	O2-C2	-2.11	1.18	1.23
29	j	301	CDL	OA6-CA5	2.11	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	p	201	CDL	OB8-CB6	-2.11	1.40	1.45
29	I	302	CDL	OA6-CA5	2.11	1.40	1.34
29	r	201	CDL	OB6-CB5	2.11	1.40	1.34
29	L	302	CDL	OB8-CB6	-2.10	1.40	1.45
29	f	303	CDL	OB8-CB6	-2.10	1.40	1.45
29	k	201	CDL	OB8-CB6	-2.09	1.40	1.45
29	B	404	CDL	OA8-CA6	-2.09	1.40	1.45
37	D1	501	ADP	C2-N3	2.09	1.35	1.32
37	B1	603	ADP	C2-N3	2.09	1.35	1.32
29	f	304	CDL	OB6-CB5	2.09	1.40	1.34
29	K	202	CDL	OB6-CB5	2.09	1.40	1.34
29	K	201	CDL	OB8-CB6	-2.09	1.40	1.45
37	B2	603	ADP	C2-N3	2.09	1.35	1.32
35	J	303	PEE	O2-C10	2.08	1.40	1.34
33	C1	601	ATP	C5'-C4'	2.08	1.58	1.51
29	b	401	CDL	OA6-CA5	2.08	1.40	1.34
29	J	302	CDL	OA8-CA6	-2.08	1.40	1.45
29	b	401	CDL	OA8-CA6	-2.08	1.40	1.45
29	I	301	CDL	OB6-CB5	2.08	1.40	1.34
29	k	202	CDL	OA8-CA6	-2.08	1.40	1.45
29	I	301	CDL	OA8-CA6	-2.08	1.40	1.45
29	a	501	CDL	OB8-CB6	-2.07	1.40	1.45
29	p	201	CDL	OA8-CA6	-2.07	1.40	1.45
29	J	301	CDL	OA8-CA6	-2.07	1.40	1.45
29	i	301	CDL	OA8-CA6	-2.07	1.40	1.45
29	f	302	CDL	OA8-CA6	-2.07	1.40	1.45
29	a	501	CDL	OA6-CA5	2.07	1.40	1.34
33	A2	601	ATP	C5'-C4'	2.07	1.58	1.51
29	a	502	CDL	OB6-CB5	2.07	1.40	1.34
30	G	303	PC1	O21-C21	2.06	1.40	1.34
29	B	404	CDL	OB8-CB6	-2.06	1.40	1.45
33	B1	601	ATP	C5'-C4'	2.06	1.58	1.51
29	L	301	CDL	OA8-CA6	-2.06	1.40	1.45
29	L	302	CDL	OB6-CB5	2.06	1.40	1.34
29	k	201	CDL	OA8-CA6	-2.06	1.40	1.45
29	P	201	CDL	OA6-CA5	2.06	1.40	1.34
29	J	302	CDL	OB8-CB6	-2.06	1.40	1.45
29	j	301	CDL	OA8-CA6	-2.05	1.40	1.45
30	g	304	PC1	O31-C3	-2.05	1.40	1.45
30	G	304	PC1	O31-C3	-2.05	1.40	1.45
36	e	900	NAD	PA-O5B	2.05	1.67	1.59
29	J	302	CDL	OA6-CA5	2.05	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	K	201	CDL	OA8-CA6	-2.04	1.40	1.45
29	b	401	CDL	OB6-CB5	2.04	1.40	1.34
29	r	201	CDL	OB8-CB6	-2.04	1.40	1.45
29	F	302	CDL	OB8-CB6	-2.04	1.40	1.45
29	I	301	CDL	OB8-CB6	-2.04	1.40	1.45
37	D2	501	ADP	C2-N3	2.04	1.35	1.32
33	B2	601	ATP	C5'-C4'	2.03	1.57	1.51
29	I	302	CDL	OA8-CA6	-2.03	1.40	1.45
29	B	402	CDL	OA6-CA5	2.03	1.40	1.34
33	C2	601	ATP	C5'-C4'	2.03	1.57	1.51
36	E	900	NAD	PA-O5B	2.03	1.67	1.59
33	A1	601	ATP	C5'-C4'	2.02	1.57	1.51
36	e	900	NAD	C2A-N3A	2.02	1.35	1.32
30	g	303	PC1	O21-C21	2.02	1.40	1.34
29	r	201	CDL	OA6-CA5	2.01	1.40	1.34
33	B1	601	ATP	C2-N3	2.01	1.35	1.32

All (286) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D1	501	ADP	C1'-N9-C4	15.98	154.72	126.64
37	B1	603	ADP	C1'-N9-C4	14.91	152.83	126.64
37	B2	603	ADP	C1'-N9-C4	14.89	152.81	126.64
37	D2	501	ADP	C1'-N9-C4	14.61	152.31	126.64
36	e	900	NAD	C1B-N9A-C4A	-8.49	111.73	126.64
36	E	900	NAD	C1B-N9A-C4A	-8.29	112.07	126.64
36	E	900	NAD	C5A-C6A-N6A	7.98	132.47	120.35
36	e	900	NAD	C5A-C6A-N6A	7.91	132.38	120.35
33	A1	601	ATP	C5-C6-N6	7.60	131.91	120.35
33	B1	601	ATP	C5-C6-N6	7.59	131.89	120.35
33	B2	601	ATP	C5-C6-N6	7.58	131.87	120.35
33	C2	601	ATP	C5-C6-N6	7.57	131.85	120.35
37	B1	603	ADP	C5-C6-N6	7.53	131.79	120.35
33	A2	601	ATP	C5-C6-N6	7.52	131.78	120.35
37	D1	501	ADP	C5-C6-N6	7.50	131.75	120.35
33	C1	601	ATP	C5-C6-N6	7.49	131.74	120.35
37	D2	501	ADP	C5-C6-N6	7.48	131.72	120.35
37	B2	603	ADP	C5-C6-N6	7.47	131.71	120.35
33	g	301	ATP	C5-C6-N6	7.39	131.59	120.35
33	G	301	ATP	C5-C6-N6	7.36	131.54	120.35
33	G	301	ATP	C1'-N9-C4	5.70	136.65	126.64
33	A2	601	ATP	C1'-N9-C4	5.64	136.55	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	A1	601	ATP	C1'-N9-C4	5.63	136.54	126.64
33	B2	601	ATP	C1'-N9-C4	5.63	136.54	126.64
33	C2	601	ATP	C1'-N9-C4	5.63	136.53	126.64
33	g	301	ATP	C1'-N9-C4	5.60	136.48	126.64
33	B1	601	ATP	C1'-N9-C4	5.57	136.43	126.64
33	C1	601	ATP	C1'-N9-C4	5.56	136.41	126.64
37	B2	603	ADP	N3-C2-N1	-5.56	119.99	128.68
37	D2	501	ADP	N3-C2-N1	-5.54	120.03	128.68
37	B1	603	ADP	N3-C2-N1	-5.53	120.04	128.68
33	C2	601	ATP	N3-C2-N1	-5.53	120.04	128.68
33	B1	601	ATP	N3-C2-N1	-5.50	120.08	128.68
37	D1	501	ADP	N3-C2-N1	-5.50	120.08	128.68
33	C1	601	ATP	N3-C2-N1	-5.50	120.09	128.68
33	A1	601	ATP	N3-C2-N1	-5.49	120.09	128.68
33	A2	601	ATP	N3-C2-N1	-5.48	120.11	128.68
33	B2	601	ATP	N3-C2-N1	-5.47	120.13	128.68
33	G	301	ATP	N3-C2-N1	-5.42	120.20	128.68
33	g	301	ATP	N3-C2-N1	-5.40	120.25	128.68
36	e	900	NAD	N3A-C2A-N1A	-5.39	120.26	128.68
36	E	900	NAD	N3A-C2A-N1A	-5.39	120.26	128.68
36	E	900	NAD	N6A-C6A-N1A	-5.37	107.42	118.57
36	e	900	NAD	N6A-C6A-N1A	-5.34	107.49	118.57
29	l	302	CDL	OB6-CB5-C51	5.32	122.97	111.50
33	B1	601	ATP	N6-C6-N1	-5.05	108.10	118.57
32	I	303	UQ8	C25-C24-C26	5.05	123.76	115.27
33	A1	601	ATP	N6-C6-N1	-5.03	108.13	118.57
37	B1	603	ADP	N6-C6-N1	-5.02	108.15	118.57
33	B2	601	ATP	N6-C6-N1	-5.02	108.16	118.57
37	D1	501	ADP	N6-C6-N1	-5.00	108.20	118.57
33	C2	601	ATP	N6-C6-N1	-4.99	108.22	118.57
33	A2	601	ATP	N6-C6-N1	-4.98	108.24	118.57
37	D2	501	ADP	N6-C6-N1	-4.98	108.24	118.57
37	B2	603	ADP	N6-C6-N1	-4.97	108.25	118.57
33	g	301	ATP	N6-C6-N1	-4.97	108.25	118.57
33	C1	601	ATP	N6-C6-N1	-4.96	108.29	118.57
33	G	301	ATP	N6-C6-N1	-4.92	108.37	118.57
29	B	402	CDL	OB6-CB5-C51	4.79	121.82	111.50
29	F	302	CDL	OB6-CB5-C51	4.61	121.45	111.50
29	f	304	CDL	OA6-CA5-C11	4.59	121.40	111.50
29	B	401	CDL	OA6-CA5-C11	4.50	121.20	111.50
29	j	301	CDL	OA6-CA5-C11	4.31	120.80	111.50
30	d	301	PC1	O21-C21-C22	4.27	120.71	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	502	CDL	OA6-CA5-C11	4.26	120.68	111.50
29	k	201	CDL	OA6-CA5-C11	4.21	120.58	111.50
29	J	301	CDL	OA6-CA5-C11	4.21	120.56	111.50
29	A	502	CDL	OB6-CB5-C51	4.20	120.56	111.50
29	a	501	CDL	OB6-CB5-C51	4.19	120.53	111.50
29	k	202	CDL	OB6-CB5-C51	4.18	120.50	111.50
29	B	403	CDL	OA6-CA5-C11	4.16	120.46	111.50
29	f	302	CDL	OA6-CA5-C11	4.14	120.42	111.50
30	G	304	PC1	O21-C21-C22	4.14	120.42	111.50
29	K	201	CDL	OA6-CA5-C11	4.09	120.31	111.50
35	A	501	PEE	O2-C10-C11	4.08	120.30	111.50
29	b	401	CDL	OB6-CB5-C51	4.07	120.27	111.50
30	D	301	PC1	O21-C21-C22	4.05	120.23	111.50
29	P	201	CDL	OB6-CB5-C51	4.04	120.21	111.50
29	p	201	CDL	OB6-CB5-C51	4.04	120.21	111.50
29	k	202	CDL	OA6-CA5-C11	4.02	120.16	111.50
29	f	303	CDL	OA6-CA5-C11	4.01	120.15	111.50
29	P	201	CDL	OA6-CA5-C11	4.01	120.14	111.50
29	J	301	CDL	OB6-CB5-C51	4.01	120.14	111.50
29	i	301	CDL	OB6-CB5-C51	3.99	120.10	111.50
35	L	303	PEE	O2-C10-C11	3.97	120.07	111.50
33	G	301	ATP	C3'-C2'-C1'	3.95	106.92	100.98
29	F	302	CDL	OA6-CA5-C11	3.94	120.00	111.50
29	I	302	CDL	OB6-CB5-C51	3.94	120.00	111.50
35	J	303	PEE	O2-C10-C11	3.91	119.94	111.50
29	j	301	CDL	OB6-CB5-C51	3.91	119.93	111.50
29	B	404	CDL	OA6-CA5-C11	3.91	119.92	111.50
30	G	303	PC1	O21-C21-C22	3.90	119.91	111.50
29	f	303	CDL	OB6-CB5-C51	3.90	119.90	111.50
29	b	401	CDL	OA6-CA5-C11	3.88	119.87	111.50
29	f	302	CDL	OB6-CB5-C51	3.87	119.83	111.50
29	B	404	CDL	OB6-CB5-C51	3.86	119.83	111.50
29	I	302	CDL	OA6-CA5-C11	3.86	119.83	111.50
32	i	302	UQ8	C25-C24-C26	3.86	121.76	115.27
29	L	302	CDL	OB6-CB5-C51	3.84	119.78	111.50
33	g	301	ATP	C3'-C2'-C1'	3.83	106.75	100.98
37	D1	501	ADP	C3'-C2'-C1'	3.82	106.73	100.98
29	J	302	CDL	OB6-CB5-C51	3.79	119.67	111.50
29	i	301	CDL	OA6-CA5-C11	3.79	119.66	111.50
30	g	303	PC1	O21-C21-C22	3.78	119.64	111.50
29	l	301	CDL	OA6-CA5-C11	3.78	119.64	111.50
29	r	201	CDL	OA6-CA5-C11	3.77	119.62	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	K	202	CDL	OA6-CA5-C11	3.74	119.56	111.50
29	L	302	CDL	OA6-CA5-C11	3.68	119.44	111.50
29	l	301	CDL	OB6-CB5-C51	3.68	119.44	111.50
29	p	201	CDL	OA6-CA5-C11	3.68	119.44	111.50
37	B1	603	ADP	C3'-C2'-C1'	3.67	106.50	100.98
29	I	301	CDL	OA6-CA5-C11	3.66	119.40	111.50
29	f	304	CDL	OB6-CB5-C51	3.66	119.39	111.50
29	L	301	CDL	OB6-CB5-C51	3.65	119.37	111.50
29	a	501	CDL	OA6-CA5-C11	3.65	119.36	111.50
29	k	201	CDL	OB6-CB5-C51	3.65	119.36	111.50
29	K	201	CDL	OB6-CB5-C51	3.63	119.33	111.50
32	i	302	UQ8	C30-C29-C31	3.63	121.38	115.27
29	B	403	CDL	OB6-CB5-C51	3.62	119.31	111.50
29	L	301	CDL	OA6-CA5-C11	3.60	119.27	111.50
37	B2	603	ADP	C3'-C2'-C1'	3.60	106.39	100.98
32	I	303	UQ8	C40-C39-C41	3.57	121.28	115.27
29	j	302	CDL	OB6-CB5-C51	3.57	119.19	111.50
29	K	202	CDL	OB6-CB5-C51	3.57	119.19	111.50
29	B	402	CDL	OA6-CA5-C11	3.55	119.15	111.50
29	A	502	CDL	OA6-CA5-C11	3.54	119.13	111.50
29	j	302	CDL	OA6-CA5-C11	3.51	119.07	111.50
30	g	304	PC1	O21-C21-C22	3.50	119.05	111.50
32	i	302	UQ8	C17-C18-C19	-3.49	119.27	127.66
29	I	301	CDL	OB6-CB5-C51	3.44	118.91	111.50
29	J	302	CDL	OA6-CA5-C11	3.38	118.79	111.50
32	I	303	UQ8	C20-C19-C21	3.38	120.96	115.27
32	I	303	UQ8	C17-C18-C19	-3.37	119.54	127.66
29	r	201	CDL	OB6-CB5-C51	3.36	118.75	111.50
29	B	401	CDL	OB6-CB5-C51	3.36	118.75	111.50
35	m	301	PEE	O2-C10-C11	3.36	118.74	111.50
33	B2	601	ATP	C3'-C2'-C1'	3.28	105.92	100.98
33	B1	601	ATP	C3'-C2'-C1'	3.28	105.91	100.98
32	i	302	UQ8	C22-C23-C24	-3.24	119.87	127.66
29	a	502	CDL	OB6-CB5-C51	3.21	118.43	111.50
32	I	303	UQ8	C7-C8-C9	-3.17	121.52	126.79
29	l	302	CDL	OA6-CA5-C11	3.17	118.32	111.50
33	G	301	ATP	PB-O3B-PG	-3.13	122.08	132.83
32	i	302	UQ8	C20-C19-C21	3.09	120.47	115.27
32	i	302	UQ8	C40-C39-C41	3.09	120.47	115.27
29	i	301	CDL	OB8-CB7-C71	3.08	121.57	111.91
33	g	301	ATP	PB-O3B-PG	-3.08	122.26	132.83
32	I	303	UQ8	C22-C23-C24	-3.07	120.26	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L	301	CDL	OB8-CB7-C71	3.07	121.55	111.91
29	b	401	CDL	OA8-CA7-C31	3.00	121.32	111.91
33	C1	601	ATP	C3'-C2'-C1'	2.98	105.47	100.98
29	B	402	CDL	OA8-CA7-C31	2.95	121.15	111.91
29	K	202	CDL	OA8-CA7-C31	2.94	121.14	111.91
37	D1	501	ADP	C2'-C3'-C4'	2.94	108.35	102.64
35	J	303	PEE	O3-C30-C31	2.93	121.11	111.91
32	I	303	UQ8	C12-C13-C14	-2.92	120.63	127.66
33	C2	601	ATP	C3'-C2'-C1'	2.90	105.34	100.98
32	i	302	UQ8	C32-C33-C34	-2.88	120.72	127.66
32	i	302	UQ8	C40-C39-C38	-2.87	116.32	123.68
29	k	202	CDL	OA8-CA7-C31	2.86	120.87	111.91
29	A	502	CDL	OA8-CA7-C31	2.85	120.86	111.91
30	D	301	PC1	O31-C31-C32	2.85	120.84	111.91
36	E	900	NAD	PN-O3-PA	-2.84	123.08	132.83
29	j	301	CDL	OA8-CA7-C31	2.84	120.81	111.91
29	l	301	CDL	OB8-CB7-C71	2.82	120.77	111.91
33	A1	601	ATP	PA-O3A-PB	-2.82	123.16	132.83
29	J	301	CDL	OA8-CA7-C31	2.81	120.72	111.91
29	p	201	CDL	OB8-CB7-C71	2.79	120.67	111.91
33	C1	601	ATP	PB-O3B-PG	-2.77	123.33	132.83
33	B1	601	ATP	PB-O3B-PG	-2.76	123.36	132.83
37	D1	501	ADP	PA-O3A-PB	-2.75	123.38	132.83
37	D2	501	ADP	PA-O3A-PB	-2.75	123.39	132.83
33	A2	601	ATP	PA-O3A-PB	-2.75	123.40	132.83
29	r	201	CDL	OB8-CB7-C71	2.74	120.50	111.91
33	B2	601	ATP	PB-O3B-PG	-2.72	123.50	132.83
29	B	403	CDL	OB8-CB7-C71	2.72	120.43	111.91
30	d	301	PC1	O31-C31-C32	2.71	120.41	111.91
29	l	301	CDL	OA8-CA7-C31	2.70	120.40	111.91
32	i	302	UQ8	C7-C8-C9	-2.70	122.31	126.79
29	a	502	CDL	OB8-CB7-C71	2.69	120.36	111.91
37	B2	603	ADP	PA-O3A-PB	-2.69	123.58	132.83
33	C2	601	ATP	PB-O3B-PG	-2.69	123.60	132.83
37	B1	603	ADP	PA-O3A-PB	-2.69	123.60	132.83
35	m	301	PEE	O3-C30-C31	2.68	120.31	111.91
29	B	402	CDL	OB8-CB7-C71	2.67	120.28	111.91
29	a	501	CDL	OB8-CB7-C71	2.66	120.27	111.91
29	f	303	CDL	OB8-CB7-C71	2.66	120.27	111.91
33	C2	601	ATP	PA-O3A-PB	-2.66	123.69	132.83
37	D2	501	ADP	C2'-C3'-C4'	2.66	107.81	102.64
29	r	201	CDL	OA8-CA7-C31	2.66	120.24	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	404	CDL	OB8-CB7-C71	2.65	120.24	111.91
33	A2	601	ATP	C3'-C2'-C1'	2.65	104.97	100.98
29	F	302	CDL	OB8-CB7-C71	2.65	120.21	111.91
29	K	201	CDL	OB8-CB7-C71	2.64	120.18	111.91
29	b	401	CDL	OB8-CB7-C71	2.64	120.18	111.91
36	e	900	NAD	PN-O3-PA	-2.63	123.81	132.83
36	e	900	NAD	C3D-C2D-C1D	2.62	104.93	100.98
32	I	303	UQ8	C27-C28-C29	-2.62	121.35	127.66
33	A1	601	ATP	PB-O3B-PG	-2.61	123.86	132.83
29	j	302	CDL	OA8-CA7-C31	2.61	120.11	111.91
33	A2	601	ATP	PB-O3B-PG	-2.61	123.87	132.83
30	g	303	PC1	O31-C31-C32	2.61	120.09	111.91
29	B	402	CDL	CB6-CB4-CB3	-2.60	105.64	111.79
29	I	302	CDL	OA8-CA7-C31	2.60	120.06	111.91
29	i	301	CDL	OA8-CA7-C31	2.59	120.04	111.91
30	G	303	PC1	O31-C31-C32	2.59	120.04	111.91
37	D2	501	ADP	C3'-C2'-C1'	2.59	104.88	100.98
29	k	201	CDL	OA8-CA7-C31	2.59	120.03	111.91
29	J	301	CDL	OB8-CB7-C71	2.58	120.01	111.91
29	f	303	CDL	OA8-CA7-C31	2.58	120.01	111.91
29	k	202	CDL	CA4-OA6-CA5	-2.58	111.44	117.79
33	G	301	ATP	PA-O3A-PB	-2.56	124.03	132.83
33	C1	601	ATP	PA-O3A-PB	-2.56	124.05	132.83
32	i	302	UQ8	C27-C28-C29	-2.56	121.50	127.66
30	G	304	PC1	O31-C31-C32	2.53	119.85	111.91
29	L	301	CDL	OA8-CA7-C31	2.51	119.80	111.91
29	k	201	CDL	OB8-CB7-C71	2.51	119.79	111.91
29	f	302	CDL	OA8-CA7-C31	2.50	119.77	111.91
29	K	201	CDL	OA8-CA7-C31	2.50	119.76	111.91
29	f	304	CDL	OB8-CB7-C71	2.49	119.72	111.91
29	K	202	CDL	OB8-CB7-C71	2.49	119.72	111.91
35	A	501	PEE	O3-C30-C31	2.48	119.70	111.91
29	J	302	CDL	OB8-CB7-C71	2.48	119.70	111.91
29	I	301	CDL	OB8-CB7-C71	2.48	119.68	111.91
32	I	303	UQ8	C1M-C1-C6	-2.47	120.36	124.40
29	l	302	CDL	CB4-OB6-CB5	-2.47	111.72	117.79
29	P	201	CDL	OB8-CB7-C71	2.46	119.62	111.91
29	B	404	CDL	OA8-CA7-C31	2.46	119.61	111.91
29	f	304	CDL	OA8-CA7-C31	2.45	119.61	111.91
29	f	302	CDL	OB8-CB7-C71	2.45	119.59	111.91
29	L	302	CDL	OB8-CB7-C71	2.45	119.58	111.91
33	A1	601	ATP	C3'-C2'-C1'	2.44	104.66	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	g	304	PC1	O31-C31-C32	2.44	119.56	111.91
29	j	301	CDL	OB8-CB7-C71	2.43	119.54	111.91
29	l	302	CDL	OA8-CA7-C31	2.43	119.53	111.91
32	I	303	UQ8	C10-C9-C11	2.42	119.34	115.27
29	j	302	CDL	OB8-CB7-C71	2.41	119.48	111.91
33	B1	601	ATP	PA-O3A-PB	-2.41	124.56	132.83
29	I	302	CDL	OB8-CB7-C71	2.41	119.46	111.91
36	E	900	NAD	C3D-C2D-C1D	2.39	104.58	100.98
33	B2	601	ATP	PA-O3A-PB	-2.39	124.64	132.83
32	i	302	UQ8	C46-C44-C45	2.38	119.86	114.60
29	a	502	CDL	CA6-CA4-CA3	-2.37	106.19	111.79
33	g	301	ATP	PA-O3A-PB	-2.36	124.71	132.83
32	I	303	UQ8	C37-C38-C39	-2.35	122.00	127.66
29	k	202	CDL	OB8-CB7-C71	2.35	119.27	111.91
29	B	404	CDL	CA6-CA4-CA3	-2.35	106.24	111.79
33	B2	601	ATP	C2'-C3'-C4'	2.34	107.18	102.64
33	B1	601	ATP	C2'-C3'-C4'	2.32	107.15	102.64
29	I	301	CDL	OA8-CA7-C31	2.32	119.19	111.91
32	i	302	UQ8	C1M-C1-C6	-2.32	120.62	124.40
29	A	502	CDL	OB8-CB7-C71	2.31	119.14	111.91
29	K	202	CDL	CA4-OA6-CA5	-2.30	112.13	117.79
29	B	401	CDL	OA8-CA7-C31	2.29	119.11	111.91
29	p	201	CDL	OA8-CA7-C31	2.29	119.10	111.91
35	L	303	PEE	O3-C30-C31	2.28	119.06	111.91
29	J	302	CDL	OA8-CA7-C31	2.24	118.95	111.91
32	i	302	UQ8	C12-C13-C14	-2.23	122.30	127.66
29	a	501	CDL	OA8-CA7-C31	2.22	118.87	111.91
29	a	501	CDL	OB6-CB5-OB7	-2.22	118.35	123.70
32	I	303	UQ8	C25-C24-C23	-2.21	118.00	123.68
37	B1	603	ADP	C2'-C3'-C4'	2.21	106.94	102.64
29	P	201	CDL	OA8-CA7-C31	2.21	118.83	111.91
29	P	201	CDL	CA4-OA6-CA5	-2.20	112.36	117.79
36	e	900	NAD	C6N-N1N-C2N	-2.20	119.97	121.97
29	F	302	CDL	OA8-CA7-C31	2.20	118.80	111.91
36	E	900	NAD	C6N-N1N-C2N	-2.20	119.97	121.97
29	B	403	CDL	OA8-CA7-C31	2.17	118.73	111.91
32	I	303	UQ8	C35-C34-C33	-2.17	118.11	123.68
35	m	301	PEE	C40-C39-C38	-2.14	108.32	124.73
32	i	302	UQ8	C35-C34-C36	2.14	118.86	115.27
32	I	303	UQ8	C30-C29-C31	2.14	118.86	115.27
29	a	502	CDL	C41-C40-C39	-2.12	103.65	114.42
32	i	302	UQ8	C42-C43-C44	-2.12	120.50	127.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	502	CDL	C39-C38-C37	-2.12	103.67	114.42
29	f	303	CDL	CA6-CA4-CA3	-2.11	106.79	111.79
32	I	303	UQ8	C46-C44-C45	2.11	119.25	114.60
35	m	301	PEE	C17-C18-C19	-2.10	108.64	124.73
32	i	302	UQ8	C10-C9-C11	2.08	118.77	115.27
32	I	303	UQ8	C42-C43-C44	-2.07	120.66	127.75
35	L	303	PEE	C40-C39-C38	-2.07	108.82	124.73
37	B2	603	ADP	C2'-C3'-C4'	2.07	106.66	102.64
35	J	303	PEE	C17-C18-C19	-2.05	109.00	124.73
32	I	303	UQ8	C15-C14-C16	2.05	118.72	115.27
29	B	401	CDL	OB8-CB7-C71	2.00	118.19	111.91
29	l	301	CDL	CA4-OA6-CA5	-2.00	112.86	117.79

There are no chirality outliers.

All (1499) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	a	501	CDL	OA5-CA3-CA4-OA6
29	a	501	CDL	CB3-OB5-PB2-OB4
29	a	501	CDL	OB7-CB5-OB6-CB4
29	a	501	CDL	C51-CB5-OB6-CB4
29	a	502	CDL	CA3-OA5-PA1-OA3
29	b	401	CDL	CB3-OB5-PB2-OB4
29	b	401	CDL	OB7-CB5-OB6-CB4
29	b	401	CDL	C51-CB5-OB6-CB4
29	f	302	CDL	C1-CA2-OA2-PA1
29	f	302	CDL	CA4-CA3-OA5-PA1
29	f	302	CDL	C11-CA5-OA6-CA4
29	f	302	CDL	CB2-OB2-PB2-OB3
29	f	302	CDL	CB2-OB2-PB2-OB4
29	f	302	CDL	CB2-OB2-PB2-OB5
29	f	302	CDL	CB3-OB5-PB2-OB2
29	f	302	CDL	CB3-OB5-PB2-OB3
29	f	302	CDL	CB3-OB5-PB2-OB4
29	f	303	CDL	OA7-CA5-OA6-CA4
29	f	303	CDL	CB3-OB5-PB2-OB2
29	f	303	CDL	CB3-OB5-PB2-OB3
29	f	303	CDL	CB3-OB5-PB2-OB4
29	f	303	CDL	OB6-CB4-CB6-OB8
29	f	303	CDL	C51-CB5-OB6-CB4
29	f	304	CDL	C1-CA2-OA2-PA1
29	f	304	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
29	f	304	CDL	OA5-CA3-CA4-OA6
29	f	304	CDL	C51-CB5-OB6-CB4
29	i	301	CDL	CB3-OB5-PB2-OB2
29	i	301	CDL	CB3-OB5-PB2-OB4
29	i	301	CDL	OB7-CB5-OB6-CB4
29	k	201	CDL	CA3-OA5-PA1-OA3
29	k	201	CDL	OA7-CA5-OA6-CA4
29	k	201	CDL	C11-CA5-OA6-CA4
29	k	201	CDL	CB2-OB2-PB2-OB4
29	k	201	CDL	CB3-OB5-PB2-OB3
29	k	201	CDL	CB3-OB5-PB2-OB4
29	k	202	CDL	OA5-CA3-CA4-OA6
29	k	202	CDL	CB3-OB5-PB2-OB2
29	k	202	CDL	CB3-OB5-PB2-OB3
29	k	202	CDL	CB3-OB5-PB2-OB4
29	j	301	CDL	CB3-OB5-PB2-OB3
29	j	302	CDL	CA3-OA5-PA1-OA4
29	j	302	CDL	CB3-OB5-PB2-OB2
29	j	302	CDL	CB3-OB5-PB2-OB3
29	j	302	CDL	CB3-OB5-PB2-OB4
29	l	302	CDL	CB3-OB5-PB2-OB3
29	p	201	CDL	CA2-OA2-PA1-OA3
29	p	201	CDL	CA3-OA5-PA1-OA3
29	p	201	CDL	C11-CA5-OA6-CA4
29	p	201	CDL	CB2-OB2-PB2-OB3
29	p	201	CDL	CB3-OB5-PB2-OB2
29	p	201	CDL	CB3-OB5-PB2-OB3
29	p	201	CDL	CB3-OB5-PB2-OB4
29	r	201	CDL	CA3-OA5-PA1-OA2
29	r	201	CDL	CB2-OB2-PB2-OB3
29	A	502	CDL	C1-CA2-OA2-PA1
29	A	502	CDL	C11-CA5-OA6-CA4
29	A	502	CDL	CB3-OB5-PB2-OB2
29	A	502	CDL	CB3-OB5-PB2-OB3
29	A	502	CDL	CB3-OB5-PB2-OB4
29	A	502	CDL	C51-CB5-OB6-CB4
29	B	401	CDL	CA4-CA3-OA5-PA1
29	B	401	CDL	C11-CA5-OA6-CA4
29	B	402	CDL	OA7-CA5-OA6-CA4
29	B	402	CDL	CB3-OB5-PB2-OB2
29	B	402	CDL	CB3-OB5-PB2-OB3
29	B	402	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
29	B	402	CDL	OB7-CB5-OB6-CB4
29	B	402	CDL	C51-CB5-OB6-CB4
29	B	404	CDL	O1-C1-CB2-OB2
29	B	404	CDL	CA2-C1-CB2-OB2
29	B	404	CDL	C11-CA5-OA6-CA4
29	B	404	CDL	OA9-CA7-OA8-CA6
29	B	404	CDL	CB3-OB5-PB2-OB2
29	B	404	CDL	CB3-OB5-PB2-OB3
29	B	404	CDL	CB3-OB5-PB2-OB4
29	B	404	CDL	OB6-CB4-CB6-OB8
29	F	302	CDL	CB2-OB2-PB2-OB3
29	F	302	CDL	CB2-OB2-PB2-OB5
29	F	302	CDL	CB3-OB5-PB2-OB3
29	F	302	CDL	CB3-OB5-PB2-OB4
29	F	302	CDL	OB7-CB5-OB6-CB4
29	I	301	CDL	CB2-C1-CA2-OA2
29	I	301	CDL	CA3-OA5-PA1-OA3
29	I	301	CDL	CA3-OA5-PA1-OA4
29	I	301	CDL	CB3-OB5-PB2-OB3
29	I	301	CDL	CB3-OB5-PB2-OB4
29	I	302	CDL	CA3-OA5-PA1-OA2
29	I	302	CDL	CB3-OB5-PB2-OB2
29	I	302	CDL	CB3-OB5-PB2-OB3
29	I	302	CDL	CB3-OB5-PB2-OB4
29	I	302	CDL	OB7-CB5-OB6-CB4
29	I	302	CDL	C51-CB5-OB6-CB4
29	K	201	CDL	CA3-OA5-PA1-OA3
29	K	201	CDL	OA7-CA5-OA6-CA4
29	K	201	CDL	C11-CA5-OA6-CA4
29	K	202	CDL	OA5-CA3-CA4-OA6
29	K	202	CDL	CB3-OB5-PB2-OB3
29	K	202	CDL	CB3-OB5-PB2-OB4
29	J	301	CDL	CA2-OA2-PA1-OA3
29	J	301	CDL	OB7-CB5-OB6-CB4
29	J	301	CDL	C51-CB5-OB6-CB4
29	J	302	CDL	CB3-OB5-PB2-OB3
29	J	302	CDL	CB3-OB5-PB2-OB4
29	L	301	CDL	CA3-OA5-PA1-OA3
29	L	301	CDL	C11-CA5-OA6-CA4
29	L	301	CDL	CB3-OB5-PB2-OB3
29	L	302	CDL	CA3-OA5-PA1-OA3
29	L	302	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
29	P	201	CDL	C11-CA5-OA6-CA4
29	P	201	CDL	CB2-OB2-PB2-OB3
29	P	201	CDL	CB2-OB2-PB2-OB5
29	P	201	CDL	CB3-OB5-PB2-OB2
29	P	201	CDL	CB3-OB5-PB2-OB3
29	P	201	CDL	CB3-OB5-PB2-OB4
30	d	301	PC1	C1-O11-P-O14
30	d	301	PC1	O13-C11-C12-N
30	d	301	PC1	O22-C21-O21-C2
30	g	303	PC1	O13-C11-C12-N
30	g	303	PC1	C2-C1-O11-P
30	g	304	PC1	O22-C21-O21-C2
30	g	304	PC1	C22-C21-O21-C2
30	D	301	PC1	C1-O11-P-O14
30	D	301	PC1	O13-C11-C12-N
30	D	301	PC1	O22-C21-O21-C2
30	D	301	PC1	C22-C21-O21-C2
30	G	303	PC1	C1-O11-P-O12
30	G	304	PC1	O22-C21-O21-C2
32	i	302	UQ8	C34-C36-C37-C38
32	I	303	UQ8	C29-C31-C32-C33
33	B1	601	ATP	C5'-O5'-PA-O1A
33	A1	601	ATP	C5'-O5'-PA-O3A
33	A1	601	ATP	C3'-C4'-C5'-O5'
33	C2	601	ATP	C5'-O5'-PA-O3A
33	B2	601	ATP	C5'-O5'-PA-O1A
33	A2	601	ATP	C5'-O5'-PA-O3A
33	A2	601	ATP	C3'-C4'-C5'-O5'
35	m	301	PEE	C1-O3P-P-O2P
35	m	301	PEE	C4-O4P-P-O2P
35	m	301	PEE	C4-O4P-P-O1P
35	A	501	PEE	C1-O3P-P-O2P
35	A	501	PEE	C1-O3P-P-O1P
35	A	501	PEE	C4-O4P-P-O1P
35	J	303	PEE	O2-C2-C3-O3
35	J	303	PEE	C1-O3P-P-O2P
35	J	303	PEE	C4-O4P-P-O2P
35	J	303	PEE	C4-O4P-P-O1P
35	L	303	PEE	C1-O3P-P-O2P
35	L	303	PEE	C1-O3P-P-O1P
35	L	303	PEE	C4-O4P-P-O1P
36	e	900	NAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
36	e	900	NAD	O4D-C4D-C5D-O5D
36	E	900	NAD	C5B-O5B-PA-O1A
36	E	900	NAD	O4D-C4D-C5D-O5D
37	D1	501	ADP	C5'-O5'-PA-O1A
37	D2	501	ADP	C5'-O5'-PA-O1A
37	B2	603	ADP	PA-O3A-PB-O2B
37	B2	603	ADP	PA-O3A-PB-O3B
29	B	403	CDL	OB9-CB7-OB8-CB6
29	I	301	CDL	OB9-CB7-OB8-CB6
29	B	403	CDL	C71-CB7-OB8-CB6
35	m	301	PEE	C31-C30-O3-C3
29	f	303	CDL	OA9-CA7-OA8-CA6
29	f	303	CDL	OB9-CB7-OB8-CB6
29	j	302	CDL	OA9-CA7-OA8-CA6
29	l	302	CDL	OB9-CB7-OB8-CB6
29	r	201	CDL	OA9-CA7-OA8-CA6
29	B	404	CDL	OB9-CB7-OB8-CB6
29	I	301	CDL	OA9-CA7-OA8-CA6
29	J	302	CDL	OA9-CA7-OA8-CA6
35	m	301	PEE	O5-C30-O3-C3
35	A	501	PEE	O5-C30-O3-C3
35	L	303	PEE	O5-C30-O3-C3
29	f	302	CDL	OA7-CA5-OA6-CA4
29	f	303	CDL	OB7-CB5-OB6-CB4
29	k	202	CDL	OA7-CA5-OA6-CA4
29	p	201	CDL	OA7-CA5-OA6-CA4
29	A	502	CDL	OA7-CA5-OA6-CA4
29	A	502	CDL	OB7-CB5-OB6-CB4
29	B	401	CDL	OA7-CA5-OA6-CA4
29	B	404	CDL	OA7-CA5-OA6-CA4
29	L	301	CDL	OA7-CA5-OA6-CA4
29	f	303	CDL	C31-CA7-OA8-CA6
29	f	303	CDL	C71-CB7-OB8-CB6
29	j	302	CDL	C31-CA7-OA8-CA6
29	l	302	CDL	C71-CB7-OB8-CB6
29	r	201	CDL	C31-CA7-OA8-CA6
29	B	404	CDL	C31-CA7-OA8-CA6
29	B	404	CDL	C71-CB7-OB8-CB6
29	I	301	CDL	C71-CB7-OB8-CB6
30	d	301	PC1	C32-C31-O31-C3
29	f	303	CDL	C11-CA5-OA6-CA4
29	i	301	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
29	k	202	CDL	C11-CA5-OA6-CA4
29	B	402	CDL	C11-CA5-OA6-CA4
29	F	302	CDL	C51-CB5-OB6-CB4
30	d	301	PC1	C22-C21-O21-C2
30	G	304	PC1	C22-C21-O21-C2
29	r	201	CDL	OB9-CB7-OB8-CB6
29	f	304	CDL	C31-CA7-OA8-CA6
29	f	304	CDL	C71-CB7-OB8-CB6
29	I	301	CDL	C31-CA7-OA8-CA6
29	K	201	CDL	C71-CB7-OB8-CB6
29	K	202	CDL	C31-CA7-OA8-CA6
29	J	302	CDL	C31-CA7-OA8-CA6
35	A	501	PEE	C31-C30-O3-C3
35	L	303	PEE	C31-C30-O3-C3
29	f	304	CDL	OB7-CB5-OB6-CB4
29	P	201	CDL	OA7-CA5-OA6-CA4
29	a	502	CDL	OB9-CB7-OB8-CB6
29	f	304	CDL	OA9-CA7-OA8-CA6
29	K	201	CDL	OB9-CB7-OB8-CB6
29	K	202	CDL	OA9-CA7-OA8-CA6
29	B	402	CDL	O1-C1-CA2-OA2
29	k	201	CDL	C71-CB7-OB8-CB6
29	k	202	CDL	C31-CA7-OA8-CA6
29	r	201	CDL	C71-CB7-OB8-CB6
29	L	301	CDL	C71-CB7-OB8-CB6
29	k	201	CDL	OB9-CB7-OB8-CB6
30	d	301	PC1	O32-C31-O31-C3
29	i	301	CDL	C11-CA5-OA6-CA4
29	r	201	CDL	C11-CA5-OA6-CA4
29	K	202	CDL	C11-CA5-OA6-CA4
29	f	304	CDL	OB9-CB7-OB8-CB6
29	I	302	CDL	C76-C77-C78-C79
29	K	201	CDL	C62-C63-C64-C65
33	A1	601	ATP	O4'-C4'-C5'-O5'
33	A2	601	ATP	O4'-C4'-C5'-O5'
36	E	900	NAD	O4B-C4B-C5B-O5B
29	a	502	CDL	C71-CB7-OB8-CB6
29	k	202	CDL	OA9-CA7-OA8-CA6
29	L	301	CDL	OB9-CB7-OB8-CB6
32	I	303	UQ8	C34-C36-C37-C38
29	l	301	CDL	C31-CA7-OA8-CA6
29	l	301	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
29	I	302	CDL	C22-C23-C24-C25
29	a	502	CDL	CB2-C1-CA2-OA2
29	B	403	CDL	CB2-C1-CA2-OA2
29	K	202	CDL	OA7-CA5-OA6-CA4
29	f	304	CDL	C22-C23-C24-C25
29	B	401	CDL	C71-CB7-OB8-CB6
30	D	301	PC1	C32-C31-O31-C3
29	b	401	CDL	C16-C17-C18-C19
29	a	502	CDL	O1-C1-CA2-OA2
29	f	303	CDL	O1-C1-CB2-OB2
29	B	404	CDL	CB7-C71-C72-C73
30	D	301	PC1	O32-C31-O31-C3
29	r	201	CDL	OA7-CA5-OA6-CA4
29	f	304	CDL	C11-CA5-OA6-CA4
29	B	402	CDL	CA5-C11-C12-C13
29	i	301	CDL	C31-CA7-OA8-CA6
29	I	302	CDL	C31-CA7-OA8-CA6
29	i	301	CDL	CB5-C51-C52-C53
29	B	404	CDL	CA5-C11-C12-C13
29	f	302	CDL	CA7-C31-C32-C33
29	f	303	CDL	CB7-C71-C72-C73
29	k	201	CDL	CA7-C31-C32-C33
29	l	302	CDL	CA5-C11-C12-C13
29	B	401	CDL	CA5-C11-C12-C13
29	P	201	CDL	CA5-C11-C12-C13
35	m	301	PEE	C43-C44-C45-C46
36	e	900	NAD	C3B-C4B-C5B-O5B
36	e	900	NAD	C3D-C4D-C5D-O5D
36	E	900	NAD	C3B-C4B-C5B-O5B
36	E	900	NAD	C3D-C4D-C5D-O5D
29	l	301	CDL	C54-C55-C56-C57
29	i	301	CDL	OA7-CA5-OA6-CA4
30	g	304	PC1	C21-C22-C23-C24
29	B	401	CDL	OB9-CB7-OB8-CB6
32	i	302	UQ8	C29-C31-C32-C33
29	B	403	CDL	O1-C1-CA2-OA2
29	l	301	CDL	OA9-CA7-OA8-CA6
29	l	301	CDL	OB9-CB7-OB8-CB6
29	B	401	CDL	CB5-C51-C52-C53
29	L	301	CDL	C81-C82-C83-C84
29	i	301	CDL	OA9-CA7-OA8-CA6
29	I	302	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
29	J	301	CDL	C11-CA5-OA6-CA4
29	l	302	CDL	C20-C21-C22-C23
29	L	302	CDL	C40-C41-C42-C43
29	a	501	CDL	CB3-OB5-PB2-OB2
29	f	302	CDL	CA2-OA2-PA1-OA5
29	f	303	CDL	CB2-OB2-PB2-OB5
29	i	301	CDL	CA3-OA5-PA1-OA2
29	k	201	CDL	CB2-OB2-PB2-OB5
29	k	201	CDL	CB3-OB5-PB2-OB2
29	k	202	CDL	CB2-OB2-PB2-OB5
29	j	302	CDL	CA3-OA5-PA1-OA2
29	l	301	CDL	CA3-OA5-PA1-OA2
29	l	301	CDL	CB3-OB5-PB2-OB2
29	r	201	CDL	CB2-OB2-PB2-OB5
29	B	401	CDL	CB3-OB5-PB2-OB2
29	B	404	CDL	CB2-OB2-PB2-OB5
29	F	302	CDL	CB3-OB5-PB2-OB2
29	I	301	CDL	CA3-OA5-PA1-OA2
29	I	301	CDL	CB2-OB2-PB2-OB5
29	K	201	CDL	CB2-OB2-PB2-OB5
29	K	202	CDL	CB3-OB5-PB2-OB2
29	J	301	CDL	CB3-OB5-PB2-OB2
29	J	302	CDL	CA3-OA5-PA1-OA2
29	J	302	CDL	CB3-OB5-PB2-OB2
29	L	301	CDL	CA3-OA5-PA1-OA2
29	L	301	CDL	CB3-OB5-PB2-OB2
29	L	302	CDL	CA3-OA5-PA1-OA2
29	L	302	CDL	CB3-OB5-PB2-OB2
30	g	303	PC1	C1-O11-P-O13
35	m	301	PEE	C1-O3P-P-O4P
35	m	301	PEE	C4-O4P-P-O3P
35	A	501	PEE	C1-O3P-P-O4P
35	J	303	PEE	C4-O4P-P-O3P
35	L	303	PEE	C1-O3P-P-O4P
29	a	502	CDL	CA5-C11-C12-C13
30	G	304	PC1	C32-C31-O31-C3
29	a	501	CDL	CA7-C31-C32-C33
30	g	303	PC1	C31-C32-C33-C34
29	f	304	CDL	OA7-CA5-OA6-CA4
29	J	301	CDL	OA7-CA5-OA6-CA4
29	k	202	CDL	C71-CB7-OB8-CB6
29	j	302	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
29	K	202	CDL	C71-CB7-OB8-CB6
29	j	302	CDL	CA7-C31-C32-C33
35	A	501	PEE	C10-C11-C12-C13
35	L	303	PEE	C10-C11-C12-C13
29	j	302	CDL	C41-C42-C43-C44
29	B	402	CDL	C54-C55-C56-C57
29	K	202	CDL	C58-C59-C60-C61
29	K	202	CDL	C74-C75-C76-C77
29	P	201	CDL	C54-C55-C56-C57
29	a	501	CDL	C11-CA5-OA6-CA4
29	a	502	CDL	C11-CA5-OA6-CA4
29	f	302	CDL	C51-CB5-OB6-CB4
29	j	302	CDL	C11-CA5-OA6-CA4
29	I	301	CDL	C11-CA5-OA6-CA4
29	I	302	CDL	C11-CA5-OA6-CA4
35	J	303	PEE	C11-C10-O2-C2
29	f	302	CDL	C62-C63-C64-C65
29	j	302	CDL	C36-C37-C38-C39
29	A	502	CDL	C56-C57-C58-C59
29	B	403	CDL	C18-C19-C20-C21
29	F	302	CDL	C35-C36-C37-C38
29	K	202	CDL	C83-C84-C85-C86
30	g	303	PC1	C2D-C2E-C2F-C2G
35	J	303	PEE	C41-C42-C43-C44
35	L	303	PEE	C34-C35-C36-C37
29	b	401	CDL	C81-C82-C83-C84
29	f	302	CDL	C35-C36-C37-C38
29	k	202	CDL	C74-C75-C76-C77
29	l	302	CDL	C22-C23-C24-C25
29	l	302	CDL	C74-C75-C76-C77
29	I	302	CDL	C13-C14-C15-C16
29	J	301	CDL	C35-C36-C37-C38
29	J	301	CDL	C72-C73-C74-C75
29	P	201	CDL	C74-C75-C76-C77
29	a	501	CDL	OA7-CA5-OA6-CA4
29	a	502	CDL	OA7-CA5-OA6-CA4
29	j	302	CDL	OA7-CA5-OA6-CA4
29	I	301	CDL	OA7-CA5-OA6-CA4
29	I	302	CDL	OA7-CA5-OA6-CA4
35	J	303	PEE	O4-C10-O2-C2
29	j	301	CDL	C72-C73-C74-C75
29	j	302	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
29	B	403	CDL	C76-C77-C78-C79
29	J	302	CDL	C77-C78-C79-C80
29	L	302	CDL	C21-C22-C23-C24
29	a	501	CDL	C60-C61-C62-C63
29	b	401	CDL	C11-C12-C13-C14
29	f	303	CDL	C51-C52-C53-C54
29	B	402	CDL	C83-C84-C85-C86
29	K	201	CDL	C74-C75-C76-C77
29	L	301	CDL	C83-C84-C85-C86
30	D	301	PC1	C27-C28-C29-C2A
29	b	401	CDL	O1-C1-CA2-OA2
29	I	301	CDL	O1-C1-CA2-OA2
29	I	302	CDL	O1-C1-CA2-OA2
29	a	501	CDL	C58-C59-C60-C61
29	k	202	CDL	C19-C20-C21-C22
29	j	301	CDL	C31-C32-C33-C34
29	I	302	CDL	C82-C83-C84-C85
29	i	301	CDL	CB7-C71-C72-C73
29	B	403	CDL	CA5-C11-C12-C13
29	a	501	CDL	C53-C54-C55-C56
29	l	301	CDL	C21-C22-C23-C24
29	A	502	CDL	C14-C15-C16-C17
29	B	401	CDL	C41-C42-C43-C44
29	F	302	CDL	C52-C53-C54-C55
29	L	301	CDL	C71-C72-C73-C74
29	L	301	CDL	C74-C75-C76-C77
29	f	304	CDL	C11-C12-C13-C14
29	j	301	CDL	C11-C12-C13-C14
29	j	301	CDL	C22-C23-C24-C25
29	l	301	CDL	C34-C35-C36-C37
29	B	401	CDL	C81-C82-C83-C84
29	J	302	CDL	C38-C39-C40-C41
29	A	502	CDL	CB5-C51-C52-C53
29	F	302	CDL	CB5-C51-C52-C53
29	f	303	CDL	C76-C77-C78-C79
29	f	304	CDL	C75-C76-C77-C78
29	i	301	CDL	C19-C20-C21-C22
29	k	201	CDL	C76-C77-C78-C79
29	j	301	CDL	C16-C17-C18-C19
29	l	302	CDL	C15-C16-C17-C18
29	K	202	CDL	C43-C44-C45-C46
30	d	301	PC1	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
35	A	501	PEE	C42-C43-C44-C45
29	i	301	CDL	C74-C75-C76-C77
29	A	502	CDL	C80-C81-C82-C83
29	B	401	CDL	C38-C39-C40-C41
29	B	402	CDL	C22-C23-C24-C25
29	I	302	CDL	C72-C73-C74-C75
30	d	301	PC1	C35-C36-C37-C38
29	f	302	CDL	OB7-CB5-OB6-CB4
29	j	301	CDL	OA7-CA5-OA6-CA4
29	j	301	CDL	C11-CA5-OA6-CA4
29	f	302	CDL	C19-C20-C21-C22
29	i	301	CDL	C81-C82-C83-C84
29	k	201	CDL	C36-C37-C38-C39
29	l	302	CDL	C83-C84-C85-C86
29	B	401	CDL	C22-C23-C24-C25
29	B	404	CDL	C12-C13-C14-C15
29	r	201	CDL	CA7-C31-C32-C33
29	r	201	CDL	CB7-C71-C72-C73
29	a	501	CDL	C51-C52-C53-C54
29	b	401	CDL	C56-C57-C58-C59
29	f	302	CDL	C17-C18-C19-C20
29	k	201	CDL	C37-C38-C39-C40
29	l	302	CDL	C55-C56-C57-C58
29	p	201	CDL	C22-C23-C24-C25
29	p	201	CDL	C73-C74-C75-C76
29	B	402	CDL	C75-C76-C77-C78
29	B	403	CDL	C81-C82-C83-C84
29	B	404	CDL	C35-C36-C37-C38
29	F	302	CDL	C38-C39-C40-C41
29	F	302	CDL	C78-C79-C80-C81
29	I	301	CDL	C74-C75-C76-C77
29	I	302	CDL	C74-C75-C76-C77
29	J	301	CDL	C63-C64-C65-C66
29	L	301	CDL	C37-C38-C39-C40
29	P	201	CDL	C23-C24-C25-C26
30	g	303	PC1	C2C-C2D-C2E-C2F
30	G	304	PC1	C2C-C2D-C2E-C2F
29	a	502	CDL	C37-C38-C39-C40
29	j	301	CDL	C20-C21-C22-C23
29	j	301	CDL	C37-C38-C39-C40
29	A	502	CDL	C72-C73-C74-C75
29	B	401	CDL	C63-C64-C65-C66

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Mol	Chain	Res	Type	Atoms
29	J	302	CDL	C16-C17-C18-C19
29	f	302	CDL	C56-C57-C58-C59
29	f	302	CDL	C78-C79-C80-C81
29	K	201	CDL	C54-C55-C56-C57
29	L	301	CDL	C31-C32-C33-C34
29	L	302	CDL	C83-C84-C85-C86
30	g	304	PC1	C24-C25-C26-C27
30	G	304	PC1	C34-C35-C36-C37
29	k	202	CDL	OB9-CB7-OB8-CB6
29	j	302	CDL	OB9-CB7-OB8-CB6
29	f	303	CDL	C80-C81-C82-C83
29	j	301	CDL	C33-C34-C35-C36
29	F	302	CDL	C20-C21-C22-C23
30	G	304	PC1	C29-C2A-C2B-C2C
35	m	301	PEE	C14-C15-C16-C17
35	J	303	PEE	C23-C24-C25-C26
30	g	304	PC1	C32-C31-O31-C3
29	a	501	CDL	C38-C39-C40-C41
29	b	401	CDL	C40-C41-C42-C43
29	A	502	CDL	C21-C22-C23-C24
29	B	404	CDL	C57-C58-C59-C60
29	I	301	CDL	C60-C61-C62-C63
29	J	302	CDL	C74-C75-C76-C77
29	a	501	CDL	C43-C44-C45-C46
29	p	201	CDL	C54-C55-C56-C57
29	A	502	CDL	C74-C75-C76-C77
29	L	301	CDL	C54-C55-C56-C57
30	d	301	PC1	C37-C38-C39-C3A
35	A	501	PEE	C32-C33-C34-C35
29	f	304	CDL	CA7-C31-C32-C33
30	G	304	PC1	O32-C31-O31-C3
29	j	302	CDL	C74-C75-C76-C77
29	l	302	CDL	C36-C37-C38-C39
29	A	502	CDL	C16-C17-C18-C19
29	J	301	CDL	C33-C34-C35-C36
35	J	303	PEE	C17-C18-C19-C20
29	f	303	CDL	C35-C36-C37-C38
29	f	304	CDL	C18-C19-C20-C21
29	l	301	CDL	C37-C38-C39-C40
29	J	302	CDL	C13-C14-C15-C16
29	J	302	CDL	C31-C32-C33-C34
29	f	302	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	K	202	CDL	CA5-C11-C12-C13
29	b	401	CDL	C71-CB7-OB8-CB6
29	j	301	CDL	C51-CB5-OB6-CB4
29	r	201	CDL	CB4-CB6-OB8-CB7
29	a	501	CDL	C56-C57-C58-C59
29	a	502	CDL	C57-C58-C59-C60
29	j	301	CDL	C82-C83-C84-C85
29	A	502	CDL	C83-C84-C85-C86
29	f	302	CDL	C80-C81-C82-C83
29	k	201	CDL	C18-C19-C20-C21
29	j	302	CDL	C13-C14-C15-C16
29	K	201	CDL	C56-C57-C58-C59
35	m	301	PEE	C19-C20-C21-C22
29	K	202	CDL	OB9-CB7-OB8-CB6
29	f	304	CDL	CB5-C51-C52-C53
29	K	202	CDL	CB5-C51-C52-C53
29	j	302	CDL	C52-C53-C54-C55
29	B	404	CDL	C43-C44-C45-C46
29	L	301	CDL	C78-C79-C80-C81
29	B	404	CDL	O1-C1-CA2-OA2
29	a	502	CDL	C22-C23-C24-C25
29	L	301	CDL	C38-C39-C40-C41
29	l	302	CDL	C17-C18-C19-C20
29	I	302	CDL	C79-C80-C81-C82
29	L	302	CDL	C72-C73-C74-C75
29	f	304	CDL	CA5-C11-C12-C13
29	F	302	CDL	CB7-C71-C72-C73
29	a	501	CDL	C74-C75-C76-C77
29	b	401	CDL	C53-C54-C55-C56
29	f	303	CDL	C77-C78-C79-C80
29	f	302	CDL	C23-C24-C25-C26
29	I	302	CDL	C60-C61-C62-C63
29	J	301	CDL	C21-C22-C23-C24
29	L	302	CDL	C74-C75-C76-C77
29	L	302	CDL	C76-C77-C78-C79
29	a	501	CDL	C1-CB2-OB2-PB2
30	g	304	PC1	O32-C31-O31-C3
29	f	302	CDL	C42-C43-C44-C45
29	F	302	CDL	C39-C40-C41-C42
29	J	302	CDL	C52-C53-C54-C55
30	d	301	PC1	C2B-C2C-C2D-C2E
29	l	301	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
29	p	201	CDL	C52-C53-C54-C55
29	p	201	CDL	C58-C59-C60-C61
29	r	201	CDL	C82-C83-C84-C85
29	a	502	CDL	C51-C52-C53-C54
29	a	501	CDL	C21-C22-C23-C24
29	l	302	CDL	C62-C63-C64-C65
29	B	402	CDL	C60-C61-C62-C63
29	B	402	CDL	C71-C72-C73-C74
30	g	303	PC1	C3D-C3E-C3F-C3G
29	l	302	CDL	C71-C72-C73-C74
29	K	201	CDL	C40-C41-C42-C43
29	K	201	CDL	C71-C72-C73-C74
29	b	401	CDL	OB9-CB7-OB8-CB6
30	d	301	PC1	C24-C25-C26-C27
35	m	301	PEE	C35-C36-C37-C38
35	J	303	PEE	C19-C20-C21-C22
29	j	301	CDL	OB7-CB5-OB6-CB4
29	j	302	CDL	OB7-CB5-OB6-CB4
29	B	403	CDL	OA7-CA5-OA6-CA4
35	m	301	PEE	O4-C10-O2-C2
29	f	303	CDL	CA5-C11-C12-C13
29	k	202	CDL	CA5-C11-C12-C13
29	j	301	CDL	C31-CA7-OA8-CA6
29	I	302	CDL	C71-CB7-OB8-CB6
29	P	201	CDL	C31-CA7-OA8-CA6
29	a	502	CDL	C76-C77-C78-C79
29	i	301	CDL	C76-C77-C78-C79
29	J	301	CDL	C52-C53-C54-C55
35	A	501	PEE	C41-C42-C43-C44
29	B	401	CDL	C36-C37-C38-C39
29	B	404	CDL	C13-C14-C15-C16
30	g	303	PC1	C37-C38-C39-C3A
29	f	302	CDL	C38-C39-C40-C41
29	i	301	CDL	C36-C37-C38-C39
29	i	301	CDL	C61-C62-C63-C64
29	j	302	CDL	C72-C73-C74-C75
29	A	502	CDL	C35-C36-C37-C38
29	I	301	CDL	C78-C79-C80-C81
29	L	301	CDL	C15-C16-C17-C18
29	L	302	CDL	C42-C43-C44-C45
35	L	303	PEE	C32-C33-C34-C35
29	L	301	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
29	a	501	CDL	C83-C84-C85-C86
29	I	301	CDL	C71-C72-C73-C74
29	I	302	CDL	C56-C57-C58-C59
29	f	302	CDL	C81-C82-C83-C84
29	I	301	CDL	C19-C20-C21-C22
29	L	302	CDL	C19-C20-C21-C22
30	g	303	PC1	C24-C25-C26-C27
30	D	301	PC1	C28-C29-C2A-C2B
29	L	302	CDL	CA5-C11-C12-C13
29	j	302	CDL	C51-CB5-OB6-CB4
29	l	301	CDL	C11-CA5-OA6-CA4
29	B	403	CDL	C11-CA5-OA6-CA4
29	J	302	CDL	C51-CB5-OB6-CB4
35	m	301	PEE	C11-C10-O2-C2
29	i	301	CDL	OB5-CB3-CB4-OB6
29	k	202	CDL	C40-C41-C42-C43
29	b	401	CDL	C42-C43-C44-C45
29	f	303	CDL	C13-C14-C15-C16
29	k	201	CDL	C40-C41-C42-C43
29	L	301	CDL	CA5-C11-C12-C13
29	f	302	CDL	C77-C78-C79-C80
29	F	302	CDL	C11-C12-C13-C14
29	a	502	CDL	C43-C44-C45-C46
29	F	302	CDL	C82-C83-C84-C85
29	K	202	CDL	C77-C78-C79-C80
32	I	303	UQ8	C40-C39-C41-C42
29	f	302	CDL	C51-C52-C53-C54
29	r	201	CDL	C58-C59-C60-C61
29	j	302	CDL	C22-C23-C24-C25
29	B	401	CDL	C59-C60-C61-C62
29	J	301	CDL	C22-C23-C24-C25
29	a	501	CDL	C31-C32-C33-C34
29	J	301	CDL	C31-C32-C33-C34
30	D	301	PC1	C39-C3A-C3B-C3C
29	l	301	CDL	OA7-CA5-OA6-CA4
29	J	302	CDL	OB7-CB5-OB6-CB4
29	b	401	CDL	C38-C39-C40-C41
29	B	402	CDL	C74-C75-C76-C77
29	B	403	CDL	C52-C53-C54-C55
30	G	304	PC1	C27-C28-C29-C2A
29	a	502	CDL	CA3-OA5-PA1-OA2
29	b	401	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
29	j	301	CDL	CB3-OB5-PB2-OB2
29	p	201	CDL	CA3-OA5-PA1-OA2
29	p	201	CDL	CB2-OB2-PB2-OB5
29	B	401	CDL	CA2-OA2-PA1-OA5
29	B	403	CDL	CB2-OB2-PB2-OB5
29	I	301	CDL	CB3-OB5-PB2-OB2
30	d	301	PC1	C1-O11-P-O13
30	D	301	PC1	C1-O11-P-O13
30	G	303	PC1	C11-O13-P-O11
30	G	303	PC1	C1-O11-P-O13
35	A	501	PEE	C4-O4P-P-O3P
35	J	303	PEE	C1-O3P-P-O4P
35	L	303	PEE	C4-O4P-P-O3P
29	j	302	CDL	C20-C21-C22-C23
30	D	301	PC1	C25-C26-C27-C28
29	B	401	CDL	C1-CA2-OA2-PA1
29	a	501	CDL	OA5-CA3-CA4-CA6
29	b	401	CDL	OA5-CA3-CA4-CA6
29	f	304	CDL	OA5-CA3-CA4-CA6
29	i	301	CDL	OB5-CB3-CB4-CB6
29	r	201	CDL	OA5-CA3-CA4-CA6
29	F	302	CDL	OB5-CB3-CB4-CB6
29	K	202	CDL	OA5-CA3-CA4-CA6
29	P	201	CDL	OB5-CB3-CB4-CB6
29	B	404	CDL	C79-C80-C81-C82
29	F	302	CDL	C41-C42-C43-C44
35	L	303	PEE	C43-C44-C45-C46
29	f	302	CDL	C74-C75-C76-C77
35	J	303	PEE	C31-C32-C33-C34
29	B	401	CDL	C39-C40-C41-C42
29	f	302	CDL	C33-C34-C35-C36
29	f	303	CDL	C38-C39-C40-C41
30	d	301	PC1	C2A-C2B-C2C-C2D
30	g	304	PC1	C33-C34-C35-C36
29	j	302	CDL	C16-C17-C18-C19
29	a	501	CDL	C72-C73-C74-C75
29	k	202	CDL	C31-C32-C33-C34
29	l	301	CDL	C32-C33-C34-C35
35	A	501	PEE	C33-C34-C35-C36
29	j	301	CDL	OA9-CA7-OA8-CA6
29	b	401	CDL	C71-C72-C73-C74
29	p	201	CDL	C63-C64-C65-C66

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Mol	Chain	Res	Type	Atoms
29	b	401	CDL	CB3-CB4-CB6-OB8
29	f	303	CDL	CB3-CB4-CB6-OB8
29	j	302	CDL	CA3-CA4-CA6-OA8
29	p	201	CDL	C64-C65-C66-C67
29	r	201	CDL	CB3-CB4-CB6-OB8
29	B	404	CDL	CB3-CB4-CB6-OB8
29	I	301	CDL	CB3-CB4-CB6-OB8
29	I	302	CDL	CB3-CB4-CB6-OB8
29	K	202	CDL	CB3-CB4-CB6-OB8
29	P	201	CDL	CA3-CA4-CA6-OA8
30	G	303	PC1	C3F-C3G-C3H-C3I
29	P	201	CDL	OA9-CA7-OA8-CA6
29	f	302	CDL	C58-C59-C60-C61
29	I	302	CDL	C36-C37-C38-C39
29	a	501	CDL	C11-C12-C13-C14
29	a	502	CDL	C80-C81-C82-C83
29	p	201	CDL	C41-C42-C43-C44
29	I	301	CDL	C17-C18-C19-C20
30	D	301	PC1	C29-C2A-C2B-C2C
30	G	303	PC1	C22-C23-C24-C25
29	B	401	CDL	C32-C31-CA7-OA8
29	I	302	CDL	OB9-CB7-OB8-CB6
29	a	502	CDL	C24-C25-C26-C27
29	F	302	CDL	C51-C52-C53-C54
29	F	302	CDL	C74-C75-C76-C77
29	F	302	CDL	C83-C84-C85-C86
29	f	302	CDL	C44-C45-C46-C47
29	J	302	CDL	C59-C60-C61-C62
30	g	303	PC1	C3F-C3G-C3H-C3I
29	k	202	CDL	C79-C80-C81-C82
29	r	201	CDL	C74-C75-C76-C77
29	I	301	CDL	C53-C54-C55-C56
29	J	302	CDL	C18-C19-C20-C21
29	L	302	CDL	CA7-C31-C32-C33
30	g	304	PC1	C27-C28-C29-C2A
37	B1	603	ADP	PA-O3A-PB-O1B
29	p	201	CDL	CA7-C31-C32-C33
30	G	303	PC1	C31-C32-C33-C34
29	F	302	CDL	CB4-CB6-OB8-CB7
29	p	201	CDL	C72-C73-C74-C75
29	A	502	CDL	C38-C39-C40-C41
29	K	201	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
29	f	302	CDL	C84-C85-C86-C87
29	L	302	CDL	C59-C60-C61-C62
29	A	502	CDL	OB5-CB3-CB4-OB6
29	A	502	CDL	C60-C61-C62-C63
29	j	302	CDL	C24-C25-C26-C27
29	j	301	CDL	C12-C13-C14-C15
29	K	202	CDL	C51-C52-C53-C54
29	J	301	CDL	C12-C13-C14-C15
29	a	501	CDL	C16-C17-C18-C19
29	k	201	CDL	C38-C39-C40-C41
29	I	301	CDL	CB4-CB6-OB8-CB7
29	f	303	CDL	C58-C59-C60-C61
29	I	302	CDL	C81-C82-C83-C84
30	g	304	PC1	C23-C24-C25-C26
29	a	502	CDL	C41-C42-C43-C44
29	a	502	CDL	C58-C59-C60-C61
29	f	304	CDL	C35-C36-C37-C38
29	l	302	CDL	C76-C77-C78-C79
29	L	301	CDL	C16-C17-C18-C19
29	L	301	CDL	C44-C45-C46-C47
32	I	303	UQ8	C30-C29-C31-C32
29	L	301	CDL	C33-C34-C35-C36
29	J	301	CDL	C78-C79-C80-C81
29	L	302	CDL	C31-CA7-OA8-CA6
29	B	401	CDL	C84-C85-C86-C87
29	f	302	CDL	C36-C37-C38-C39
29	A	502	CDL	CB2-C1-CA2-OA2
29	B	402	CDL	CB2-C1-CA2-OA2
29	I	302	CDL	CB2-C1-CA2-OA2
29	b	401	CDL	C11-CA5-OA6-CA4
29	f	303	CDL	C73-C74-C75-C76
29	B	404	CDL	C77-C78-C79-C80
29	L	302	CDL	C11-C12-C13-C14
30	D	301	PC1	C3F-C3G-C3H-C3I
29	p	201	CDL	C31-CA7-OA8-CA6
29	J	302	CDL	C71-CB7-OB8-CB6
29	i	301	CDL	C22-C23-C24-C25
29	I	302	CDL	C58-C59-C60-C61
29	j	302	CDL	CB5-C51-C52-C53
29	f	302	CDL	OA5-CA3-CA4-CA6
29	A	502	CDL	OB5-CB3-CB4-CB6
29	B	404	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
29	I	301	CDL	OA5-CA3-CA4-CA6
29	J	301	CDL	OA5-CA3-CA4-CA6
29	L	302	CDL	OA5-CA3-CA4-CA6
30	G	303	PC1	O11-C1-C2-C3
30	G	304	PC1	O11-C1-C2-C3
35	m	301	PEE	O3P-C1-C2-C3
29	j	301	CDL	C74-C75-C76-C77
30	G	304	PC1	C3D-C3E-C3F-C3G
29	A	502	CDL	CA7-C31-C32-C33
29	k	201	CDL	C16-C17-C18-C19
29	l	302	CDL	C31-CA7-OA8-CA6
29	B	402	CDL	C71-CB7-OB8-CB6
29	r	201	CDL	C52-C53-C54-C55
32	i	302	UQ8	C40-C39-C41-C42
29	J	301	CDL	C74-C75-C76-C77
35	L	303	PEE	C14-C15-C16-C17
29	L	302	CDL	C51-CB5-OB6-CB4
29	B	401	CDL	C31-CA7-OA8-CA6
29	a	501	CDL	C13-C14-C15-C16
29	l	302	CDL	C58-C59-C60-C61
29	B	403	CDL	C1-CB2-OB2-PB2
29	f	304	CDL	C40-C41-C42-C43
29	p	201	CDL	C59-C60-C61-C62
29	f	304	CDL	C63-C64-C65-C66
29	l	302	CDL	C64-C65-C66-C67
29	K	201	CDL	C52-C53-C54-C55
30	G	304	PC1	C2F-C2G-C2H-C2I
29	i	301	CDL	C51-C52-C53-C54
29	p	201	CDL	C61-C62-C63-C64
29	B	404	CDL	C32-C33-C34-C35
29	a	501	CDL	CB3-CB4-CB6-OB8
29	j	301	CDL	CB3-CB4-CB6-OB8
29	F	302	CDL	CB3-CB4-CB6-OB8
29	J	302	CDL	CA3-CA4-CA6-OA8
30	g	303	PC1	C1-C2-C3-O31
30	D	301	PC1	C1-C2-C3-O31
30	G	303	PC1	C1-C2-C3-O31
35	J	303	PEE	C1-C2-C3-O3
29	a	502	CDL	C52-C53-C54-C55
29	r	201	CDL	C35-C36-C37-C38
29	a	502	CDL	CA7-C31-C32-C33
29	j	301	CDL	C61-C62-C63-C64

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Mol	Chain	Res	Type	Atoms
29	l	301	CDL	C11-C12-C13-C14
29	l	302	CDL	C77-C78-C79-C80
35	A	501	PEE	C14-C15-C16-C17
29	f	303	CDL	C79-C80-C81-C82
35	J	303	PEE	C34-C35-C36-C37
29	B	404	CDL	C74-C75-C76-C77
29	I	301	CDL	C76-C77-C78-C79
29	L	301	CDL	C61-C62-C63-C64
32	I	303	UQ8	C38-C39-C41-C42
32	I	303	UQ8	C28-C29-C31-C32
29	k	201	CDL	C54-C55-C56-C57
29	B	403	CDL	C57-C58-C59-C60
29	K	202	CDL	C64-C65-C66-C67
29	P	201	CDL	C58-C59-C60-C61
29	a	502	CDL	CB2-OB2-PB2-OB5
29	A	502	CDL	CA3-OA5-PA1-OA2
29	J	301	CDL	CA2-OA2-PA1-OA5
29	J	302	CDL	CA2-OA2-PA1-OA5
29	f	303	CDL	C16-C17-C18-C19
29	I	301	CDL	C21-C22-C23-C24
29	B	402	CDL	C40-C41-C42-C43
29	a	502	CDL	OA5-CA3-CA4-OA6
29	b	401	CDL	OA5-CA3-CA4-OA6
29	b	401	CDL	OB5-CB3-CB4-OB6
29	f	302	CDL	OA5-CA3-CA4-OA6
29	j	302	CDL	OB5-CB3-CB4-OB6
29	B	403	CDL	OA5-CA3-CA4-OA6
29	I	302	CDL	OB5-CB3-CB4-OB6
29	L	302	CDL	OA5-CA3-CA4-OA6
29	k	201	CDL	CB4-CB6-OB8-CB7
29	f	302	CDL	C72-C71-CB7-OB8
29	L	302	CDL	OA9-CA7-OA8-CA6
29	i	301	CDL	C84-C85-C86-C87
29	j	301	CDL	C80-C81-C82-C83
29	l	301	CDL	C44-C45-C46-C47
29	p	201	CDL	C23-C24-C25-C26
29	r	201	CDL	C16-C17-C18-C19
35	L	303	PEE	C44-C45-C46-C47
29	a	501	CDL	OB6-CB4-CB6-OB8
29	I	301	CDL	OB6-CB4-CB6-OB8
30	d	301	PC1	O21-C2-C3-O31
30	g	303	PC1	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
29	l	301	CDL	C62-C63-C64-C65
29	l	301	CDL	C24-C25-C26-C27
29	j	301	CDL	C52-C53-C54-C55
29	a	501	CDL	C33-C34-C35-C36
29	b	401	CDL	C23-C24-C25-C26
29	k	201	CDL	C24-C25-C26-C27
29	k	201	CDL	C75-C76-C77-C78
29	B	401	CDL	C12-C13-C14-C15
29	F	302	CDL	C40-C41-C42-C43
29	i	301	CDL	C41-C42-C43-C44
29	a	502	CDL	C1-CB2-OB2-PB2
29	a	502	CDL	CB4-CB3-OB5-PB2
29	f	304	CDL	CA4-CA3-OA5-PA1
29	L	302	CDL	CA4-CA3-OA5-PA1
30	G	303	PC1	C2-C1-O11-P
35	A	501	PEE	C35-C36-C37-C38
30	D	301	PC1	C32-C33-C34-C35
29	k	201	CDL	C22-C23-C24-C25
29	l	301	CDL	C40-C41-C42-C43
29	l	302	CDL	C32-C31-CA7-OA8
29	B	402	CDL	C32-C31-CA7-OA8
29	r	201	CDL	C64-C65-C66-C67
29	b	401	CDL	OA7-CA5-OA6-CA4
29	L	302	CDL	OB7-CB5-OB6-CB4
29	p	201	CDL	C51-CB5-OB6-CB4
29	F	302	CDL	C11-CA5-OA6-CA4
29	l	301	CDL	C75-C76-C77-C78
29	J	302	CDL	C72-C73-C74-C75
29	f	303	CDL	C11-C12-C13-C14
29	B	402	CDL	C63-C64-C65-C66
29	j	302	CDL	CA5-C11-C12-C13
29	J	301	CDL	CA5-C11-C12-C13
36	e	900	NAD	PA-O3-PN-O5D
36	E	900	NAD	PA-O3-PN-O5D
29	f	303	CDL	C12-C13-C14-C15
29	F	302	CDL	C57-C58-C59-C60
29	J	302	CDL	C41-C42-C43-C44
30	d	301	PC1	C33-C34-C35-C36
29	i	301	CDL	C31-C32-C33-C34
29	a	502	CDL	OB5-CB3-CB4-CB6
29	f	302	CDL	OB5-CB3-CB4-CB6
29	k	202	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
29	j	301	CDL	OA5-CA3-CA4-CA6
29	B	401	CDL	OB5-CB3-CB4-CB6
29	B	403	CDL	OA5-CA3-CA4-CA6
35	J	303	PEE	O3P-C1-C2-C3
29	b	401	CDL	C75-C76-C77-C78
30	G	304	PC1	C37-C38-C39-C3A
29	f	304	CDL	C78-C79-C80-C81
29	l	301	CDL	C61-C62-C63-C64
29	p	201	CDL	OA9-CA7-OA8-CA6
29	j	302	CDL	C34-C35-C36-C37
33	C1	601	ATP	O4'-C4'-C5'-O5'
29	I	301	CDL	C22-C23-C24-C25
29	J	301	CDL	C82-C83-C84-C85
35	m	301	PEE	C40-C41-C42-C43
29	B	403	CDL	CB5-C51-C52-C53
29	p	201	CDL	C71-CB7-OB8-CB6
29	L	302	CDL	C71-CB7-OB8-CB6
29	L	302	CDL	C72-C71-CB7-OB8
29	j	301	CDL	C63-C64-C65-C66
29	A	502	CDL	C34-C35-C36-C37
29	j	302	CDL	CA6-CA4-OA6-CA5
29	r	201	CDL	CA6-CA4-OA6-CA5
29	B	401	CDL	CA3-CA4-OA6-CA5
29	B	403	CDL	CA6-CA4-OA6-CA5
29	I	301	CDL	CA6-CA4-OA6-CA5
29	J	302	CDL	CA6-CA4-OA6-CA5
29	F	302	CDL	OA7-CA5-OA6-CA4
29	f	304	CDL	C54-C55-C56-C57
29	A	502	CDL	C84-C85-C86-C87
29	B	403	CDL	C72-C73-C74-C75
30	G	303	PC1	C3E-C3F-C3G-C3H
29	j	301	CDL	CB5-C51-C52-C53
29	i	301	CDL	C72-C71-CB7-OB8
29	B	401	CDL	C56-C57-C58-C59
29	B	402	CDL	C33-C34-C35-C36
29	K	202	CDL	C81-C82-C83-C84
32	I	303	UQ8	C15-C14-C16-C17
32	i	302	UQ8	C13-C14-C16-C17
32	I	303	UQ8	C13-C14-C16-C17
29	l	301	CDL	C80-C81-C82-C83
29	r	201	CDL	C20-C21-C22-C23
29	f	304	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
29	k	202	CDL	CB3-CB4-CB6-OB8
29	p	201	CDL	CA3-CA4-CA6-OA8
29	B	402	CDL	C1-CA2-OA2-PA1
29	F	302	CDL	CA3-CA4-CA6-OA8
30	d	301	PC1	C1-C2-C3-O31
29	l	302	CDL	OA9-CA7-OA8-CA6
29	J	302	CDL	OB9-CB7-OB8-CB6
29	a	502	CDL	OB5-CB3-CB4-OB6
29	f	304	CDL	OB5-CB3-CB4-OB6
29	r	201	CDL	OA5-CA3-CA4-OA6
29	B	404	CDL	OA5-CA3-CA4-OA6
29	P	201	CDL	OB5-CB3-CB4-OB6
30	G	303	PC1	O11-C1-C2-O21
30	G	304	PC1	O11-C1-C2-O21
35	m	301	PEE	O3P-C1-C2-O2
35	J	303	PEE	O3P-C1-C2-O2
29	J	301	CDL	C72-C71-CB7-OB8
29	f	304	CDL	C13-C14-C15-C16
29	f	304	CDL	C39-C40-C41-C42
30	G	304	PC1	C3B-C3C-C3D-C3E
29	k	202	CDL	C83-C84-C85-C86
29	b	401	CDL	O1-C1-CB2-OB2
29	f	304	CDL	O1-C1-CA2-OA2
29	i	301	CDL	O1-C1-CA2-OA2
29	B	401	CDL	OA9-CA7-OA8-CA6
29	B	402	CDL	OB9-CB7-OB8-CB6
29	L	301	CDL	C77-C78-C79-C80
29	P	201	CDL	C11-C12-C13-C14
30	G	303	PC1	C35-C36-C37-C38
35	A	501	PEE	C43-C44-C45-C46
29	F	302	CDL	C72-C73-C74-C75
29	k	201	CDL	OB6-CB4-CB6-OB8
29	F	302	CDL	OA6-CA4-CA6-OA8
29	I	302	CDL	OB6-CB4-CB6-OB8
29	K	201	CDL	OA6-CA4-CA6-OA8
29	K	202	CDL	OB6-CB4-CB6-OB8
29	J	302	CDL	OB6-CB4-CB6-OB8
30	D	301	PC1	O21-C2-C3-O31
30	G	303	PC1	O21-C2-C3-O31
33	C1	601	ATP	C5'-O5'-PA-O3A
33	B1	601	ATP	C5'-O5'-PA-O3A
33	B2	601	ATP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
36	E	900	NAD	C5B-O5B-PA-O3
29	f	304	CDL	C51-C52-C53-C54
29	L	302	CDL	C78-C79-C80-C81
35	L	303	PEE	C35-C36-C37-C38
32	i	302	UQ8	C15-C14-C16-C17
29	l	302	CDL	OA7-CA5-OA6-CA4
29	p	201	CDL	OB7-CB5-OB6-CB4
30	D	301	PC1	C2A-C2B-C2C-C2D
33	C1	601	ATP	C3'-C4'-C5'-O5'
29	b	401	CDL	CA7-C31-C32-C33
29	I	302	CDL	C20-C21-C22-C23
29	L	302	CDL	OB9-CB7-OB8-CB6
29	r	201	CDL	C33-C34-C35-C36
30	G	303	PC1	C2F-C2G-C2H-C2I
29	f	304	CDL	C42-C43-C44-C45
29	I	301	CDL	C39-C40-C41-C42
29	a	502	CDL	C75-C76-C77-C78
29	f	302	CDL	C31-C32-C33-C34
29	l	302	CDL	CB3-OB5-PB2-OB2
29	B	402	CDL	CA3-OA5-PA1-OA2
29	K	202	CDL	CA3-OA5-PA1-OA2
30	g	303	PC1	C11-O13-P-O11
29	I	302	CDL	C38-C39-C40-C41
29	L	301	CDL	C76-C77-C78-C79
29	A	502	CDL	O1-C1-CA2-OA2
29	i	301	CDL	C57-C58-C59-C60
29	j	301	CDL	C1-CB2-OB2-PB2
29	l	302	CDL	C1-CA2-OA2-PA1
29	J	301	CDL	C1-CB2-OB2-PB2
29	a	502	CDL	CA3-OA5-PA1-OA4
29	b	401	CDL	CA3-OA5-PA1-OA3
29	b	401	CDL	CB3-OB5-PB2-OB3
29	f	302	CDL	CA2-OA2-PA1-OA4
29	f	303	CDL	CB2-OB2-PB2-OB3
29	f	303	CDL	CB2-OB2-PB2-OB4
29	i	301	CDL	CA3-OA5-PA1-OA4
29	i	301	CDL	CB3-OB5-PB2-OB3
29	k	201	CDL	CB2-OB2-PB2-OB3
29	k	202	CDL	CB2-OB2-PB2-OB4
29	l	301	CDL	CA3-OA5-PA1-OA4
29	l	301	CDL	CB3-OB5-PB2-OB3
29	l	301	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
29	l	302	CDL	CA3-OA5-PA1-OA4
29	l	302	CDL	CB3-OB5-PB2-OB4
29	p	201	CDL	CA3-OA5-PA1-OA4
29	r	201	CDL	CB3-OB5-PB2-OB3
29	B	401	CDL	CA2-OA2-PA1-OA4
29	B	401	CDL	CB3-OB5-PB2-OB3
29	B	401	CDL	CB3-OB5-PB2-OB4
29	B	404	CDL	CB2-OB2-PB2-OB3
29	B	404	CDL	CB2-OB2-PB2-OB4
29	F	302	CDL	CA2-OA2-PA1-OA4
29	F	302	CDL	CB2-OB2-PB2-OB4
29	I	301	CDL	CB2-OB2-PB2-OB3
29	I	301	CDL	CB2-OB2-PB2-OB4
29	K	201	CDL	CB2-OB2-PB2-OB3
29	K	201	CDL	CB3-OB5-PB2-OB4
29	J	301	CDL	CB3-OB5-PB2-OB3
29	J	301	CDL	CB3-OB5-PB2-OB4
29	J	302	CDL	CA3-OA5-PA1-OA4
29	L	301	CDL	CA3-OA5-PA1-OA4
29	L	301	CDL	CB3-OB5-PB2-OB4
29	L	302	CDL	CB3-OB5-PB2-OB3
29	L	302	CDL	CB3-OB5-PB2-OB4
29	P	201	CDL	CA3-OA5-PA1-OA4
30	g	303	PC1	C1-O11-P-O14
30	G	303	PC1	C11-O13-P-O12
30	G	303	PC1	C11-O13-P-O14
30	G	303	PC1	C1-O11-P-O14
33	A1	601	ATP	C5'-O5'-PA-O2A
33	C2	601	ATP	C5'-O5'-PA-O2A
33	A2	601	ATP	C5'-O5'-PA-O2A
35	m	301	PEE	C1-O3P-P-O1P
35	A	501	PEE	C4-O4P-P-O2P
35	J	303	PEE	C1-O3P-P-O1P
35	L	303	PEE	C4-O4P-P-O2P
29	a	502	CDL	OA5-CA3-CA4-CA6
29	f	304	CDL	OB5-CB3-CB4-CB6
29	I	302	CDL	OB5-CB3-CB4-CB6
30	g	304	PC1	O11-C1-C2-C3
29	B	401	CDL	C72-C73-C74-C75
29	B	404	CDL	C22-C23-C24-C25
35	m	301	PEE	O4P-C4-C5-N
35	J	303	PEE	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
29	p	201	CDL	C39-C40-C41-C42
29	k	202	CDL	C15-C16-C17-C18
35	L	303	PEE	C12-C13-C14-C15
29	k	201	CDL	C57-C58-C59-C60
29	j	301	CDL	C18-C19-C20-C21
29	B	401	CDL	C72-C71-CB7-OB8
29	K	202	CDL	C61-C62-C63-C64
29	J	302	CDL	C20-C21-C22-C23
29	A	502	CDL	C71-CB7-OB8-CB6
29	f	303	CDL	CA2-C1-CB2-OB2
29	B	404	CDL	C72-C73-C74-C75
29	L	301	CDL	C11-C12-C13-C14
29	b	401	CDL	CB7-C71-C72-C73
29	f	302	CDL	OB5-CB3-CB4-OB6
29	j	301	CDL	OA5-CA3-CA4-OA6
29	j	301	CDL	OB5-CB3-CB4-OB6
29	l	302	CDL	OB5-CB3-CB4-OB6
29	B	401	CDL	OB5-CB3-CB4-OB6
29	B	403	CDL	OB5-CB3-CB4-OB6
29	F	302	CDL	OB5-CB3-CB4-OB6
29	J	301	CDL	OA5-CA3-CA4-OA6
29	B	403	CDL	C19-C20-C21-C22
29	p	201	CDL	OB9-CB7-OB8-CB6
29	f	302	CDL	C64-C65-C66-C67
29	r	201	CDL	C84-C85-C86-C87
29	F	302	CDL	C43-C44-C45-C46
29	K	202	CDL	C31-C32-C33-C34
30	d	301	PC1	C3C-C3D-C3E-C3F
29	l	301	CDL	C72-C71-CB7-OB8
29	I	302	CDL	C72-C71-CB7-OB8
29	K	202	CDL	C17-C18-C19-C20
29	A	502	CDL	C13-C14-C15-C16
29	J	302	CDL	C61-C62-C63-C64
29	k	201	CDL	CB3-CB4-CB6-OB8
29	K	201	CDL	CA3-CA4-CA6-OA8
30	g	304	PC1	O13-C11-C12-N
30	G	304	PC1	O13-C11-C12-N
29	f	304	CDL	OA6-CA4-CA6-OA8
29	j	301	CDL	OB6-CB4-CB6-OB8
29	r	201	CDL	OB6-CB4-CB6-OB8
29	J	301	CDL	OA6-CA4-CA6-OA8
29	J	301	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
29	J	302	CDL	OA6-CA4-CA6-OA8
29	j	301	CDL	C34-C35-C36-C37
29	j	302	CDL	C31-C32-C33-C34
35	J	303	PEE	C33-C34-C35-C36
29	p	201	CDL	C36-C37-C38-C39
29	A	502	CDL	C40-C41-C42-C43
30	G	303	PC1	C25-C26-C27-C28
29	k	202	CDL	C13-C14-C15-C16
29	j	301	CDL	C13-C14-C15-C16
29	b	401	CDL	C32-C31-CA7-OA8
29	J	301	CDL	C17-C18-C19-C20
29	P	201	CDL	C37-C38-C39-C40
30	d	301	PC1	C38-C39-C3A-C3B
29	f	303	CDL	CA4-CA3-OA5-PA1
29	I	302	CDL	CB4-CB3-OB5-PB2
29	L	302	CDL	C1-CA2-OA2-PA1
29	L	302	CDL	C36-C37-C38-C39
29	K	201	CDL	C33-C34-C35-C36
29	A	502	CDL	C61-C62-C63-C64
29	a	501	CDL	C75-C76-C77-C78
29	K	202	CDL	C55-C56-C57-C58
35	J	303	PEE	C14-C15-C16-C17
29	i	301	CDL	C71-CB7-OB8-CB6
29	B	403	CDL	C22-C23-C24-C25
29	P	201	CDL	C34-C35-C36-C37
29	B	404	CDL	C17-C18-C19-C20
29	I	301	CDL	C15-C16-C17-C18
29	l	302	CDL	C11-CA5-OA6-CA4
29	k	201	CDL	C20-C21-C22-C23
29	I	301	CDL	C44-C45-C46-C47
29	L	302	CDL	C24-C25-C26-C27
35	A	501	PEE	C12-C13-C14-C15
29	j	301	CDL	C72-C71-CB7-OB8
29	A	502	CDL	C32-C31-CA7-OA8
29	a	501	CDL	C34-C35-C36-C37
29	B	402	CDL	C16-C17-C18-C19
32	i	302	UQ8	C38-C39-C41-C42
29	j	301	CDL	C55-C56-C57-C58
35	J	303	PEE	C12-C13-C14-C15
29	p	201	CDL	C11-C12-C13-C14
29	a	502	CDL	CA6-CA4-OA6-CA5
29	l	302	CDL	CA6-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
29	p	201	CDL	CA6-CA4-OA6-CA5
29	B	404	CDL	CA3-CA4-OA6-CA5
30	D	301	PC1	C3-C2-O21-C21
29	B	403	CDL	OB5-CB3-CB4-CB6
29	f	302	CDL	CB2-C1-CA2-OA2
29	K	201	CDL	C75-C76-C77-C78
29	L	302	CDL	C33-C34-C35-C36
29	f	303	CDL	C72-C73-C74-C75
29	L	302	CDL	C34-C35-C36-C37
29	b	401	CDL	C61-C62-C63-C64
29	f	302	CDL	C22-C23-C24-C25
29	l	302	CDL	CB4-CB3-OB5-PB2
29	k	202	CDL	C80-C81-C82-C83
29	A	502	CDL	OB9-CB7-OB8-CB6
29	A	502	CDL	OA5-CA3-CA4-OA6
29	a	501	CDL	C15-C16-C17-C18
29	P	201	CDL	CB7-C71-C72-C73
29	L	301	CDL	C31-CA7-OA8-CA6
29	L	301	CDL	OA9-CA7-OA8-CA6
29	I	301	CDL	C43-C44-C45-C46
29	b	401	CDL	OB6-CB4-CB6-OB8
29	j	302	CDL	OA6-CA4-CA6-OA8
29	P	201	CDL	OA6-CA4-CA6-OA8
29	b	401	CDL	CA3-OA5-PA1-OA2
29	f	304	CDL	CA2-OA2-PA1-OA5
29	i	301	CDL	CB2-OB2-PB2-OB5
29	k	202	CDL	CA3-OA5-PA1-OA2
29	l	302	CDL	CA3-OA5-PA1-OA2
29	l	302	CDL	CB2-OB2-PB2-OB5
29	L	301	CDL	CB2-OB2-PB2-OB5
29	P	201	CDL	CA3-OA5-PA1-OA2
29	j	302	CDL	C58-C59-C60-C61
29	A	502	CDL	C33-C34-C35-C36
29	l	301	CDL	C33-C34-C35-C36
29	l	301	CDL	CA7-C31-C32-C33
29	F	302	CDL	C14-C15-C16-C17
30	g	304	PC1	C32-C33-C34-C35
30	g	304	PC1	C3C-C3D-C3E-C3F
29	i	301	CDL	OB9-CB7-OB8-CB6
29	r	201	CDL	C78-C79-C80-C81
29	k	201	CDL	C14-C15-C16-C17
29	I	301	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	f	304	CDL	C36-C37-C38-C39
33	C2	601	ATP	PB-O3A-PA-O2A
29	I	301	CDL	C14-C15-C16-C17
29	L	302	CDL	C44-C45-C46-C47
29	B	404	CDL	C14-C15-C16-C17
29	f	304	CDL	C72-C73-C74-C75
29	I	302	CDL	C31-C32-C33-C34
29	l	302	CDL	C16-C17-C18-C19
29	j	302	CDL	CB4-CB3-OB5-PB2
29	l	301	CDL	CA4-CA3-OA5-PA1
29	L	301	CDL	C1-CA2-OA2-PA1
29	L	302	CDL	CB4-CB3-OB5-PB2
29	f	304	CDL	C53-C54-C55-C56
30	d	301	PC1	C3B-C3C-C3D-C3E
29	J	302	CDL	C22-C23-C24-C25
30	G	303	PC1	C3D-C3E-C3F-C3G
30	D	301	PC1	C34-C35-C36-C37
29	b	401	CDL	C60-C61-C62-C63
29	l	301	CDL	C17-C18-C19-C20
29	k	201	CDL	C31-CA7-OA8-CA6
29	k	201	CDL	C12-C13-C14-C15
29	B	401	CDL	C24-C25-C26-C27
29	I	302	CDL	C34-C35-C36-C37
35	J	303	PEE	C18-C19-C20-C21
29	k	201	CDL	OA9-CA7-OA8-CA6
29	r	201	CDL	C22-C23-C24-C25
29	L	302	CDL	C31-C32-C33-C34
29	J	302	CDL	OB5-CB3-CB4-OB6
29	f	303	CDL	C23-C24-C25-C26
29	k	201	CDL	C59-C60-C61-C62
30	G	303	PC1	C33-C34-C35-C36
29	P	201	CDL	C72-C71-CB7-OB8
30	G	304	PC1	O31-C31-C32-C33
29	B	404	CDL	C20-C21-C22-C23
30	G	303	PC1	C23-C24-C25-C26
29	f	303	CDL	O1-C1-CA2-OA2
29	r	201	CDL	C11-C12-C13-C14
29	B	403	CDL	C56-C57-C58-C59
29	B	404	CDL	C78-C79-C80-C81
29	k	202	CDL	C52-C53-C54-C55
29	A	502	CDL	OB6-CB4-CB6-OB8
29	B	403	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
29	B	401	CDL	C32-C31-CA7-OA9
29	J	302	CDL	C72-C71-CB7-OB8
29	k	202	CDL	C58-C59-C60-C61
29	l	302	CDL	C19-C20-C21-C22
30	g	303	PC1	C3E-C3F-C3G-C3H
29	j	302	CDL	C18-C19-C20-C21
29	J	301	CDL	C39-C40-C41-C42
29	B	402	CDL	C72-C71-CB7-OB8
29	l	302	CDL	C14-C15-C16-C17
29	B	401	CDL	C11-C12-C13-C14
29	k	202	CDL	C56-C57-C58-C59
29	B	401	CDL	C35-C36-C37-C38
29	J	301	CDL	CB3-CB4-CB6-OB8
29	J	302	CDL	CB3-CB4-CB6-OB8
29	B	401	CDL	C20-C21-C22-C23
29	P	201	CDL	C76-C77-C78-C79
29	B	401	CDL	C71-C72-C73-C74
29	p	201	CDL	C37-C38-C39-C40
29	f	302	CDL	CA6-CA4-OA6-CA5
29	B	402	CDL	CB6-CB4-OB6-CB5
29	F	302	CDL	CB3-CB4-OB6-CB5
29	F	302	CDL	CB6-CB4-OB6-CB5
29	L	301	CDL	CA6-CA4-OA6-CA5
30	d	301	PC1	C3-C2-O21-C21
29	b	401	CDL	C21-C22-C23-C24
29	P	201	CDL	C40-C41-C42-C43
29	p	201	CDL	C78-C79-C80-C81
29	B	404	CDL	C58-C59-C60-C61
29	B	403	CDL	C11-C12-C13-C14
29	L	301	CDL	C17-C18-C19-C20
29	B	403	CDL	CB4-CB3-OB5-PB2
29	J	301	CDL	C41-C42-C43-C44
29	J	302	CDL	C24-C25-C26-C27
29	I	301	CDL	OA5-CA3-CA4-OA6
29	j	302	CDL	C72-C71-CB7-OB8
29	A	502	CDL	C53-C54-C55-C56
35	m	301	PEE	C15-C16-C17-C18
35	L	303	PEE	C19-C20-C21-C22
29	A	502	CDL	OA5-CA3-CA4-CA6
30	g	303	PC1	O11-C1-C2-C3
35	m	301	PEE	C36-C37-C38-C39
29	a	502	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
29	k	201	CDL	C72-C73-C74-C75
29	A	502	CDL	C20-C21-C22-C23
29	K	201	CDL	C60-C61-C62-C63
29	L	302	CDL	CB5-C51-C52-C53
29	K	201	CDL	C37-C38-C39-C40
30	g	304	PC1	C2F-C2G-C2H-C2I
35	L	303	PEE	C20-C21-C22-C23
29	F	302	CDL	OB6-CB4-CB6-OB8
29	i	301	CDL	C24-C25-C26-C27
29	P	201	CDL	C59-C60-C61-C62
30	g	304	PC1	O31-C31-C32-C33
29	B	402	CDL	C41-C42-C43-C44
29	B	403	CDL	C53-C54-C55-C56
29	f	303	CDL	C20-C21-C22-C23
30	G	304	PC1	C3A-C3B-C3C-C3D
29	J	302	CDL	C11-C12-C13-C14
29	f	304	CDL	CB2-C1-CA2-OA2
29	i	301	CDL	CB2-C1-CA2-OA2
29	K	201	CDL	CB2-C1-CA2-OA2
30	d	301	PC1	C3F-C3G-C3H-C3I
29	a	502	CDL	C11-C12-C13-C14
29	f	304	CDL	C83-C84-C85-C86
29	j	302	CDL	C32-C33-C34-C35
29	K	201	CDL	C72-C73-C74-C75
35	J	303	PEE	C38-C39-C40-C41
29	J	302	CDL	C15-C16-C17-C18
29	r	201	CDL	C81-C82-C83-C84
29	A	502	CDL	C52-C53-C54-C55
30	g	303	PC1	C23-C24-C25-C26
29	l	301	CDL	C13-C14-C15-C16
30	d	301	PC1	C22-C23-C24-C25
29	p	201	CDL	C82-C83-C84-C85
29	K	201	CDL	C16-C17-C18-C19
29	f	302	CDL	C24-C25-C26-C27
29	f	303	CDL	C14-C15-C16-C17
30	g	304	PC1	C39-C3A-C3B-C3C
35	A	501	PEE	C34-C35-C36-C37
30	g	304	PC1	O11-C1-C2-O21
29	K	202	CDL	C73-C74-C75-C76
29	k	201	CDL	C56-C57-C58-C59
29	F	302	CDL	C63-C64-C65-C66
29	J	302	CDL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
29	J	301	CDL	C59-C60-C61-C62
30	G	303	PC1	C2C-C2D-C2E-C2F
29	P	201	CDL	C80-C81-C82-C83
29	j	302	CDL	OB5-CB3-CB4-CB6
29	l	302	CDL	OB5-CB3-CB4-CB6
29	B	401	CDL	C12-C11-CA5-OA6
29	a	502	CDL	C55-C56-C57-C58
29	f	302	CDL	C72-C73-C74-C75
29	J	301	CDL	C34-C35-C36-C37
29	i	301	CDL	C58-C59-C60-C61
29	j	302	CDL	C1-CB2-OB2-PB2
29	b	401	CDL	CB2-C1-CA2-OA2
29	L	302	CDL	OA6-CA4-CA6-OA8
29	B	403	CDL	OB7-CB5-OB6-CB4
29	k	202	CDL	C53-C54-C55-C56
29	P	201	CDL	C61-C62-C63-C64
29	J	302	CDL	C82-C83-C84-C85
29	f	304	CDL	C12-C11-CA5-OA6
29	A	502	CDL	C36-C37-C38-C39
29	B	401	CDL	C33-C34-C35-C36
29	B	404	CDL	C54-C55-C56-C57
29	b	401	CDL	C44-C45-C46-C47
29	b	401	CDL	CA5-C11-C12-C13
29	b	401	CDL	C52-C51-CB5-OB6
29	L	302	CDL	C32-C31-CA7-OA8
30	g	303	PC1	O31-C31-C32-C33
30	G	303	PC1	O21-C21-C22-C23
29	B	401	CDL	C54-C55-C56-C57
29	l	301	CDL	C58-C59-C60-C61
29	F	302	CDL	C36-C37-C38-C39
35	J	303	PEE	C13-C14-C15-C16
29	k	202	CDL	C12-C11-CA5-OA6
29	B	402	CDL	C52-C51-CB5-OB6
35	J	303	PEE	C36-C37-C38-C39
30	d	301	PC1	C1-C2-O21-C21
29	A	502	CDL	C44-C45-C46-C47
29	J	301	CDL	C80-C81-C82-C83
29	F	302	CDL	C13-C14-C15-C16
29	f	303	CDL	C72-C71-CB7-OB8
29	f	304	CDL	C72-C71-CB7-OB8
29	p	201	CDL	C72-C71-CB7-OB8
29	A	502	CDL	C52-C51-CB5-OB6

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Mol	Chain	Res	Type	Atoms
29	P	201	CDL	C12-C11-CA5-OA6
29	B	403	CDL	C63-C64-C65-C66
29	P	201	CDL	C41-C42-C43-C44
29	k	202	CDL	C72-C71-CB7-OB8
29	F	302	CDL	C72-C71-CB7-OB8
35	L	303	PEE	C36-C37-C38-C39
29	b	401	CDL	C73-C74-C75-C76
29	l	302	CDL	C12-C13-C14-C15
29	B	402	CDL	C84-C85-C86-C87
29	B	402	CDL	CB3-CB4-CB6-OB8
29	K	201	CDL	CB3-CB4-CB6-OB8
29	J	301	CDL	CA3-CA4-CA6-OA8
29	F	302	CDL	C22-C23-C24-C25
29	f	304	CDL	C16-C17-C18-C19
29	k	201	CDL	C42-C43-C44-C45
29	B	404	CDL	C16-C17-C18-C19
29	F	302	CDL	C60-C61-C62-C63
35	L	303	PEE	C38-C39-C40-C41
29	i	301	CDL	C60-C61-C62-C63
29	f	302	CDL	CA4-CA6-OA8-CA7
30	G	304	PC1	C22-C23-C24-C25
29	l	302	CDL	C24-C25-C26-C27
29	b	401	CDL	OB5-CB3-CB4-CB6
29	j	301	CDL	OB5-CB3-CB4-CB6
29	K	202	CDL	OB5-CB3-CB4-CB6
29	I	302	CDL	C41-C42-C43-C44
29	b	401	CDL	C72-C71-CB7-OB8
29	B	404	CDL	C72-C71-CB7-OB8
29	f	302	CDL	OA6-CA4-CA6-OA8
29	B	402	CDL	OB6-CB4-CB6-OB8
29	a	501	CDL	C32-C31-CA7-OA8
29	r	201	CDL	C72-C71-CB7-OB8
29	K	202	CDL	C72-C71-CB7-OB8
29	a	502	CDL	C53-C54-C55-C56
29	l	301	CDL	C12-C13-C14-C15
37	D1	501	ADP	C5'-O5'-PA-O3A
37	D2	501	ADP	C5'-O5'-PA-O3A
30	g	303	PC1	C2A-C2B-C2C-C2D
30	D	301	PC1	C24-C25-C26-C27
29	f	302	CDL	C72-C71-CB7-OB9
35	L	303	PEE	O2-C10-C11-C12
29	J	301	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
29	f	304	CDL	CB4-CB3-OB5-PB2
29	J	302	CDL	CA4-CA3-OA5-PA1
29	B	402	CDL	C52-C53-C54-C55
35	A	501	PEE	C36-C37-C38-C39
29	B	403	CDL	C51-C52-C53-C54
29	p	201	CDL	C34-C35-C36-C37
29	I	301	CDL	C20-C21-C22-C23
29	A	502	CDL	C52-C51-CB5-OB7
33	C1	601	ATP	PB-O3A-PA-O2A
33	A1	601	ATP	PB-O3A-PA-O1A
33	C2	601	ATP	PB-O3A-PA-O1A
33	A2	601	ATP	PB-O3A-PA-O1A
29	p	201	CDL	C79-C80-C81-C82
30	G	303	PC1	C3B-C3C-C3D-C3E
29	B	403	CDL	C51-CB5-OB6-CB4
29	i	301	CDL	CA5-C11-C12-C13
32	i	302	UQ8	C21-C22-C23-C24
32	I	303	UQ8	C16-C17-C18-C19
29	K	202	CDL	C12-C11-CA5-OA6
30	G	303	PC1	O31-C31-C32-C33
29	a	502	CDL	C64-C65-C66-C67
29	I	302	CDL	C64-C65-C66-C67
29	P	201	CDL	C52-C53-C54-C55
35	m	301	PEE	O2-C10-C11-C12
29	l	301	CDL	C16-C17-C18-C19
29	L	302	CDL	C32-C31-CA7-OA9
29	B	401	CDL	C16-C17-C18-C19
29	B	401	CDL	C31-C32-C33-C34
29	K	201	CDL	C44-C45-C46-C47
29	P	201	CDL	C31-C32-C33-C34
29	b	401	CDL	C52-C51-CB5-OB7
29	f	302	CDL	C52-C51-CB5-OB6
35	A	501	PEE	O2-C10-C11-C12
29	b	401	CDL	C20-C21-C22-C23
32	i	302	UQ8	C16-C17-C18-C19
29	p	201	CDL	C75-C76-C77-C78
29	K	202	CDL	C56-C57-C58-C59
29	k	202	CDL	C12-C11-CA5-OA7
30	G	303	PC1	O22-C21-C22-C23
29	f	304	CDL	C72-C71-CB7-OB9
29	F	302	CDL	C72-C71-CB7-OB9
30	g	303	PC1	O32-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
30	G	303	PC1	O32-C31-C32-C33
29	f	302	CDL	C59-C60-C61-C62
29	L	301	CDL	C59-C60-C61-C62
29	L	302	CDL	C13-C14-C15-C16
29	I	301	CDL	C72-C71-CB7-OB8
35	J	303	PEE	C2-C1-O3P-P
30	g	303	PC1	C32-C33-C34-C35
29	B	402	CDL	CB5-C51-C52-C53
29	k	202	CDL	C72-C71-CB7-OB9
29	K	202	CDL	C72-C71-CB7-OB9
29	B	404	CDL	C38-C39-C40-C41
29	L	301	CDL	C18-C19-C20-C21
35	J	303	PEE	C16-C17-C18-C19
29	f	302	CDL	CA2-OA2-PA1-OA3
29	f	304	CDL	CA2-OA2-PA1-OA3
29	k	202	CDL	CA2-OA2-PA1-OA3
29	k	202	CDL	CB2-OB2-PB2-OB3
29	j	301	CDL	CA2-OA2-PA1-OA3
29	j	301	CDL	CB2-OB2-PB2-OB3
29	K	202	CDL	CA2-OA2-PA1-OA3
29	L	302	CDL	CB2-OB2-PB2-OB3
29	P	201	CDL	CA2-OA2-PA1-OA3
30	g	304	PC1	C1-O11-P-O14
30	G	304	PC1	C1-O11-P-O14
33	C1	601	ATP	C5'-O5'-PA-O2A
36	e	900	NAD	C5B-O5B-PA-O1A
29	f	303	CDL	C72-C71-CB7-OB9
29	l	302	CDL	C32-C31-CA7-OA9
29	B	402	CDL	C52-C51-CB5-OB7
29	J	302	CDL	OB5-CB3-CB4-CB6
29	f	304	CDL	C57-C58-C59-C60
29	K	202	CDL	C12-C11-CA5-OA7
29	P	201	CDL	C12-C11-CA5-OA7
29	f	304	CDL	C34-C35-C36-C37
29	l	302	CDL	C53-C54-C55-C56
29	r	201	CDL	C72-C71-CB7-OB9
29	B	402	CDL	C32-C31-CA7-OA9
29	p	201	CDL	C43-C44-C45-C46
30	G	303	PC1	C2B-C2C-C2D-C2E
35	m	301	PEE	C32-C33-C34-C35
29	B	404	CDL	C72-C71-CB7-OB9
29	L	302	CDL	C72-C71-CB7-OB9

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Mol	Chain	Res	Type	Atoms
29	B	403	CDL	C20-C21-C22-C23
29	B	402	CDL	CB3-CB4-OB6-CB5
29	B	404	CDL	CA6-CA4-OA6-CA5
30	g	304	PC1	C12-C11-O13-P
29	J	301	CDL	C18-C19-C20-C21
29	J	301	CDL	C32-C31-CA7-OA8
30	g	303	PC1	O21-C21-C22-C23
29	B	402	CDL	C11-C12-C13-C14
29	a	501	CDL	C32-C31-CA7-OA9
29	a	502	CDL	C42-C43-C44-C45
30	D	301	PC1	C22-C23-C24-C25
29	l	301	CDL	C32-C31-CA7-OA8
29	r	201	CDL	C12-C13-C14-C15
29	J	301	CDL	C51-C52-C53-C54
29	j	301	CDL	C32-C31-CA7-OA8
29	B	404	CDL	C32-C31-CA7-OA8
29	a	502	CDL	C12-C13-C14-C15
29	L	302	CDL	C58-C59-C60-C61
29	a	502	CDL	C54-C55-C56-C57
30	G	303	PC1	C29-C2A-C2B-C2C
29	j	302	CDL	CA4-CA3-OA5-PA1
35	m	301	PEE	C2-C1-O3P-P
29	J	302	CDL	C83-C84-C85-C86
29	I	301	CDL	C72-C71-CB7-OB9
29	J	301	CDL	C32-C33-C34-C35
29	f	302	CDL	C12-C11-CA5-OA6
29	p	201	CDL	C31-C32-C33-C34
29	J	301	CDL	C32-C31-CA7-OA9
35	A	501	PEE	O4-C10-C11-C12
35	L	303	PEE	O4-C10-C11-C12
29	l	301	CDL	C52-C53-C54-C55
29	F	302	CDL	C52-C51-CB5-OB6
29	r	201	CDL	C17-C18-C19-C20
29	A	502	CDL	C71-C72-C73-C74
29	l	301	CDL	C52-C51-CB5-OB6
29	f	304	CDL	C64-C65-C66-C67
29	L	301	CDL	C14-C15-C16-C17
29	l	301	CDL	C32-C31-CA7-OA9
29	B	404	CDL	C32-C31-CA7-OA9
35	m	301	PEE	O4-C10-C11-C12
29	i	301	CDL	C56-C57-C58-C59
29	B	402	CDL	C19-C20-C21-C22

*Continued on next page...*

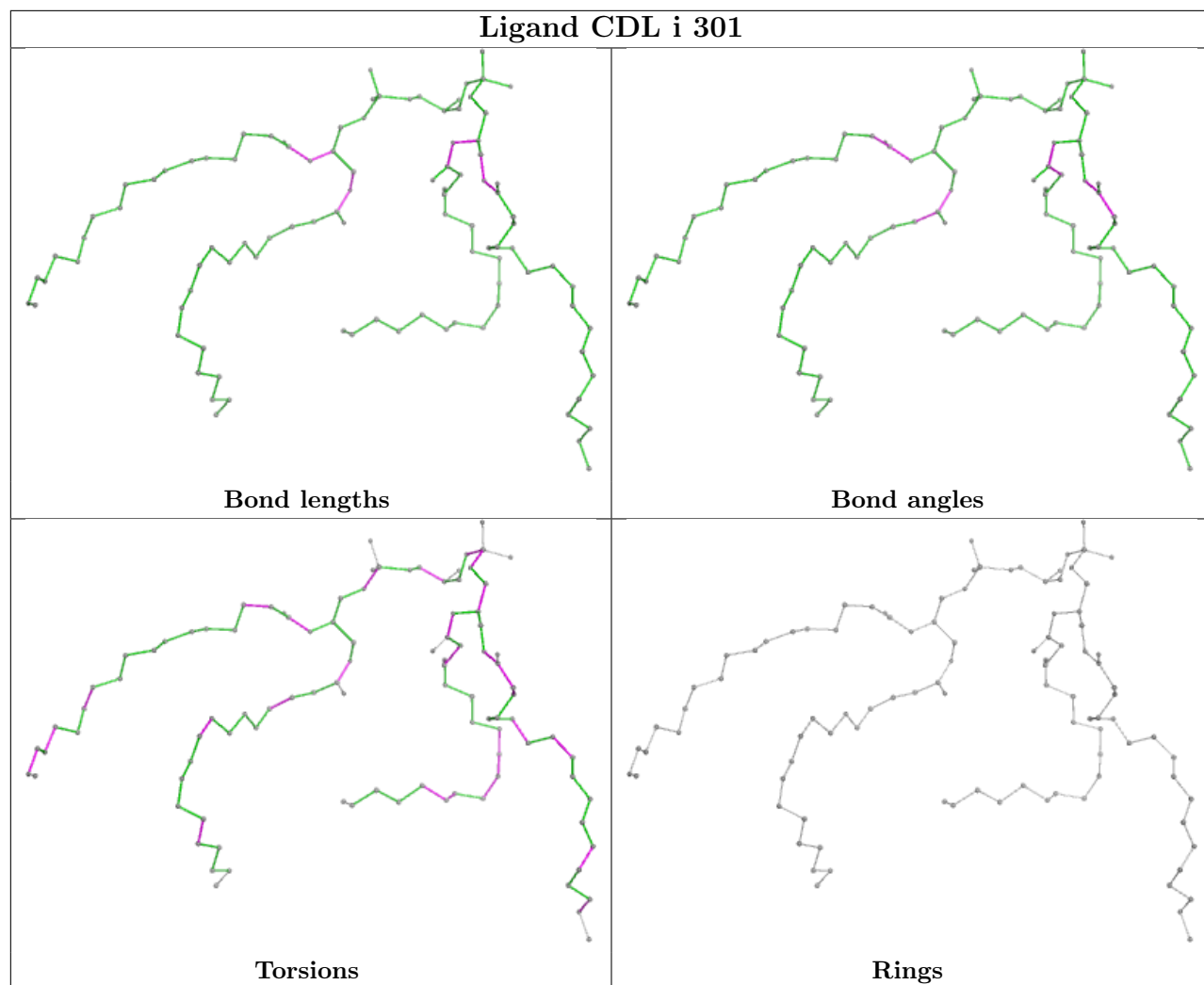
*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	l	301	CDL	C20-C21-C22-C23
29	k	201	CDL	C32-C31-CA7-OA8
29	j	301	CDL	C12-C11-CA5-OA6
35	J	303	PEE	O2-C10-C11-C12

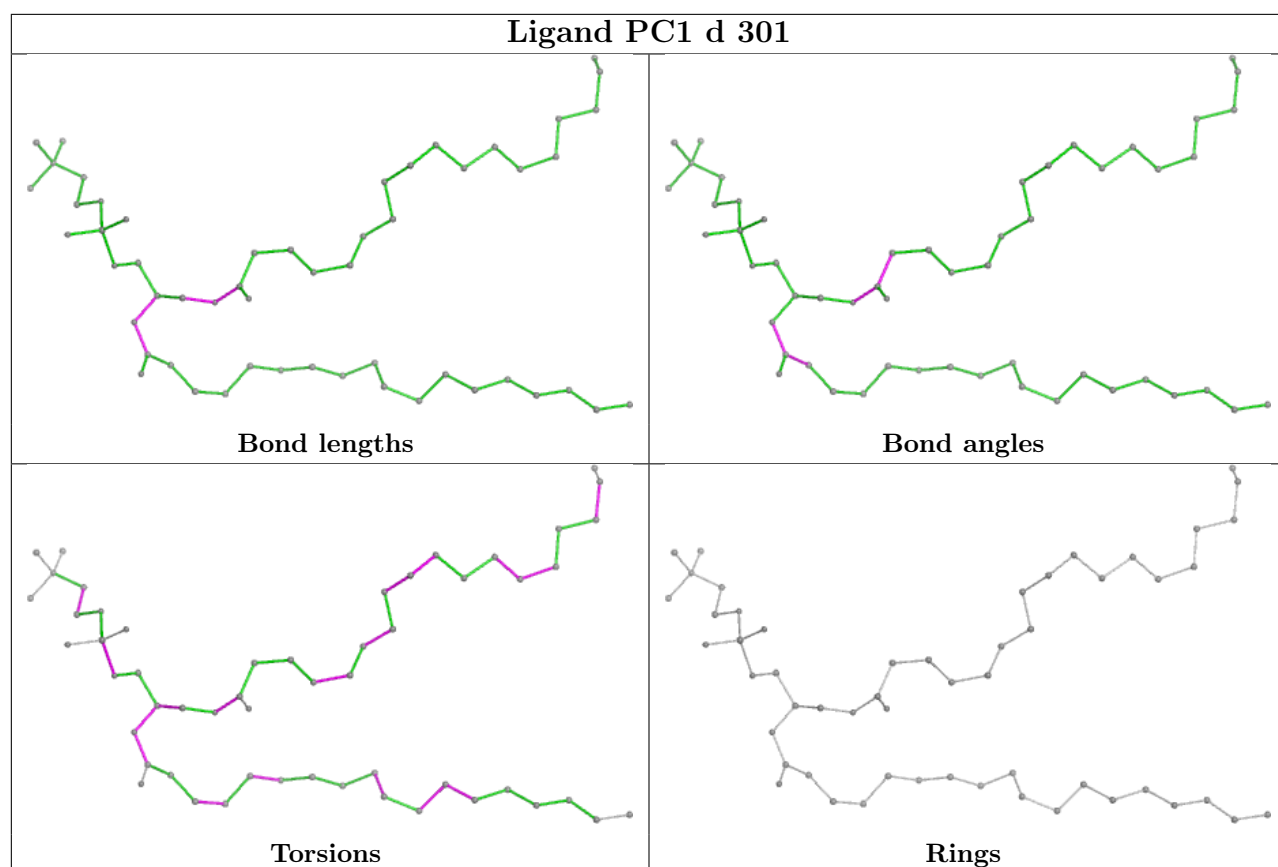
There are no ring outliers.

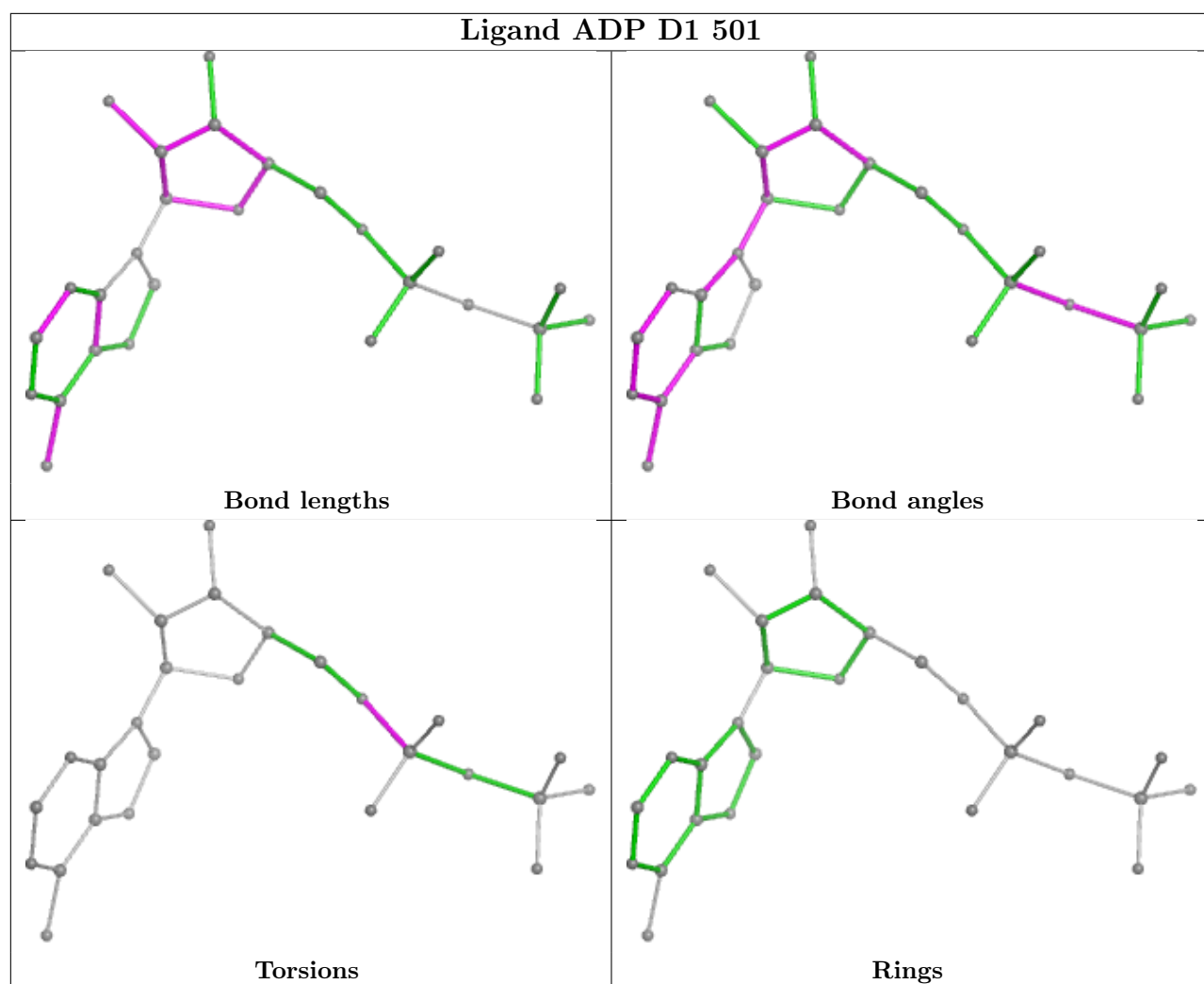
No monomer is involved in short contacts.

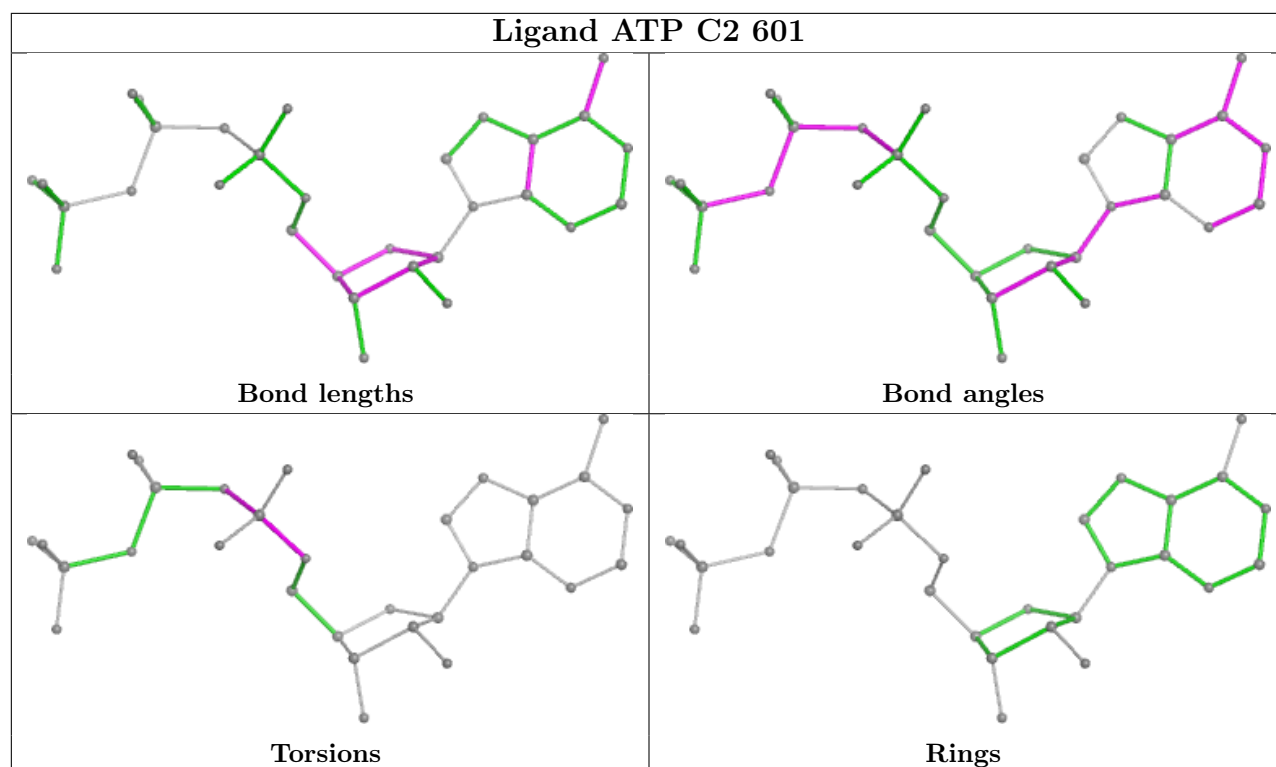
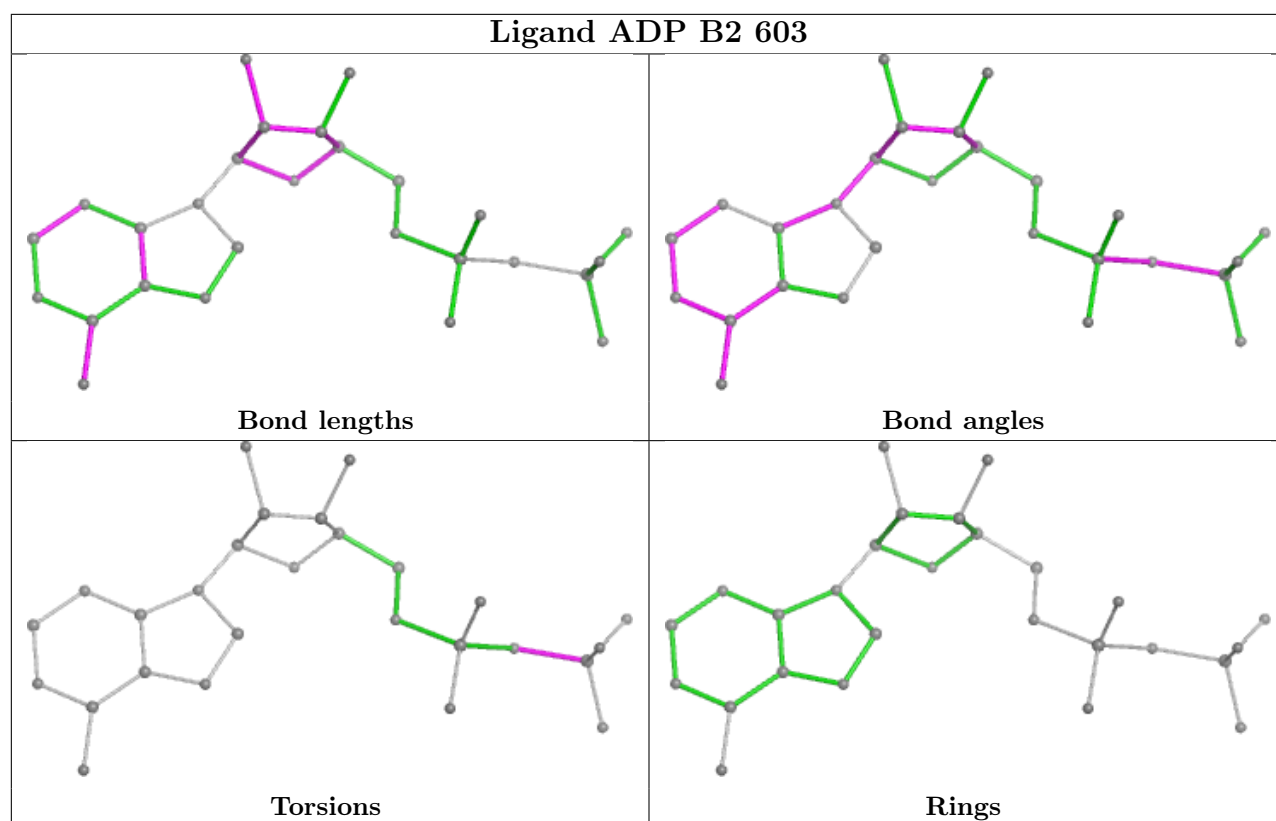
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

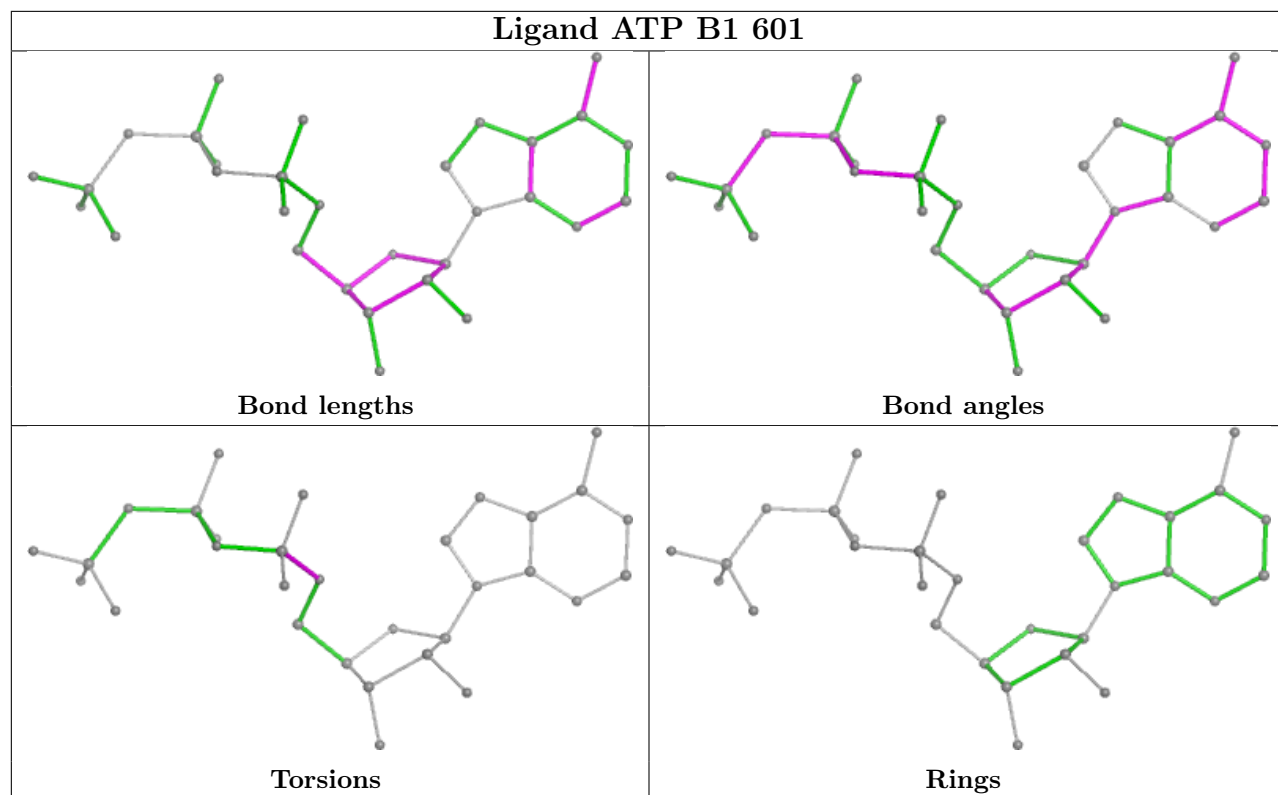


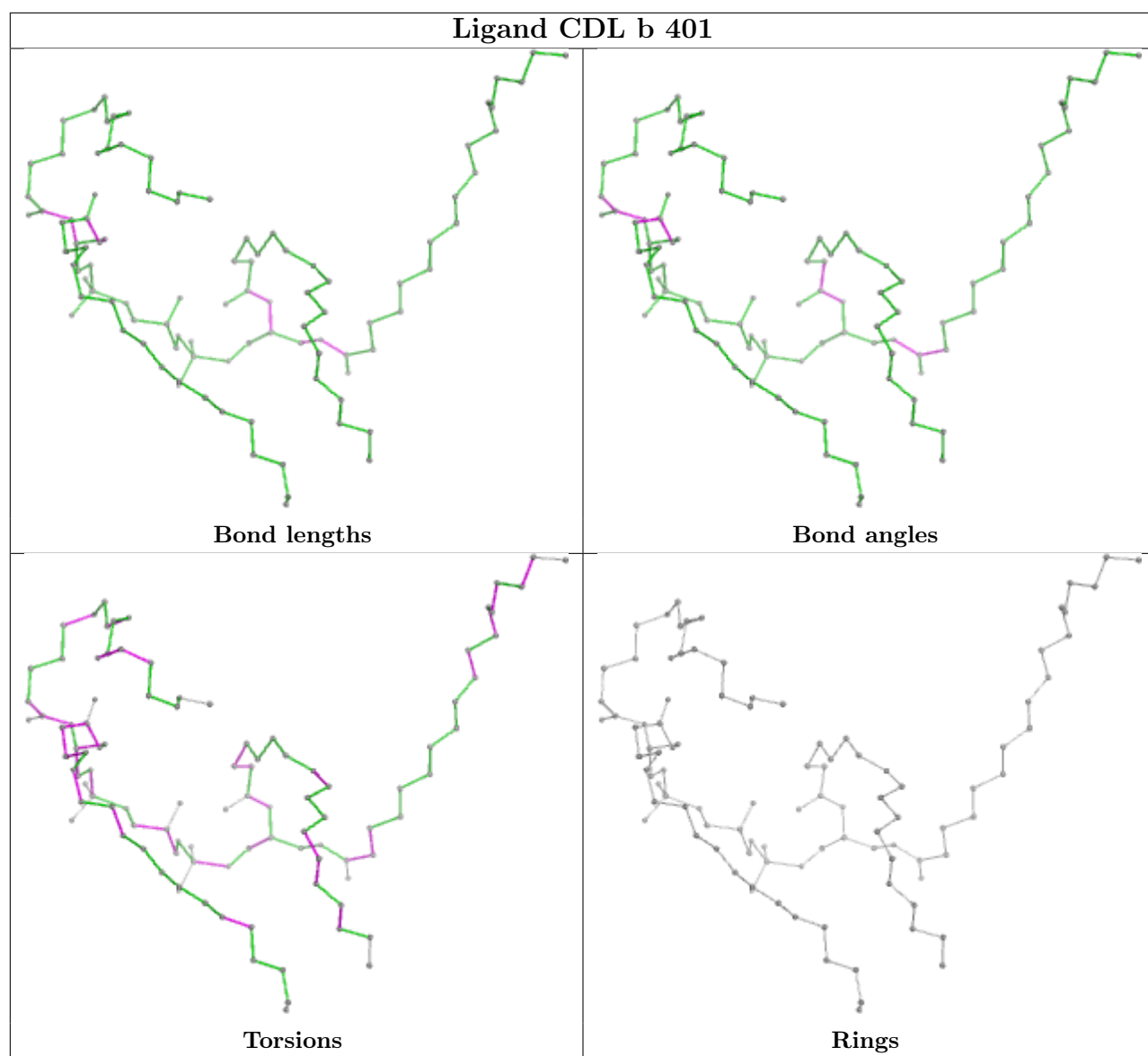


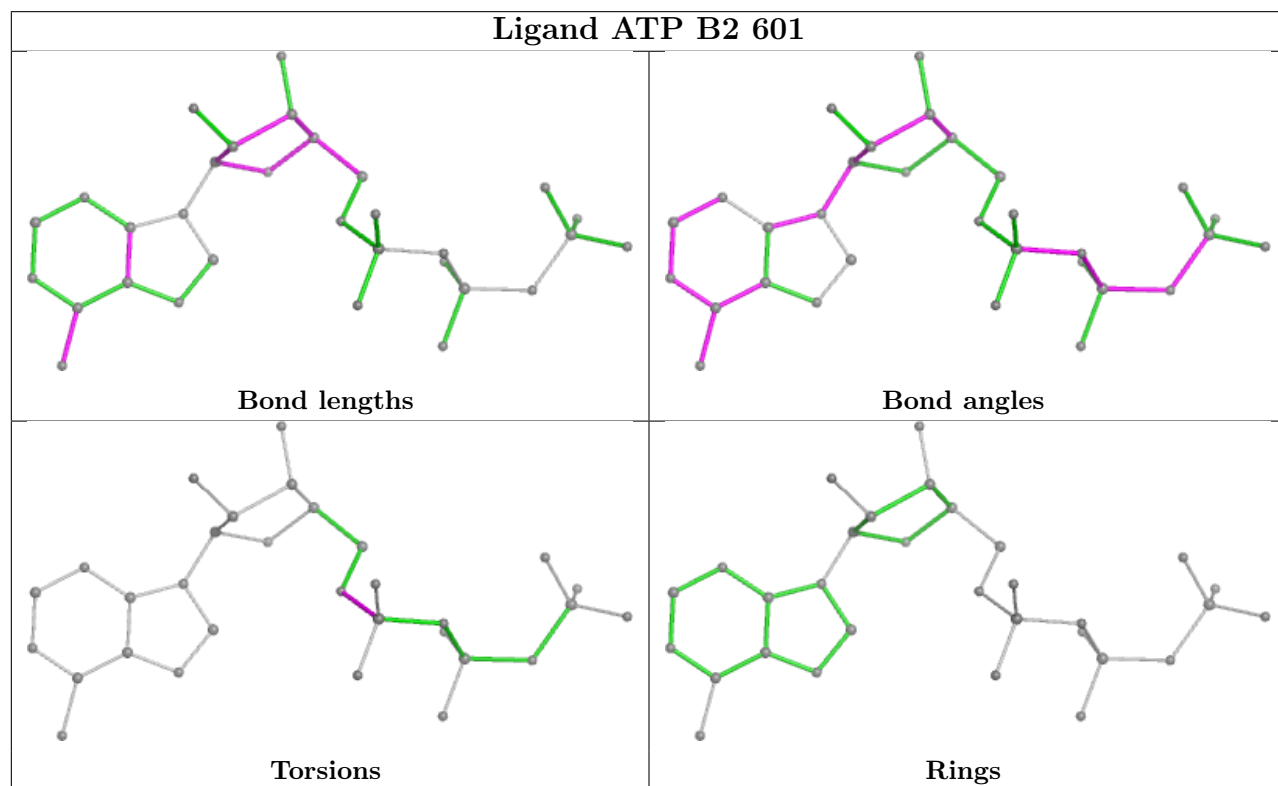
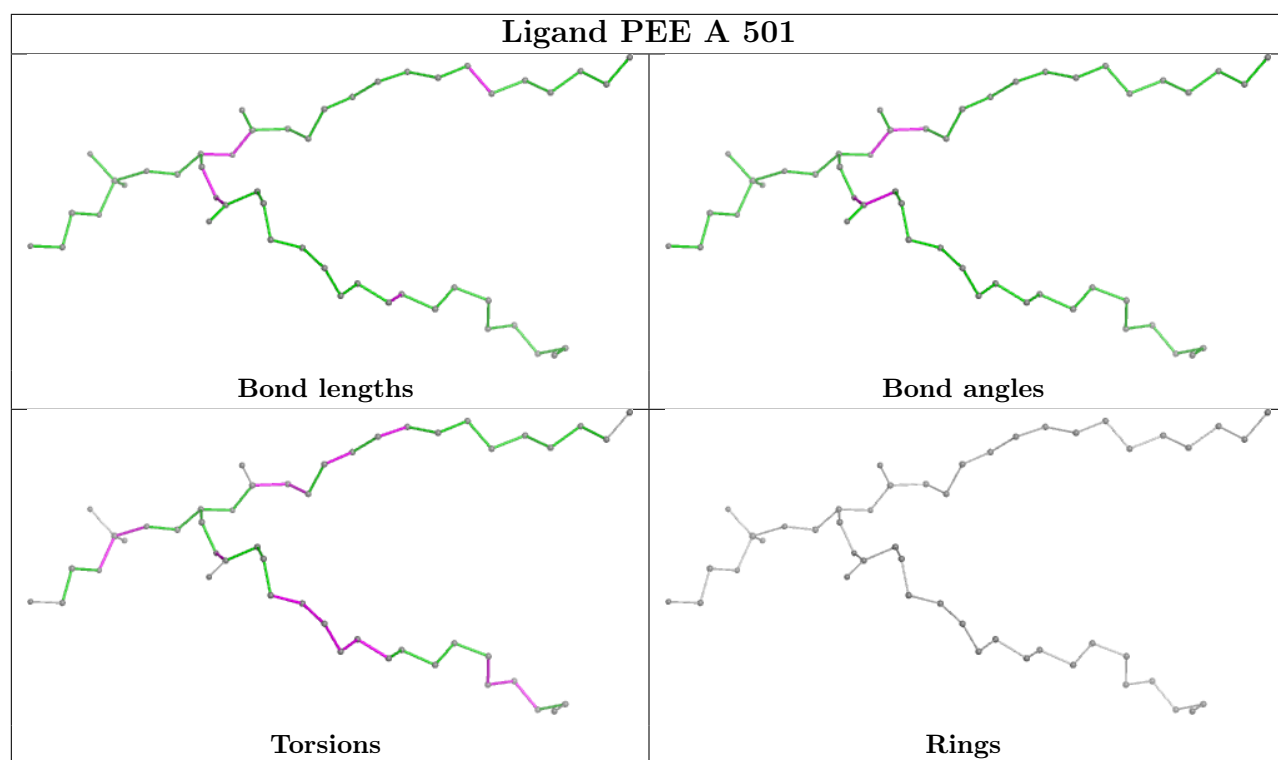


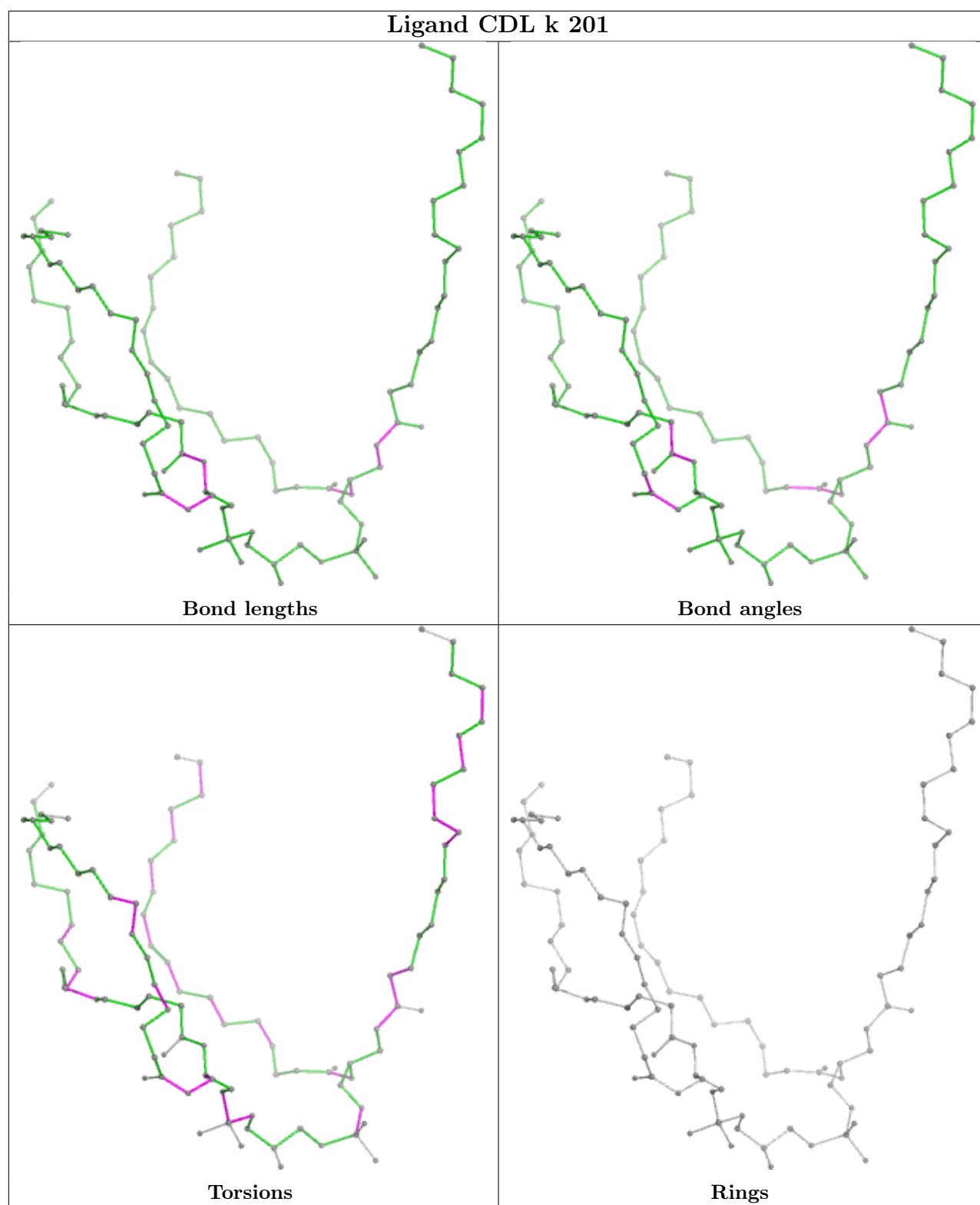


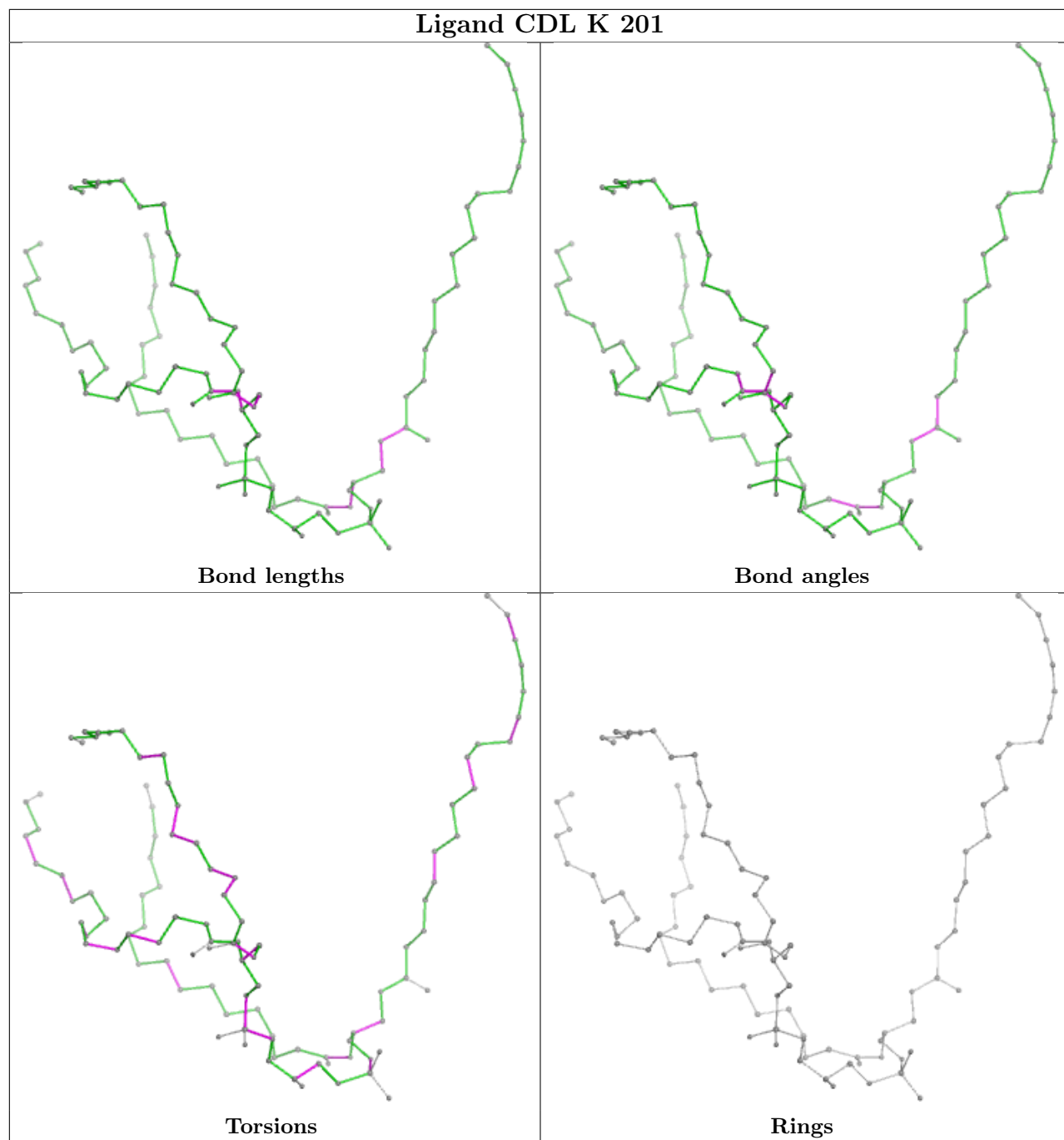




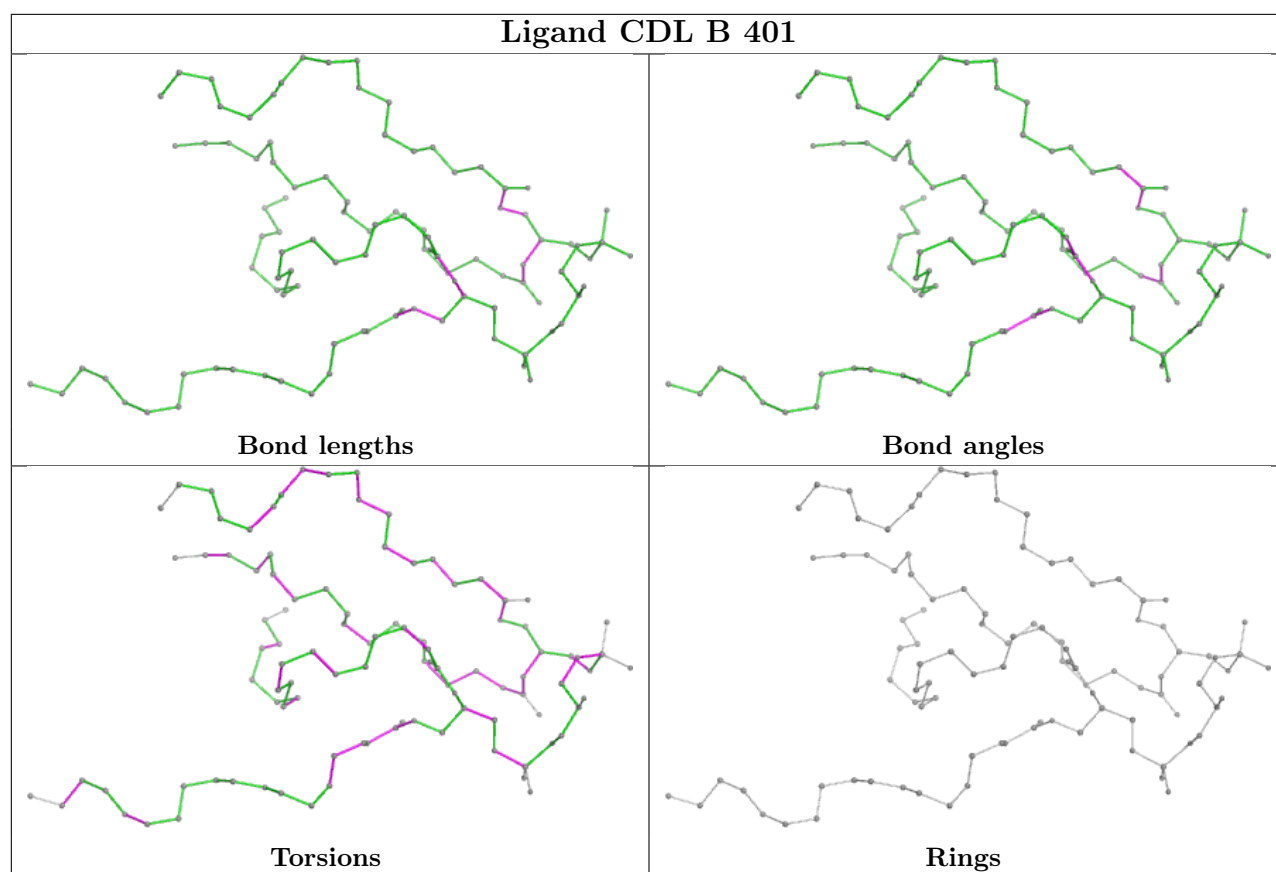


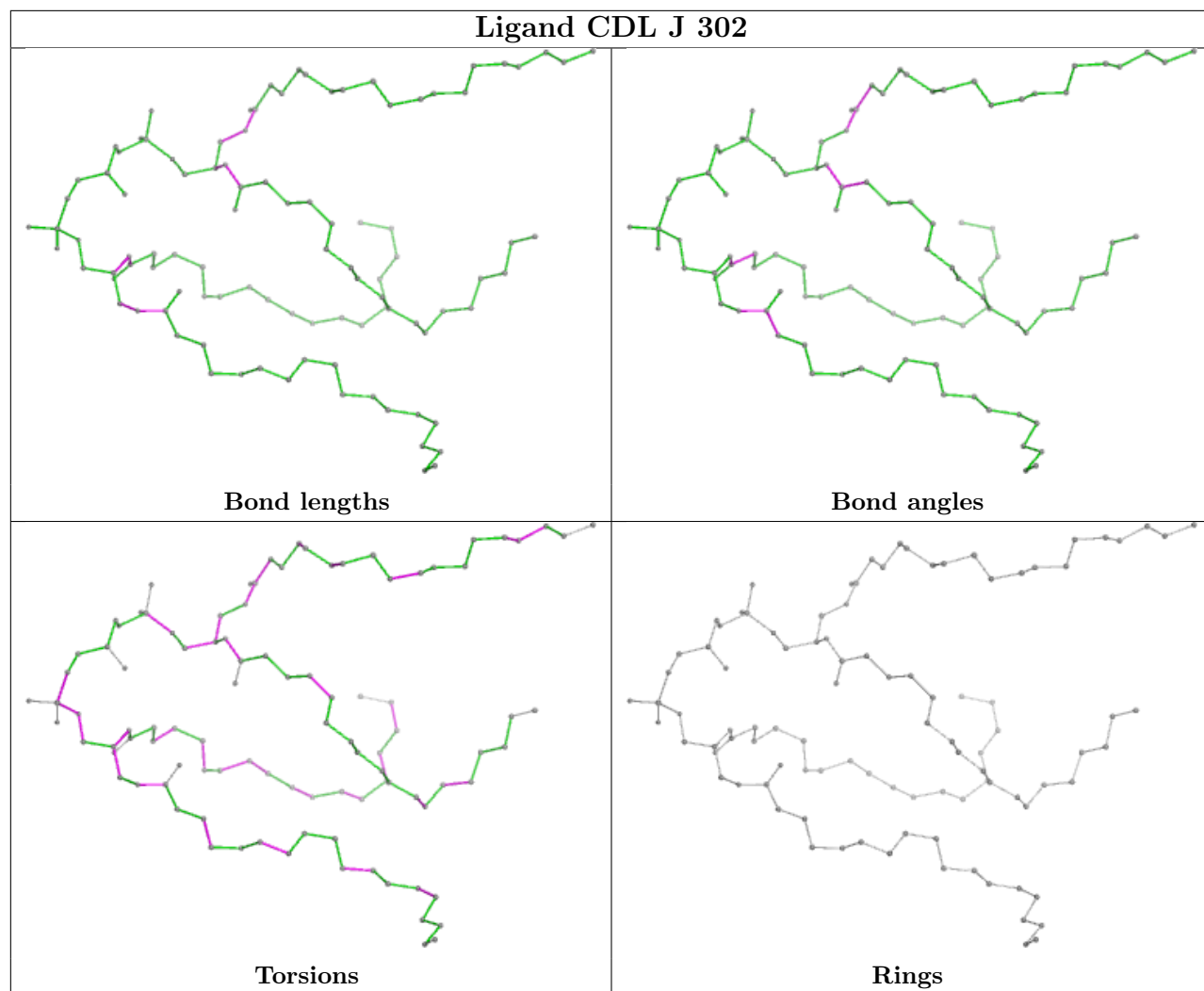


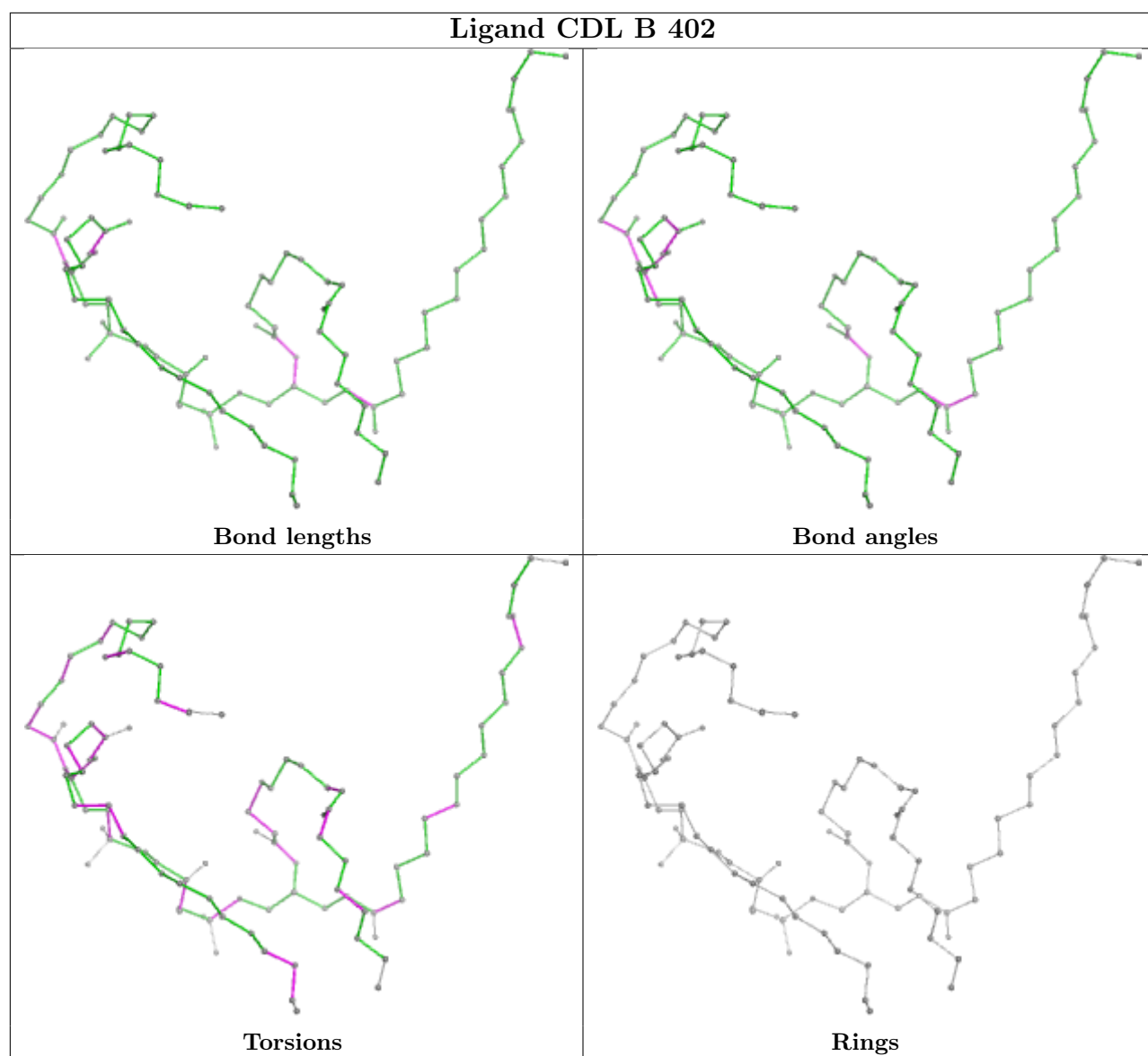


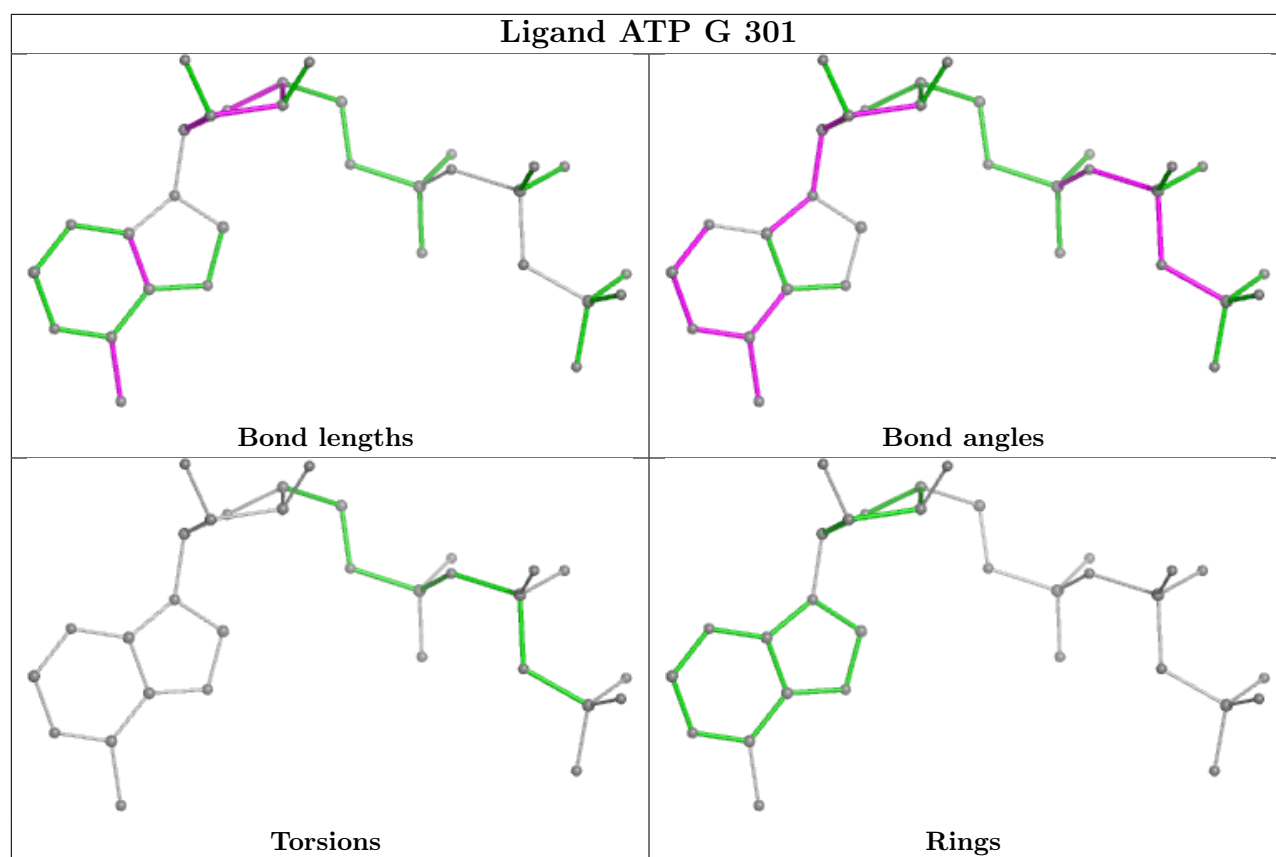


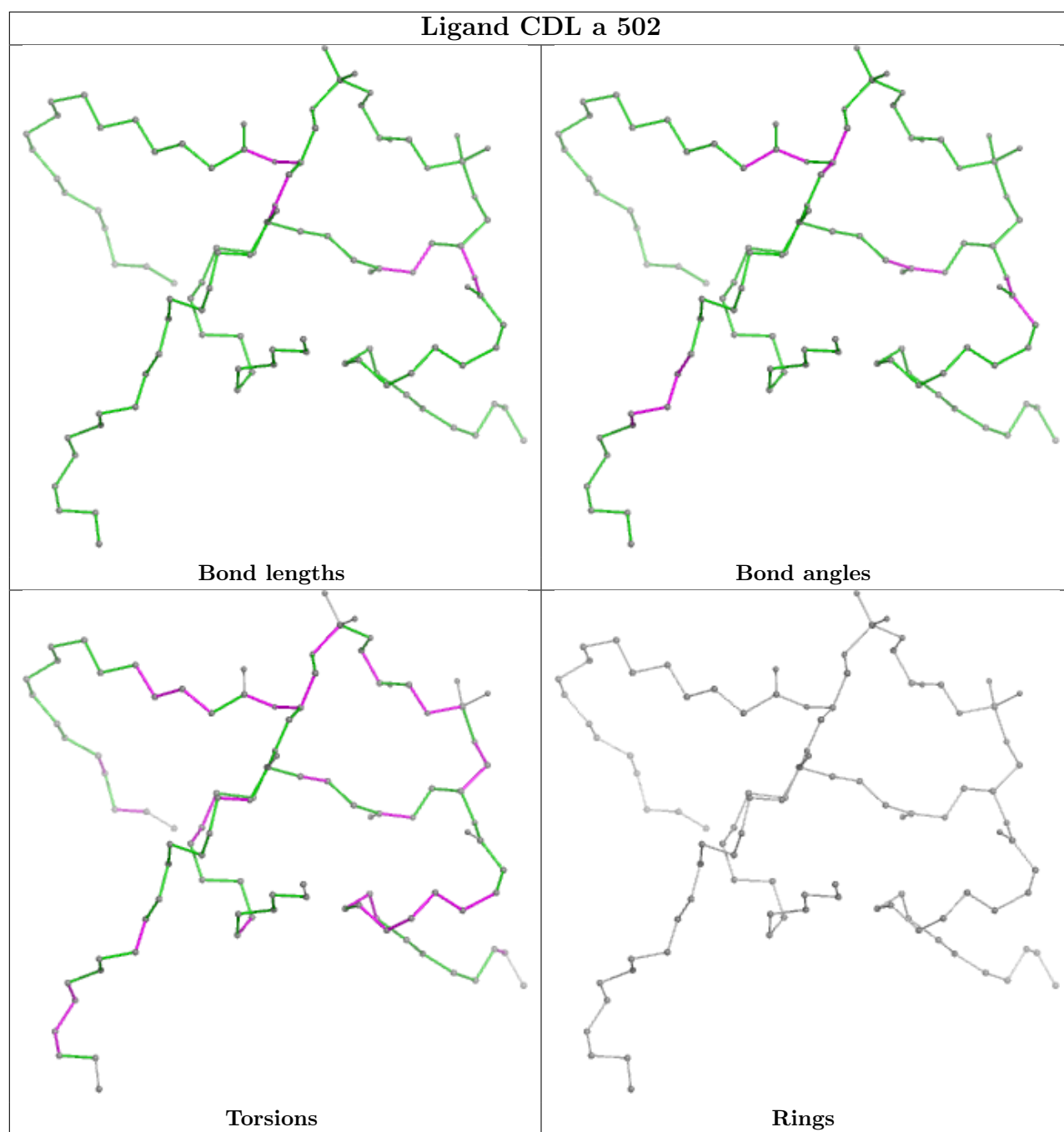


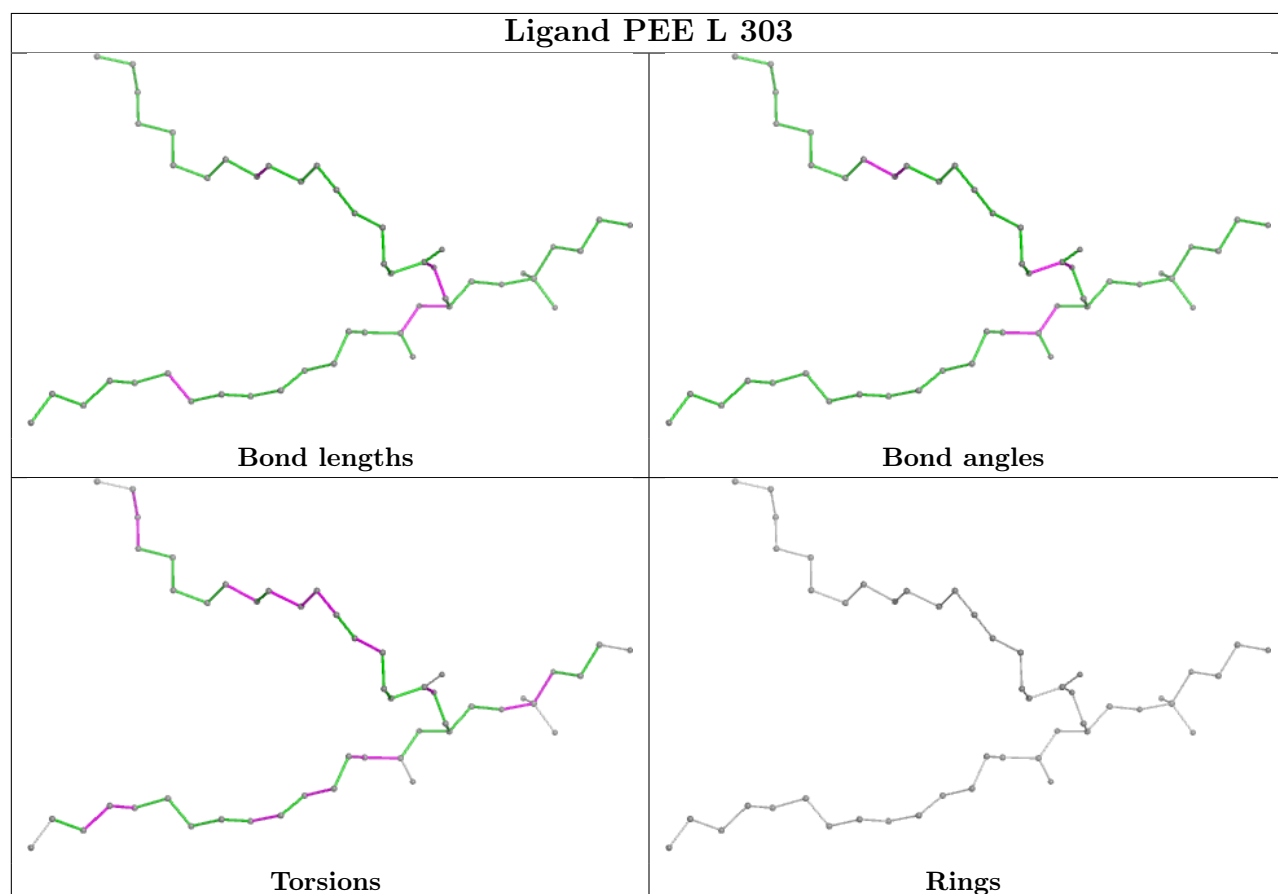
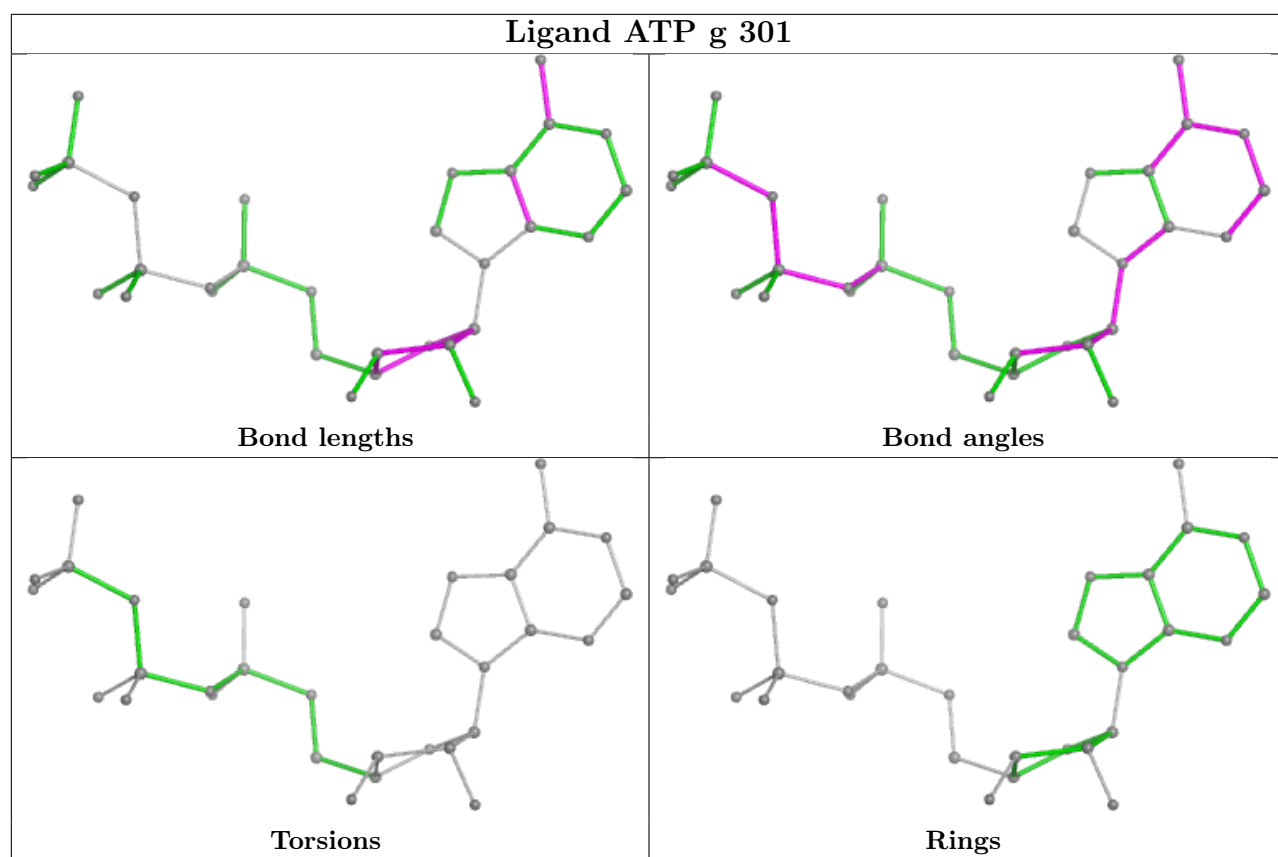


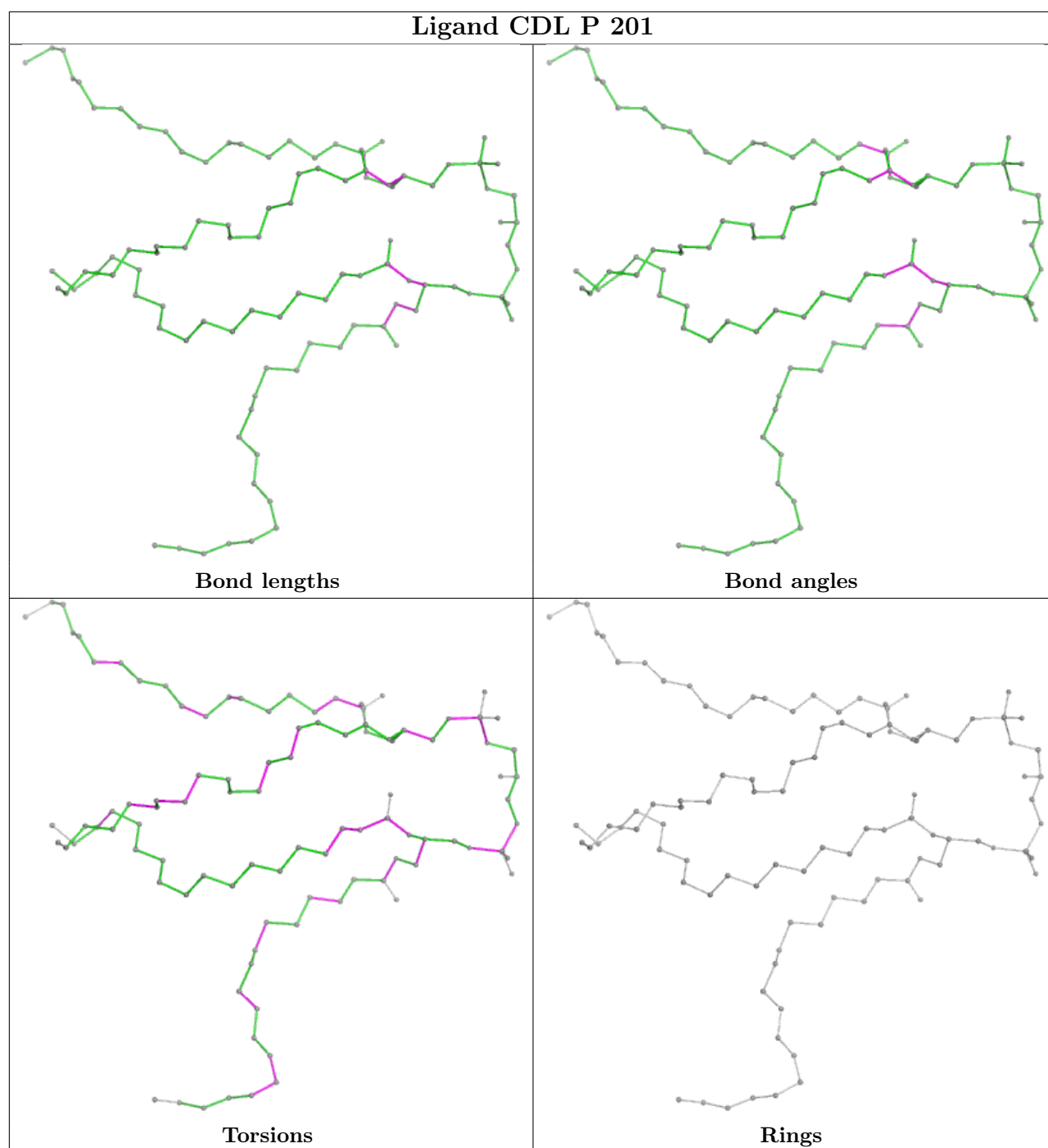




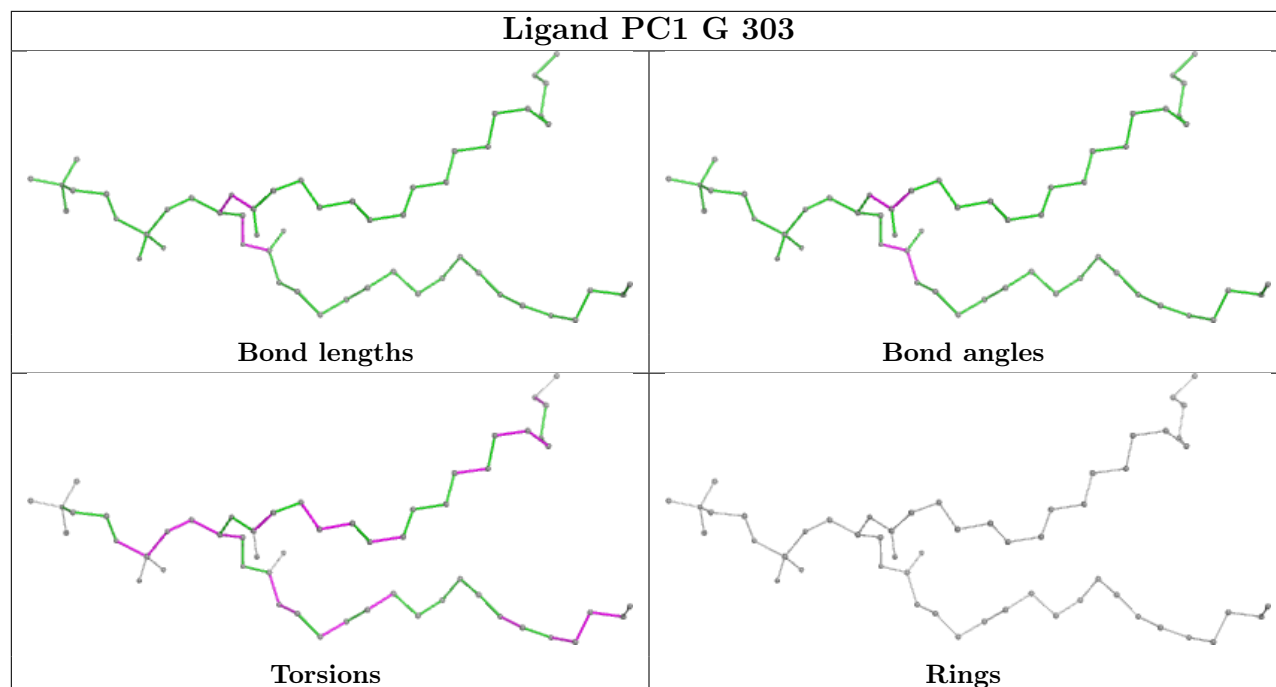




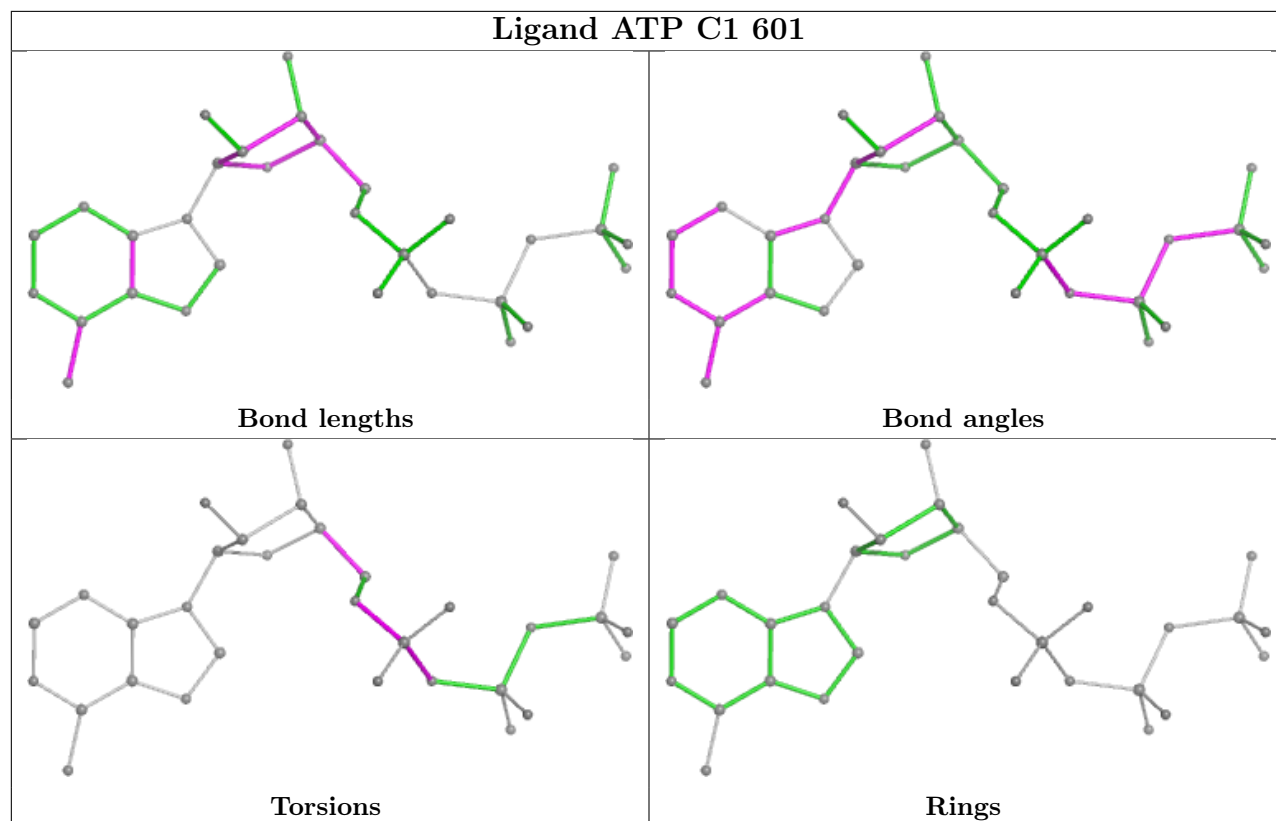




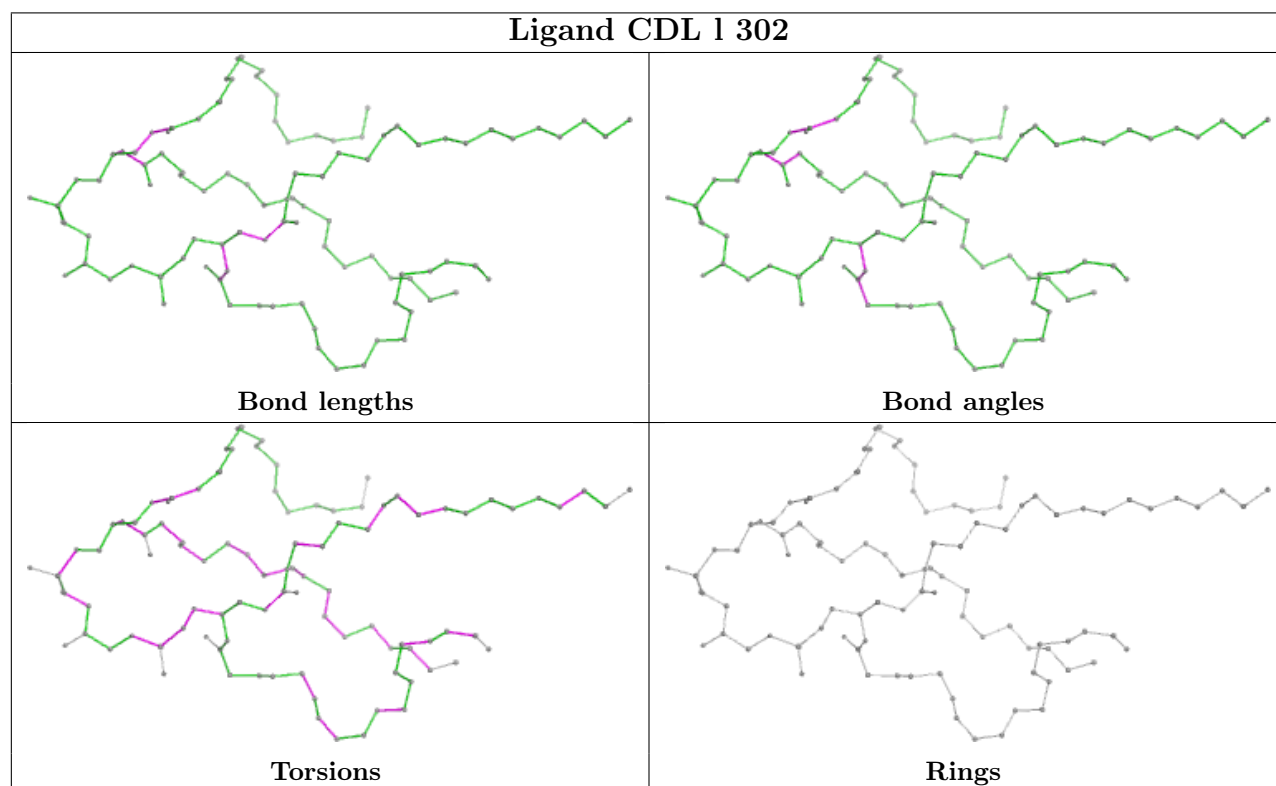
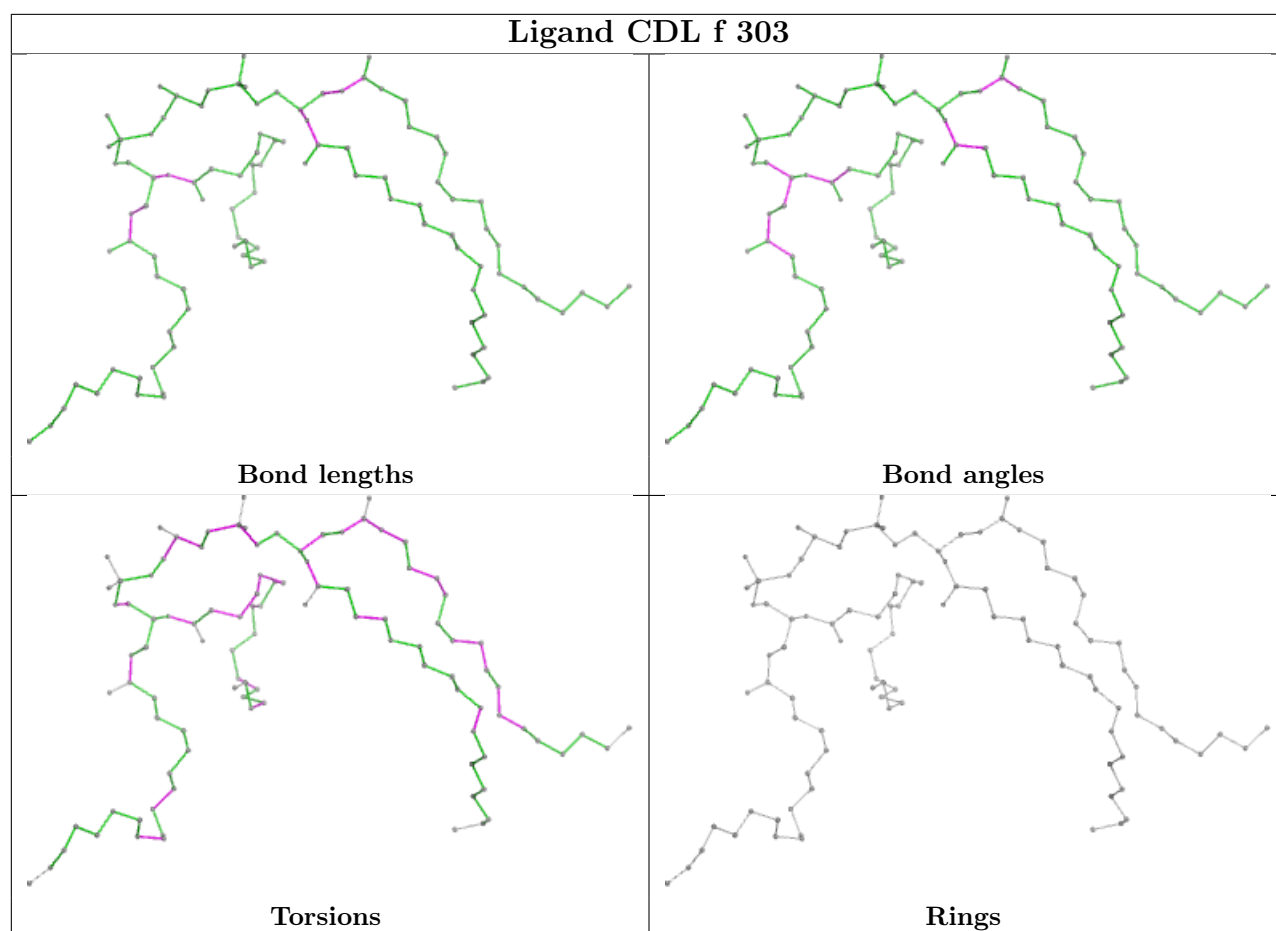
## Ligand PC1 G 303

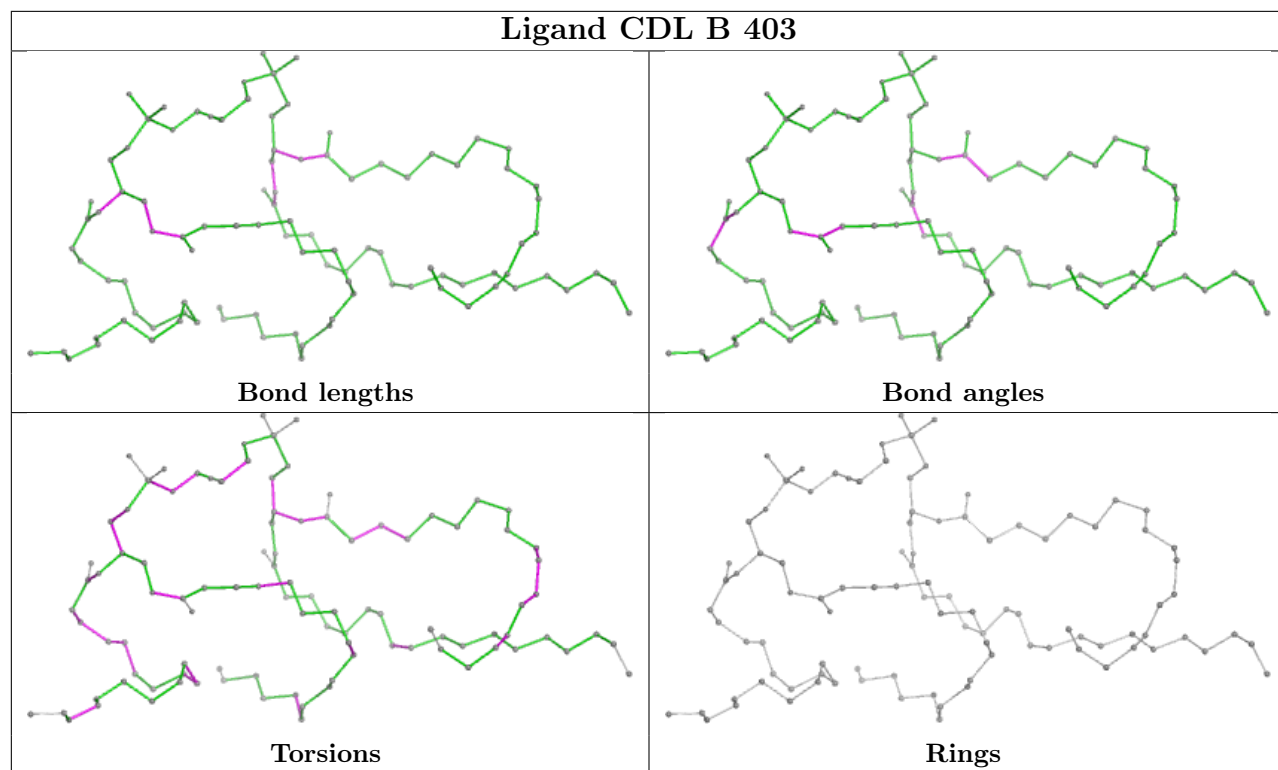


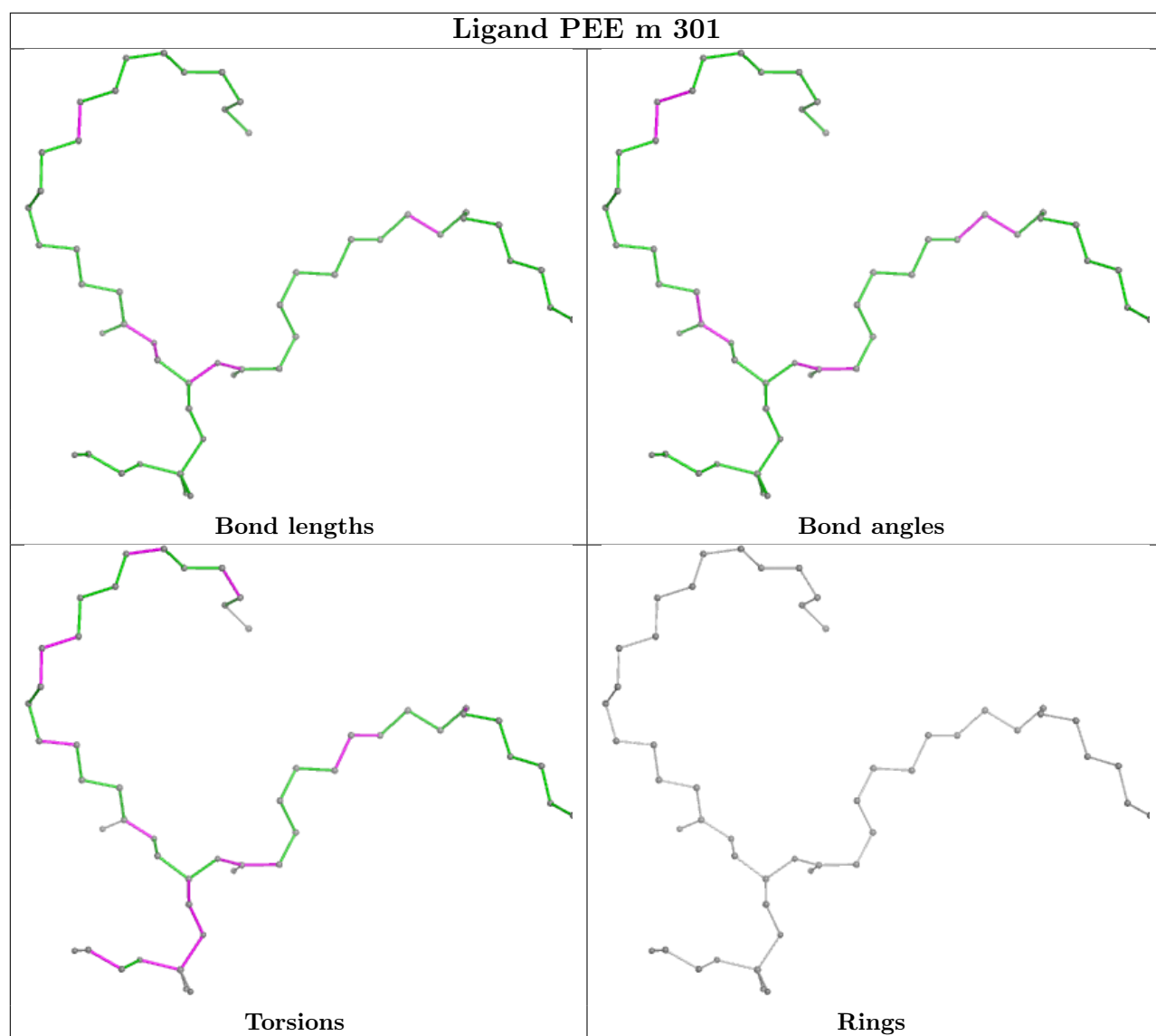
## Ligand ATP C1 601



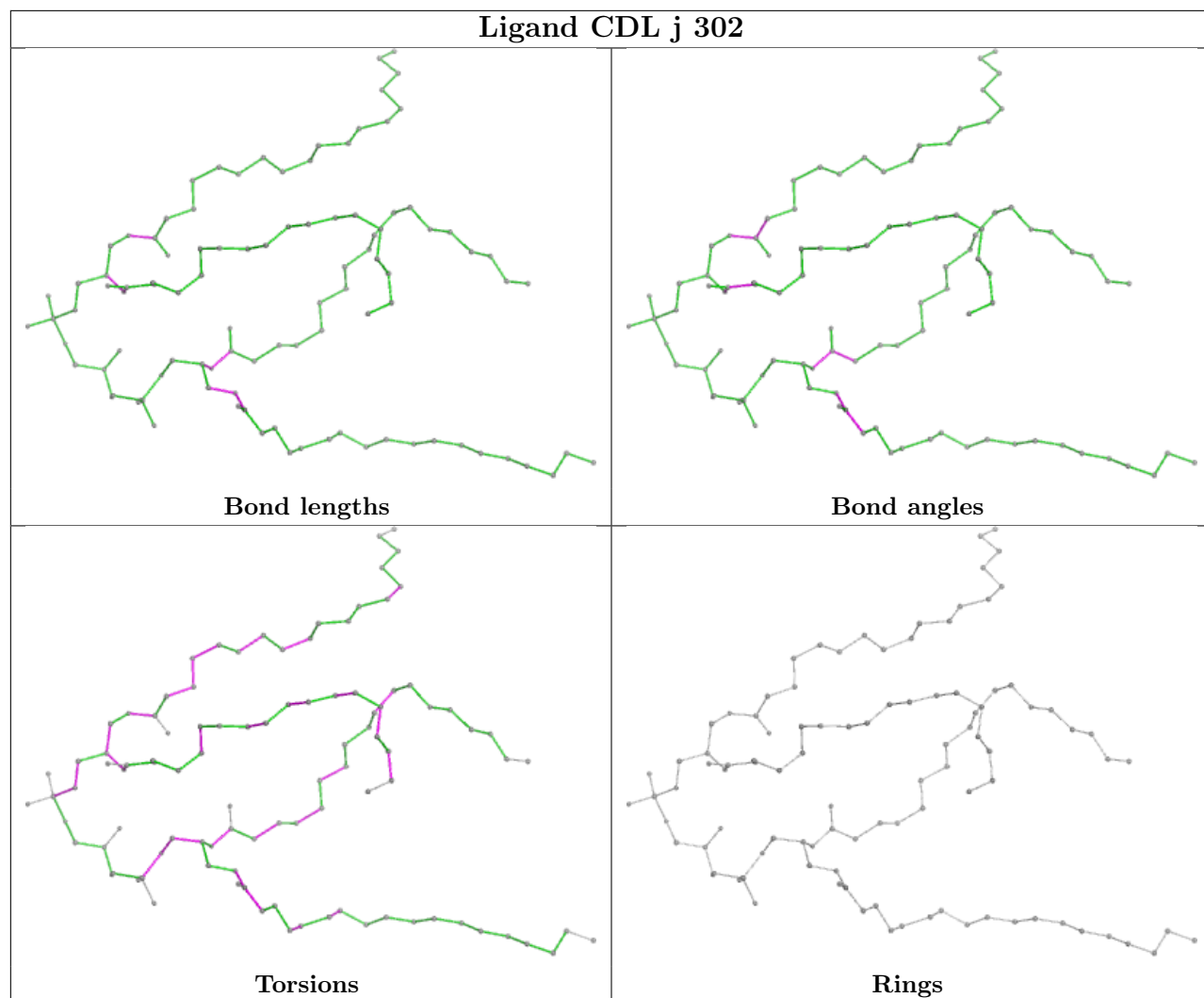


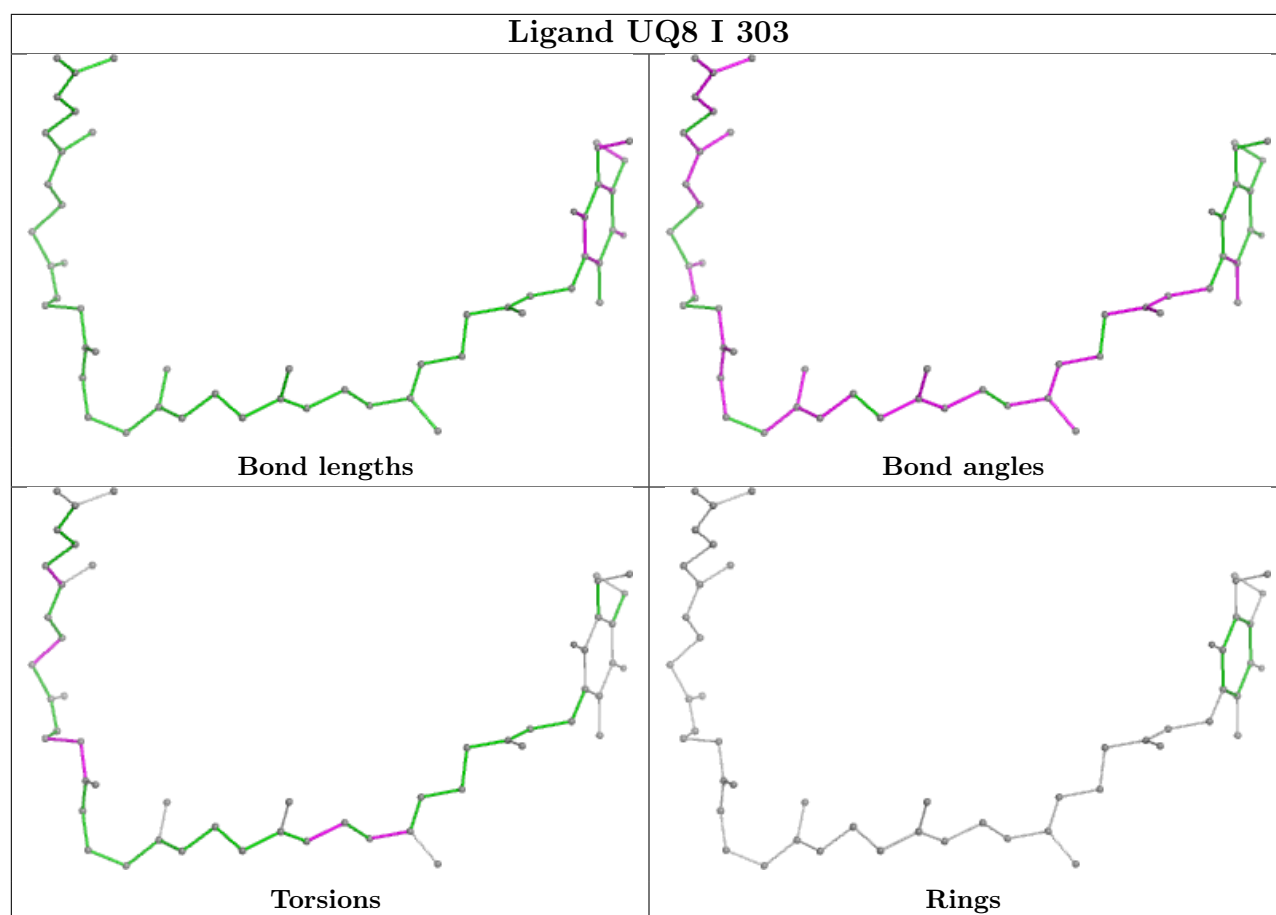


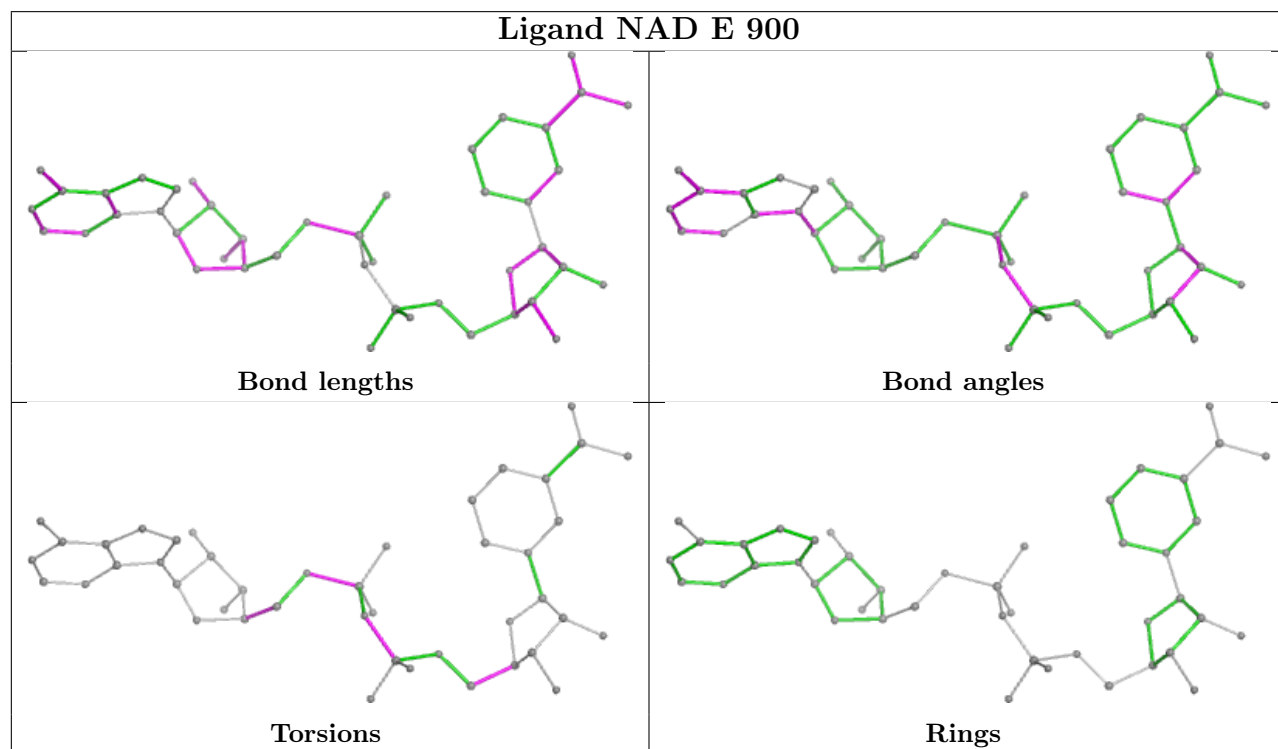
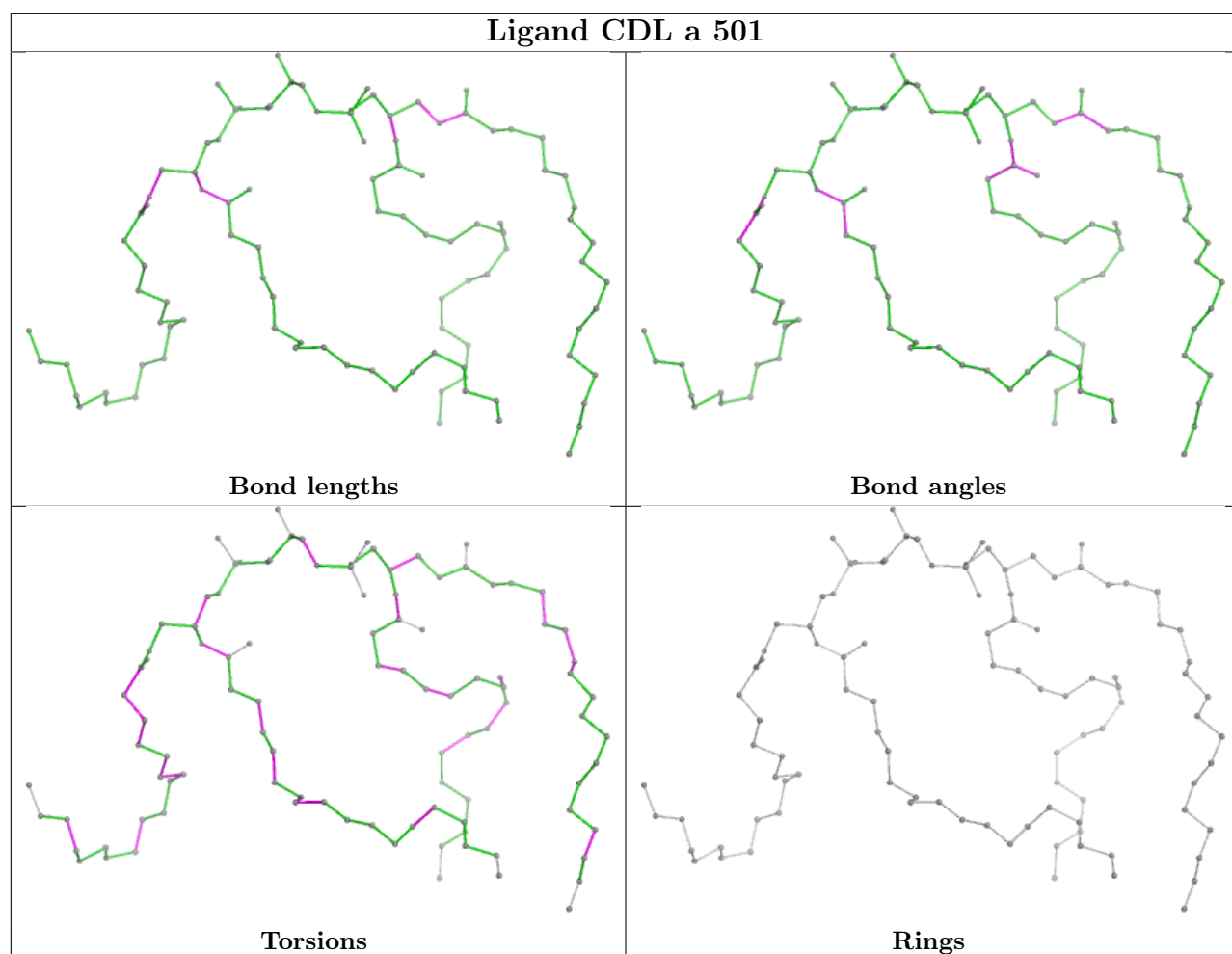


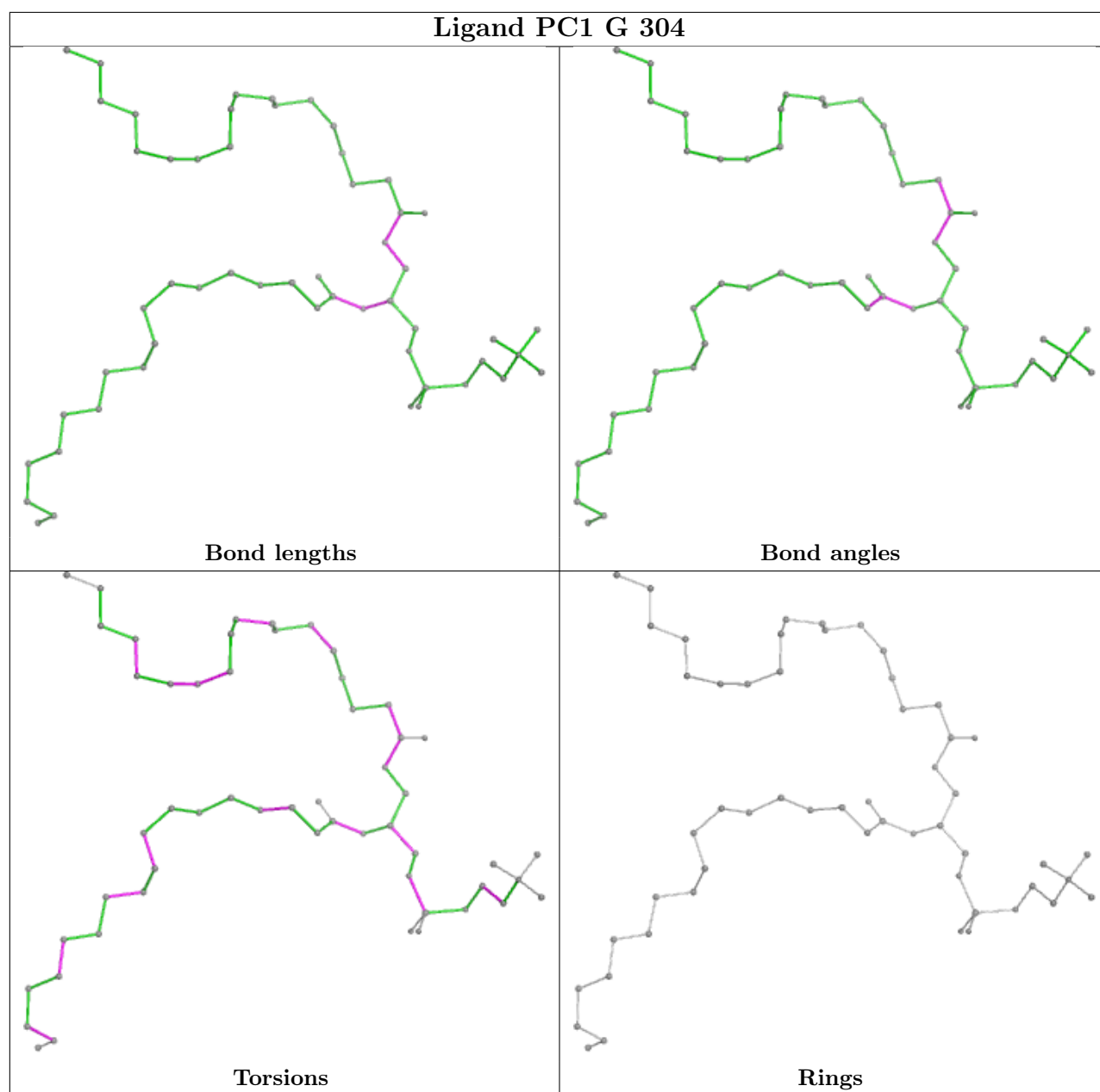


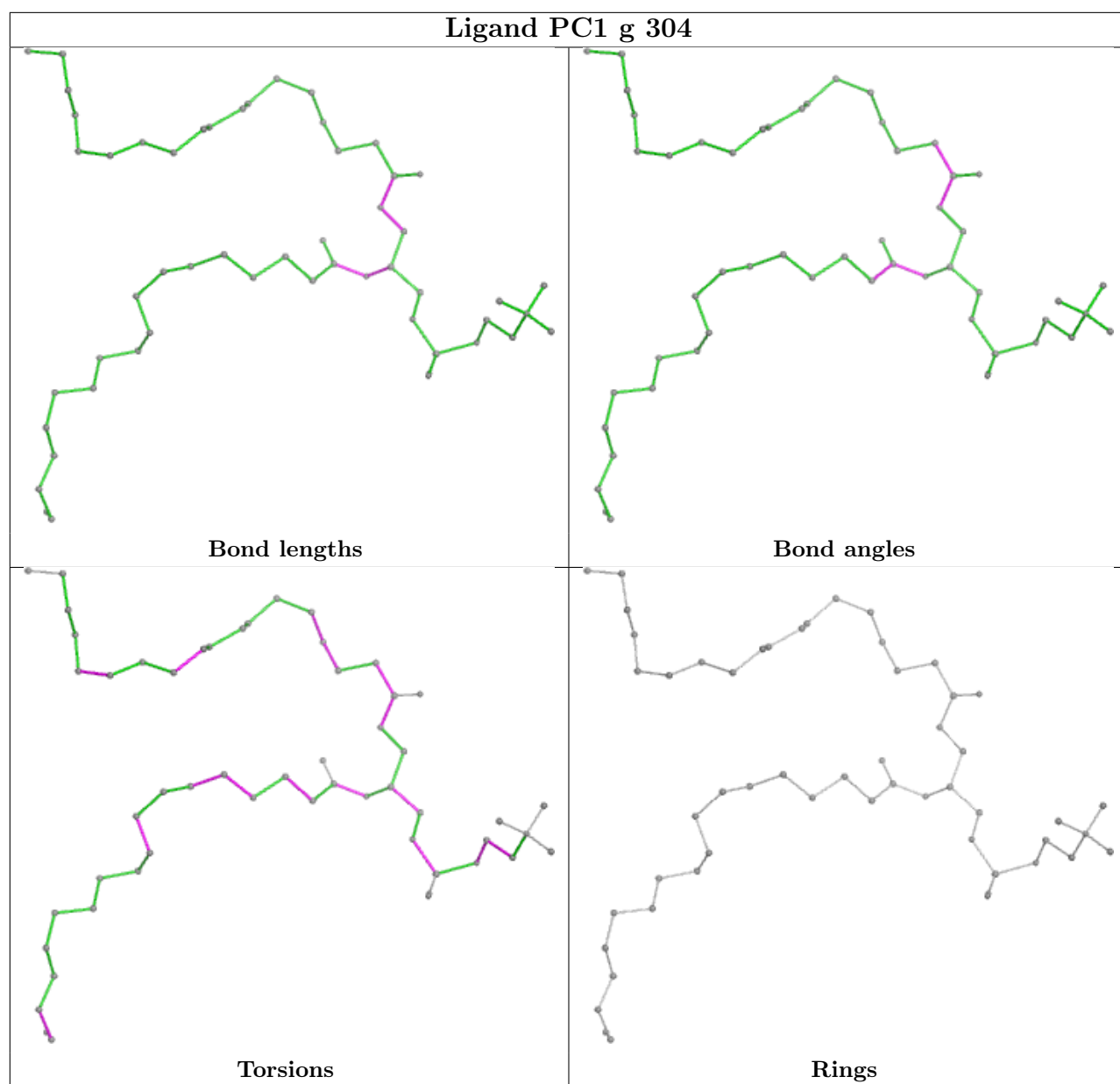
## Ligand CDL j 302



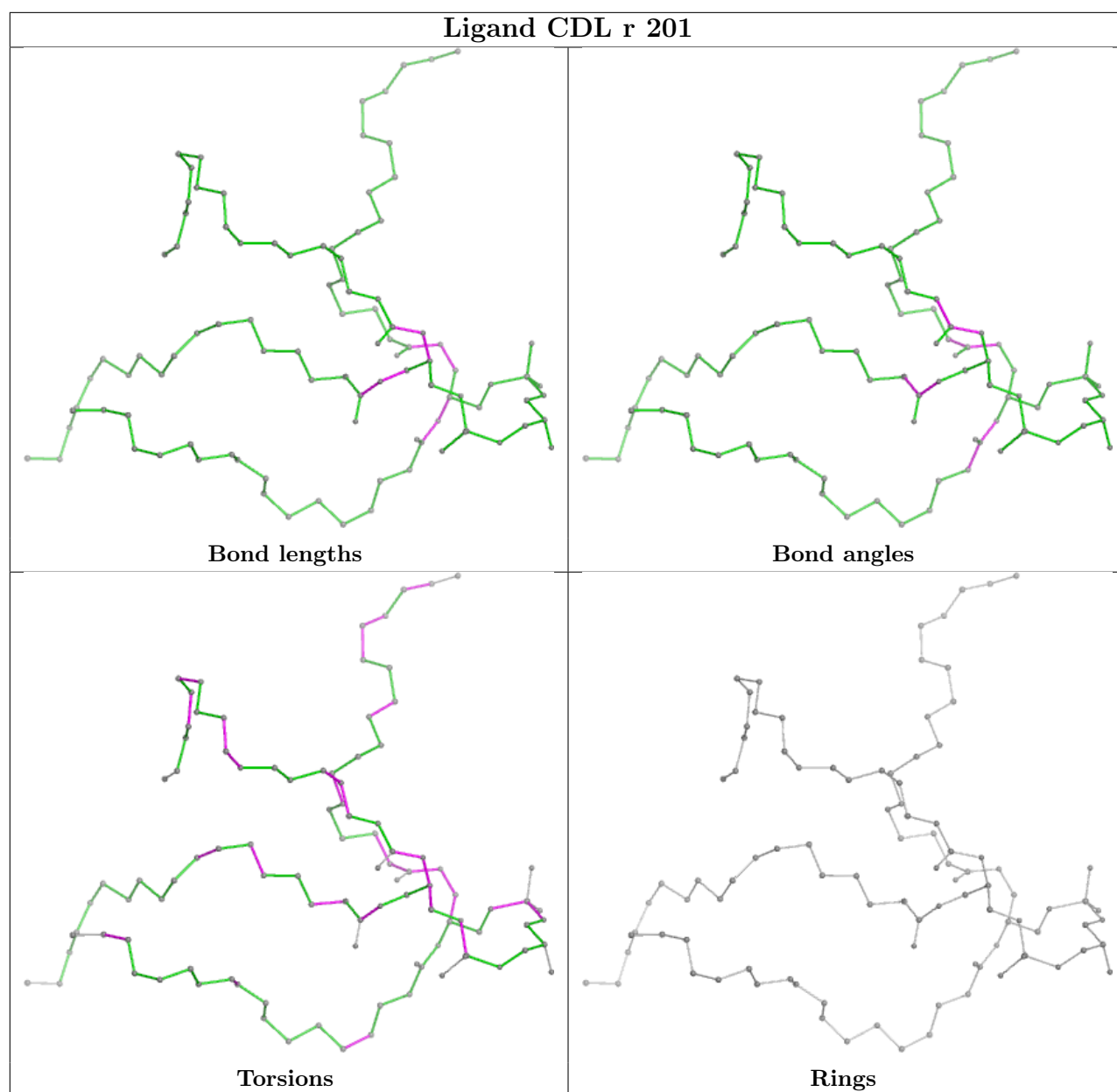


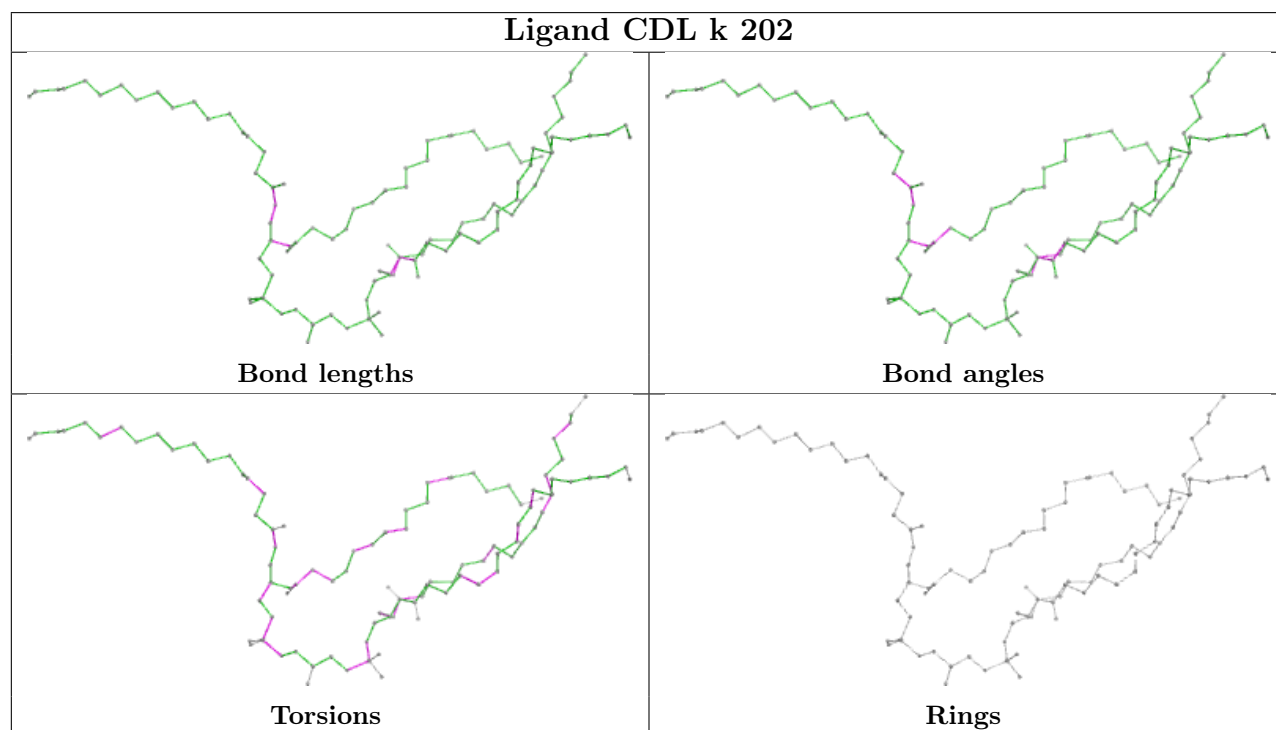
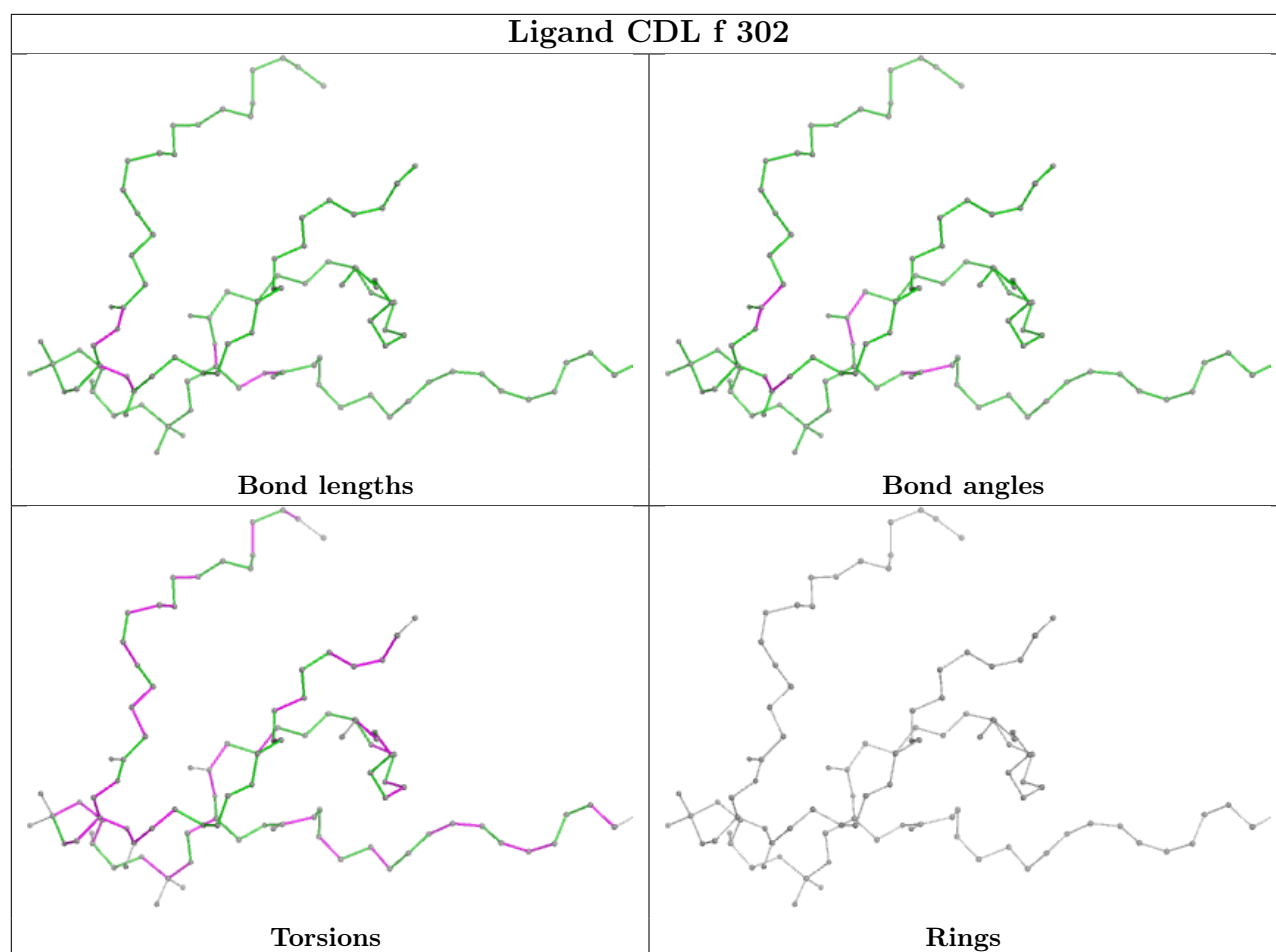


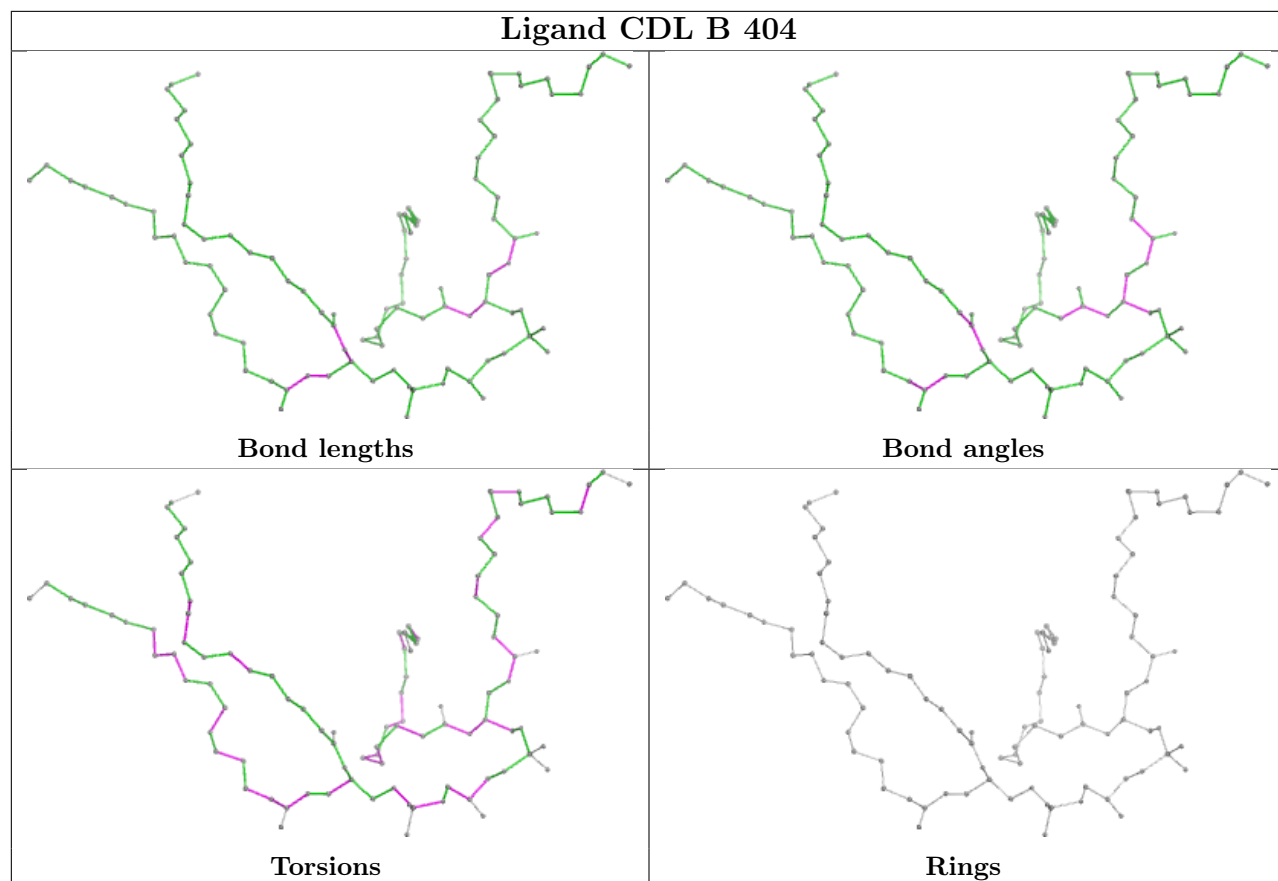




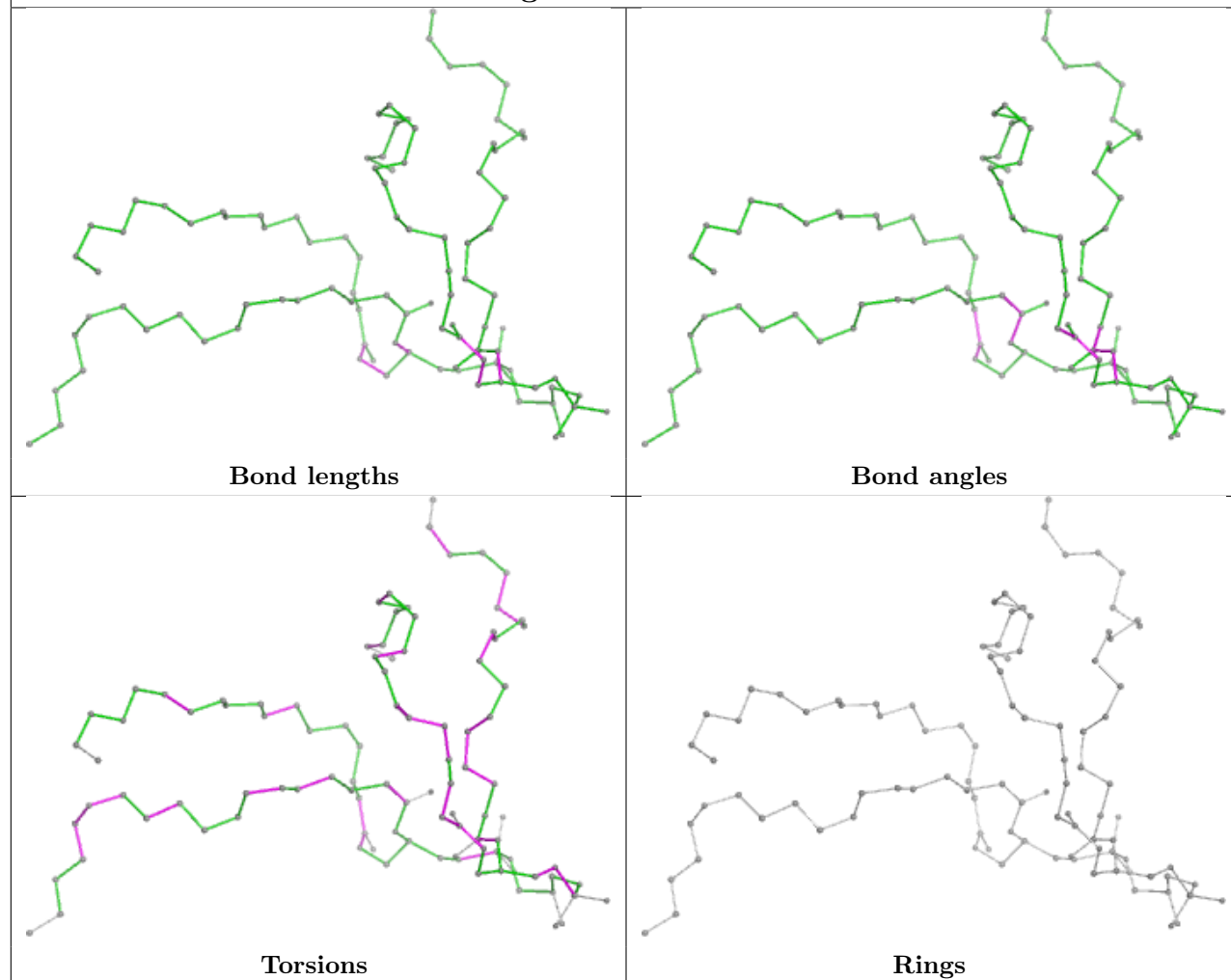




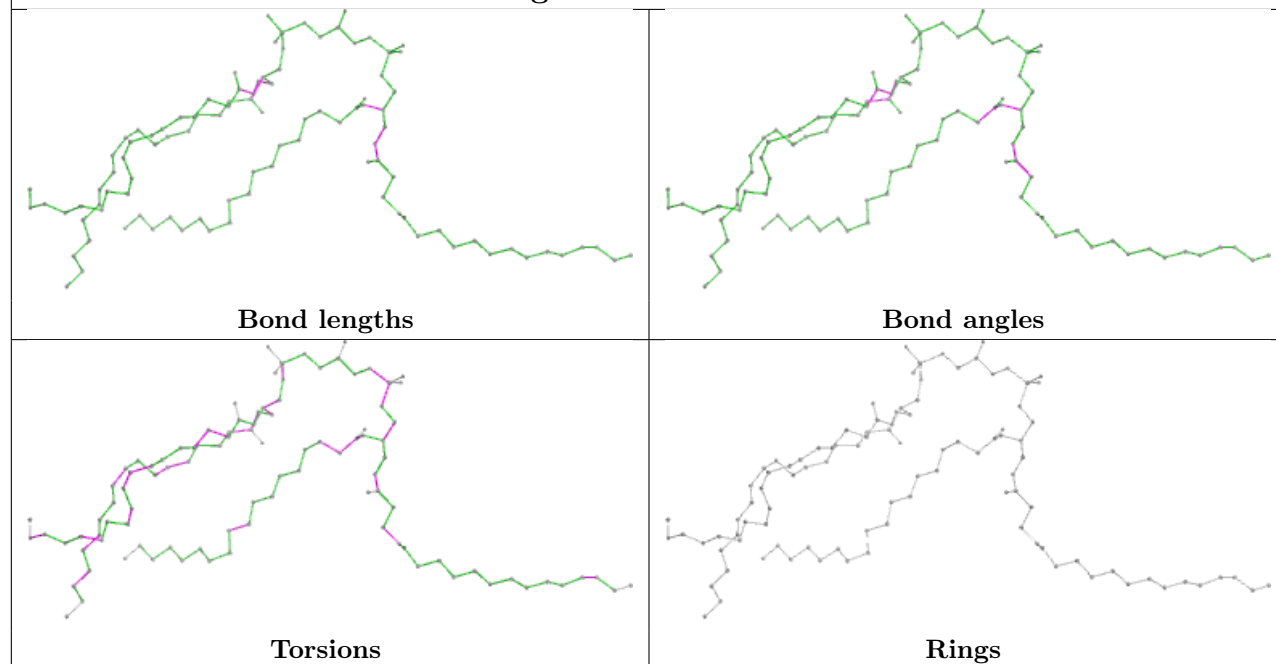


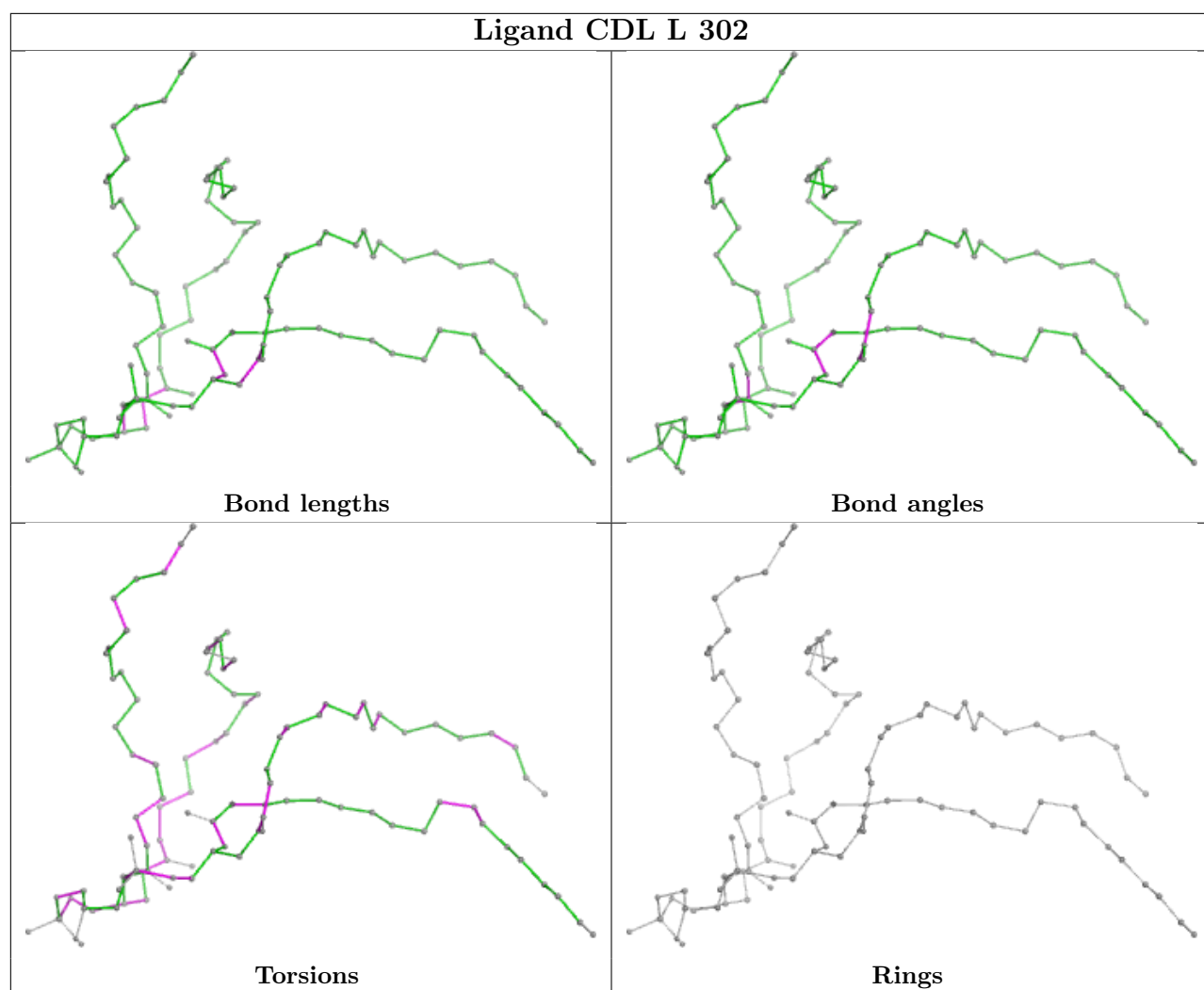


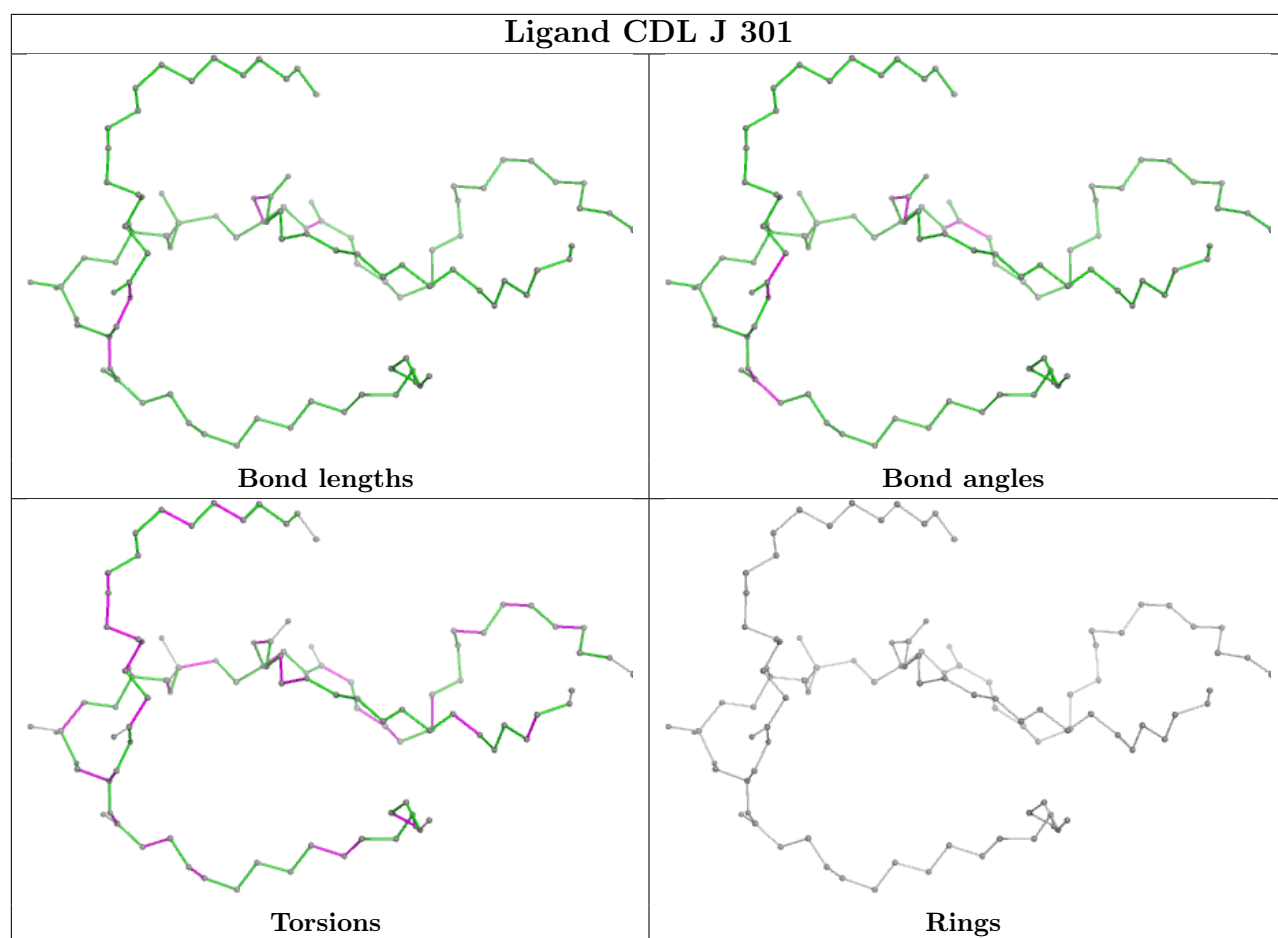
## Ligand CDL I 301

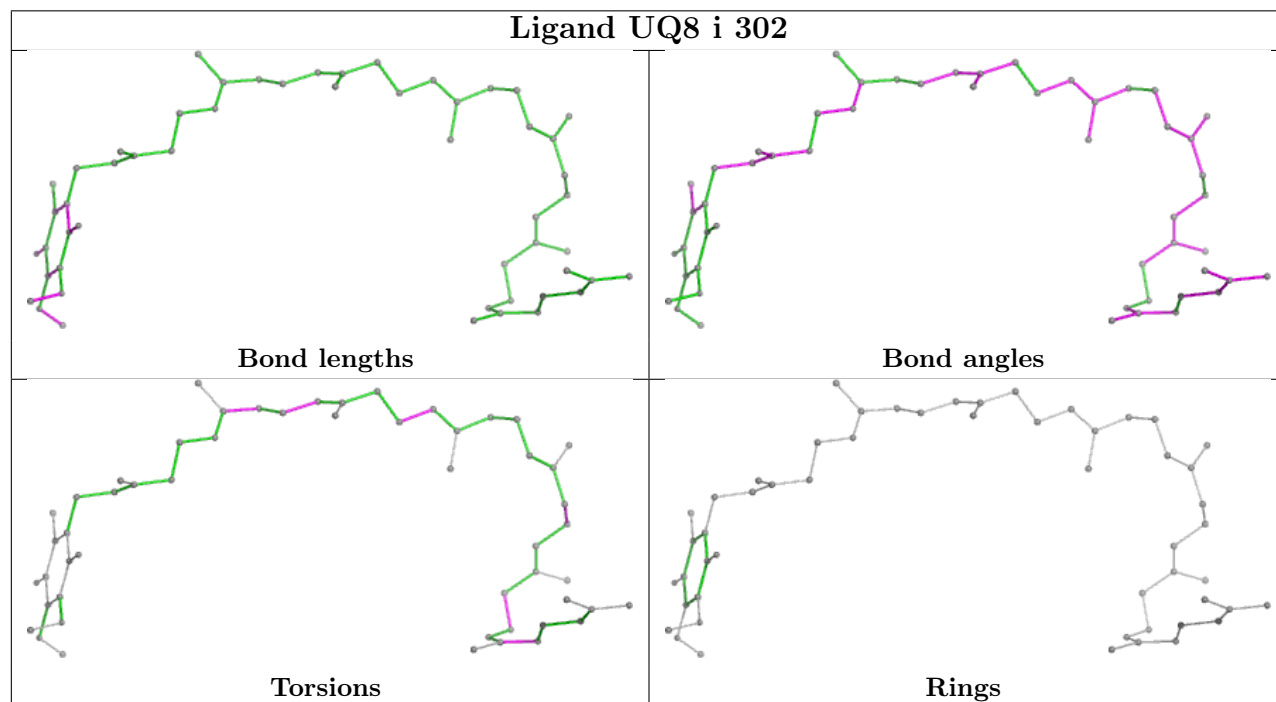
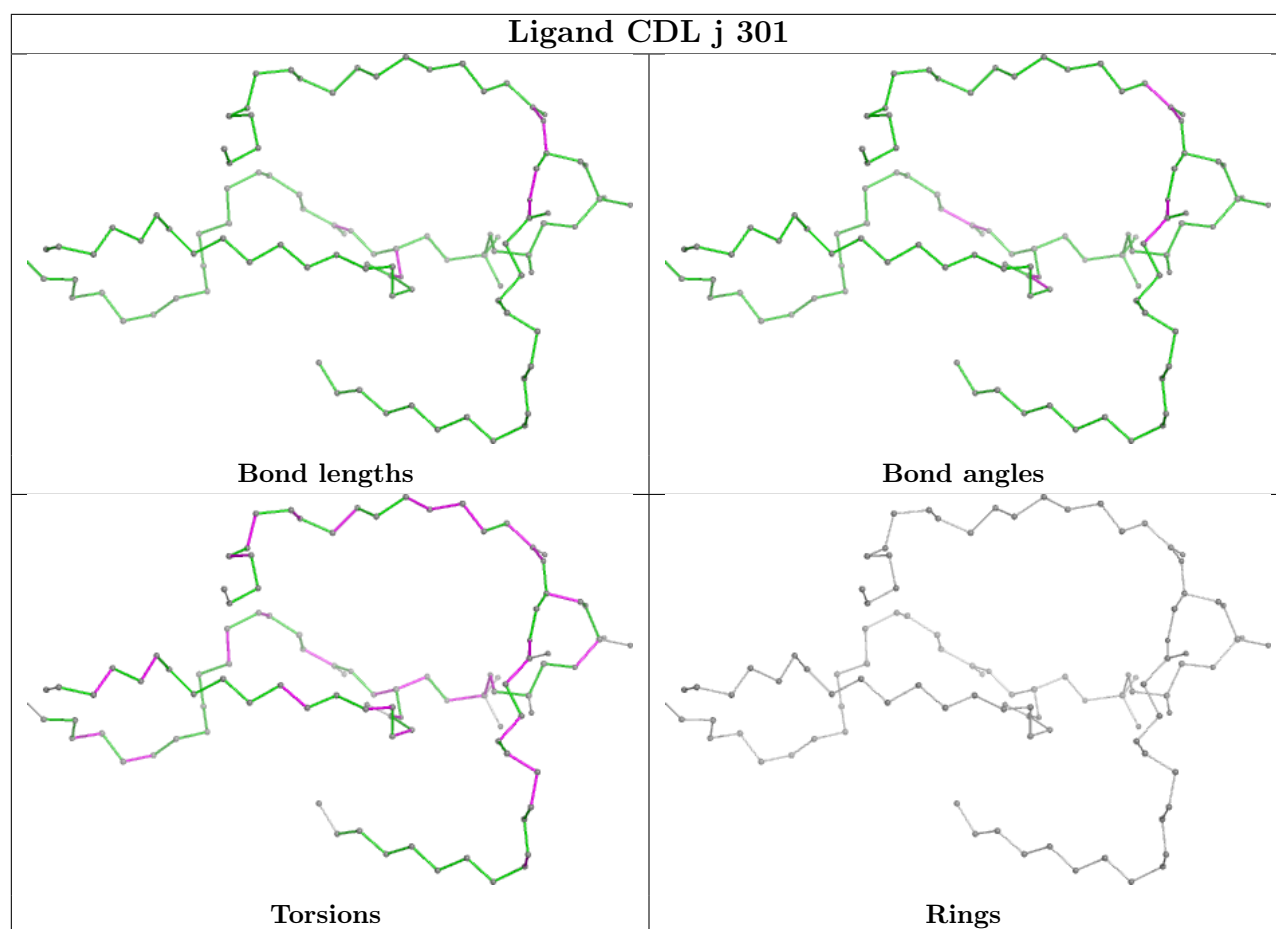


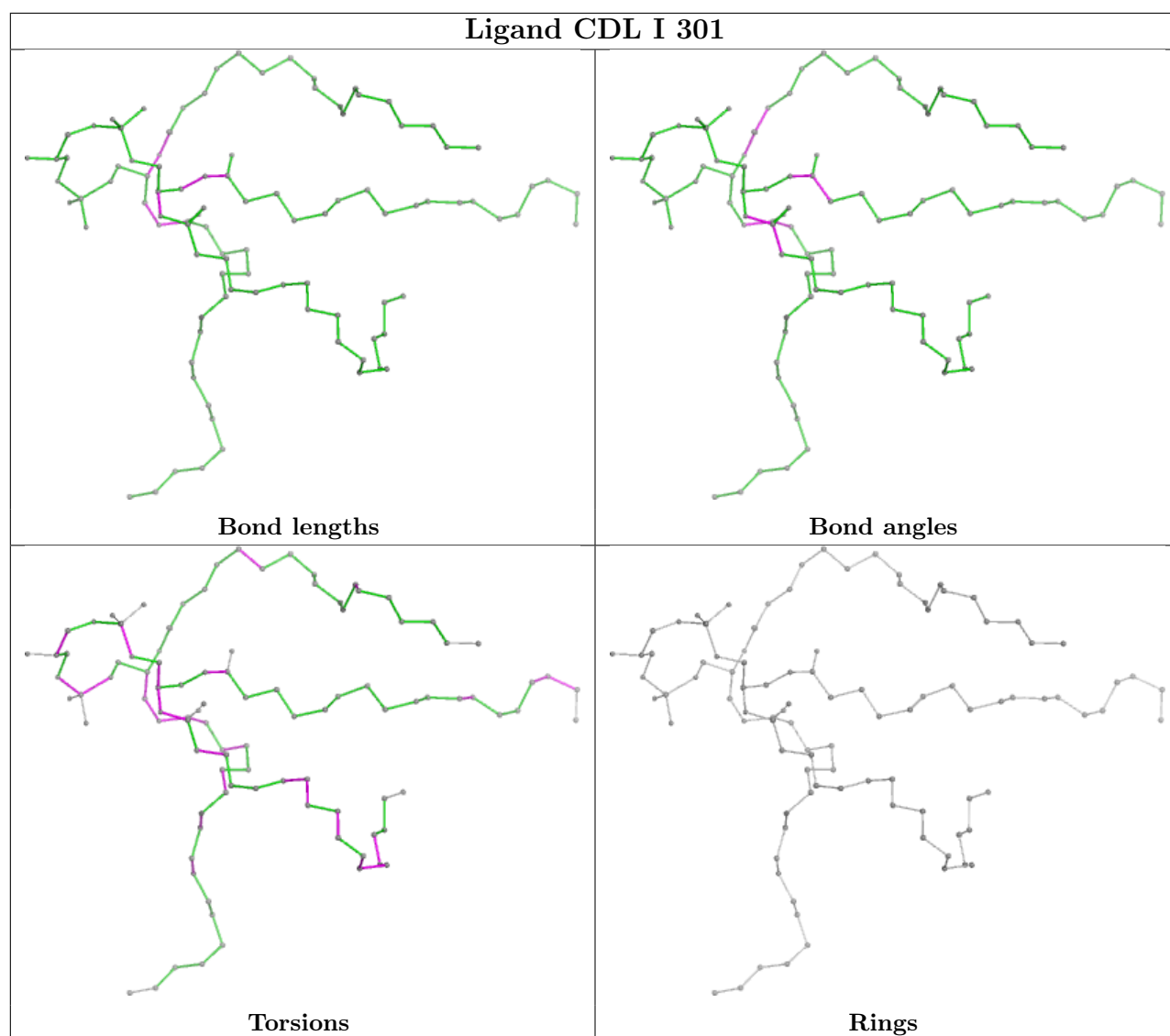
## Ligand CDL K 202



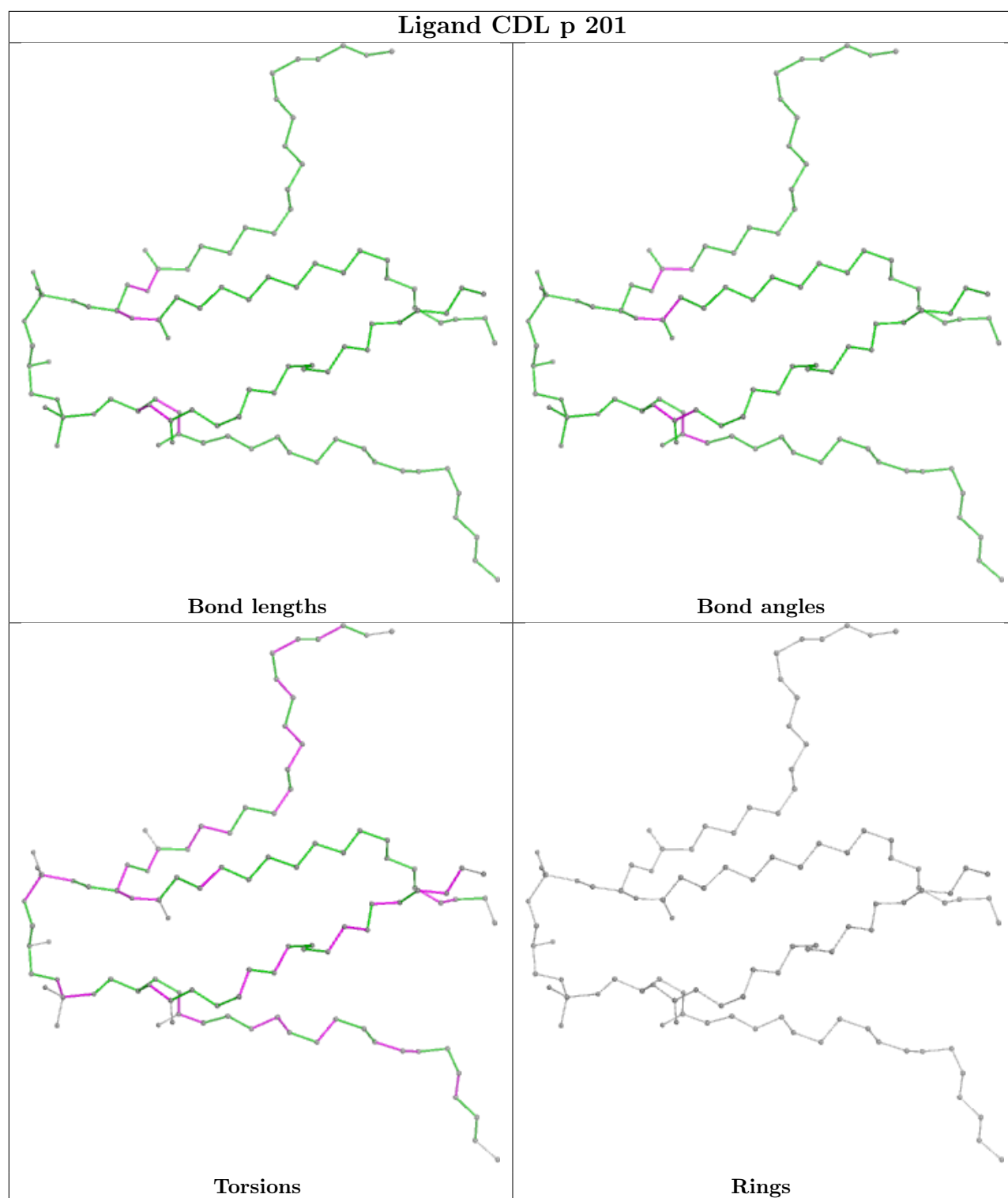


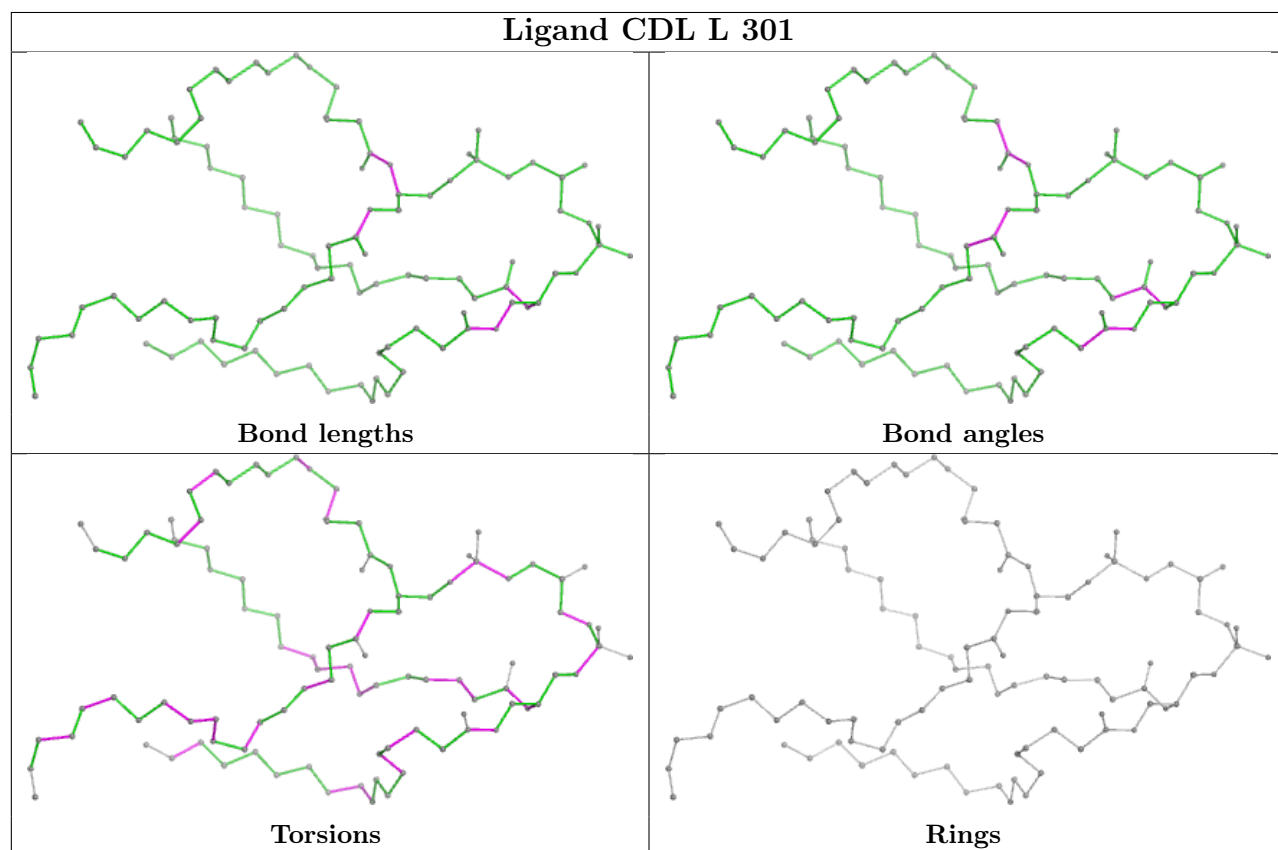
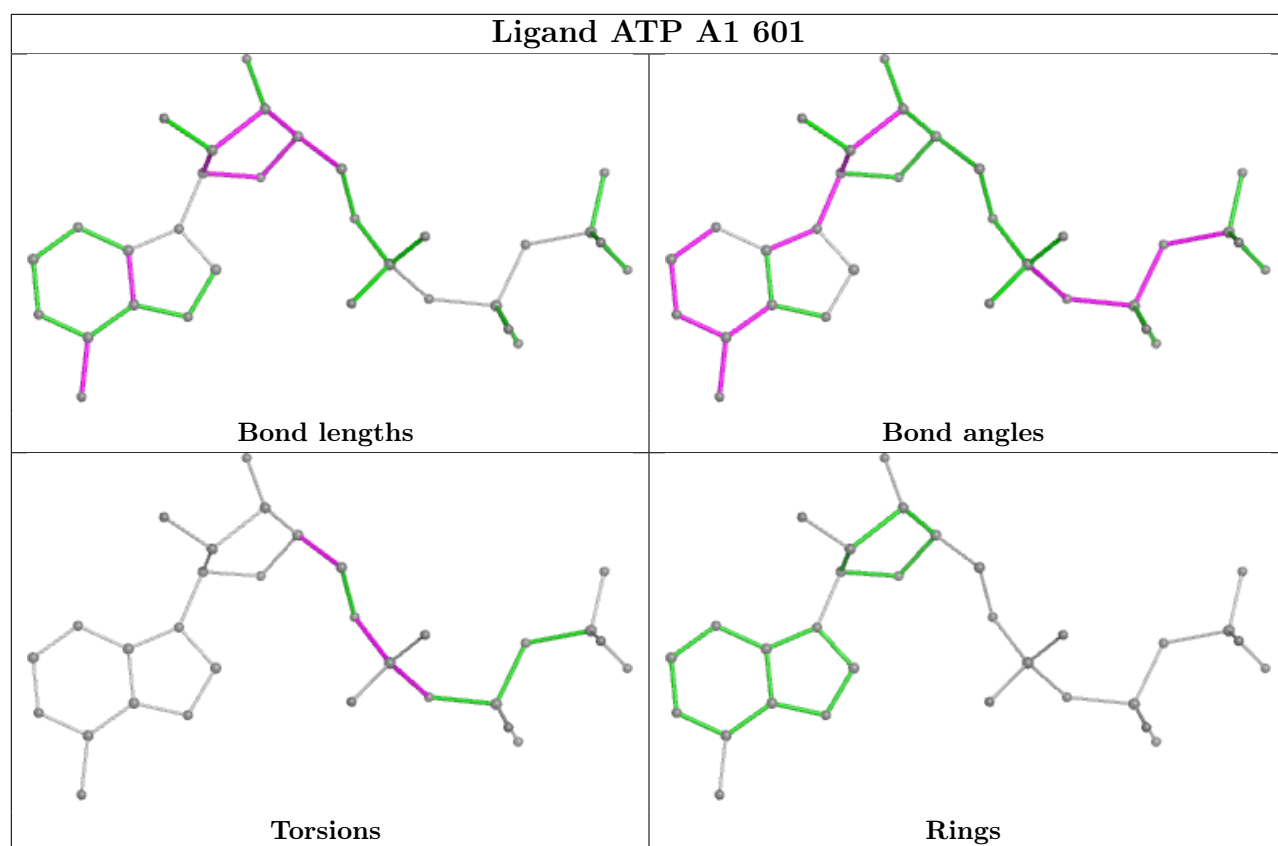


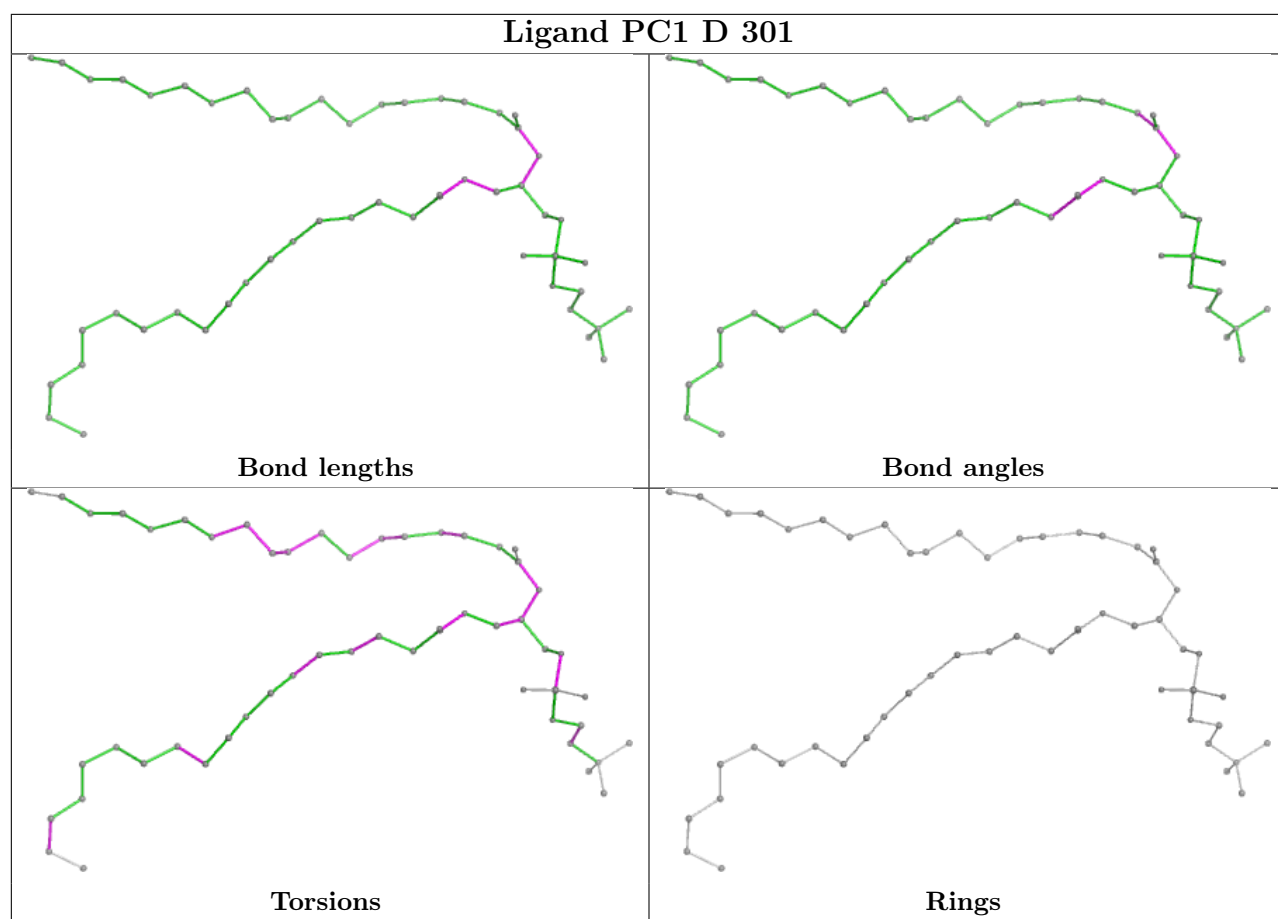


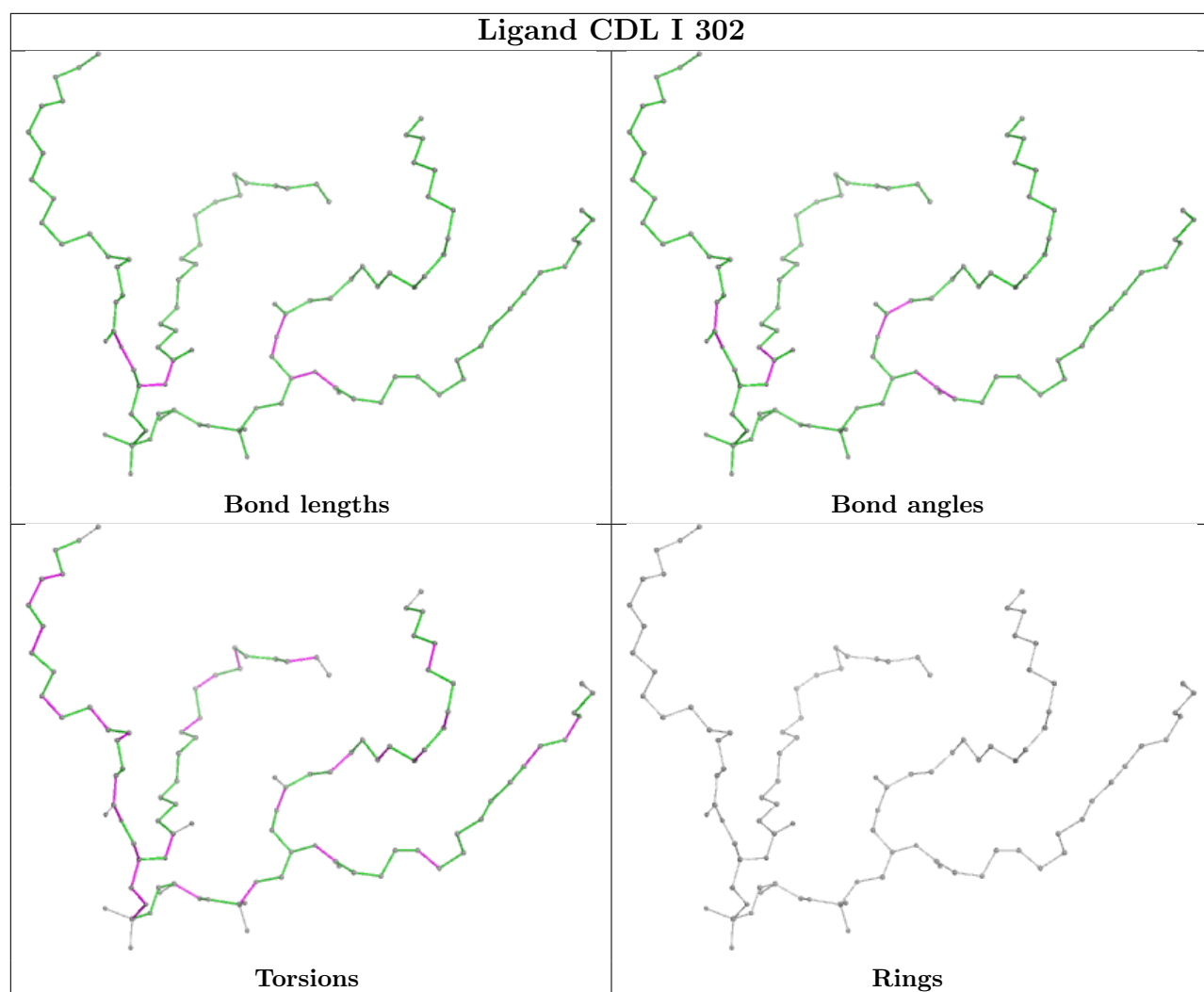


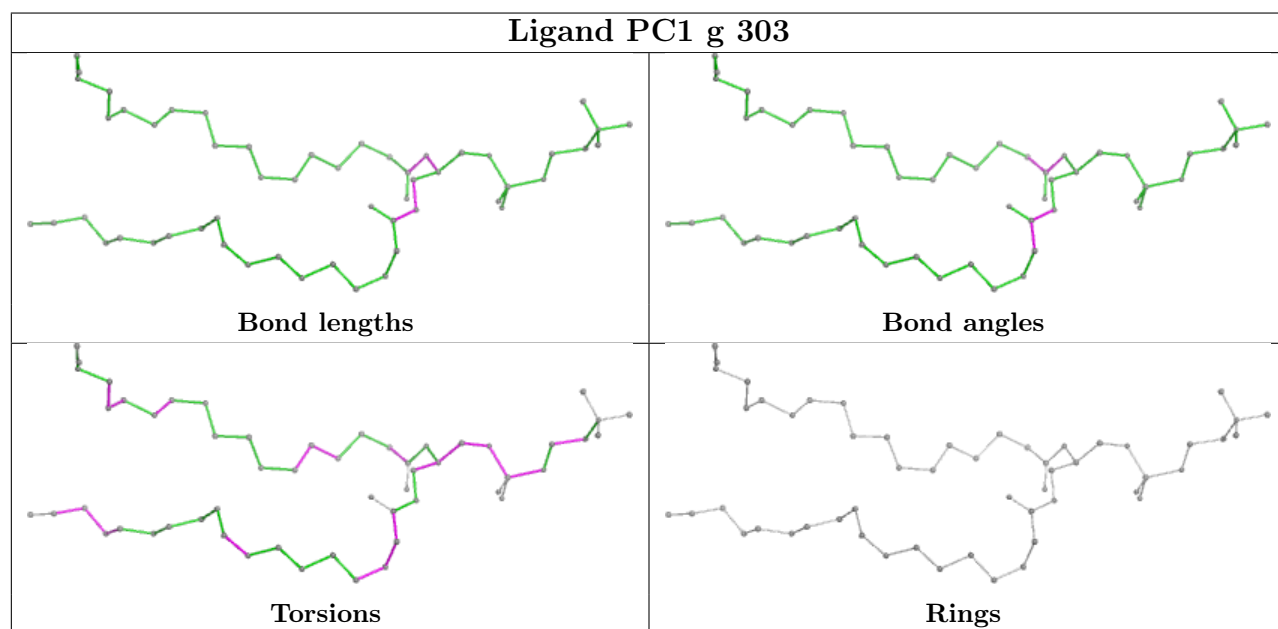
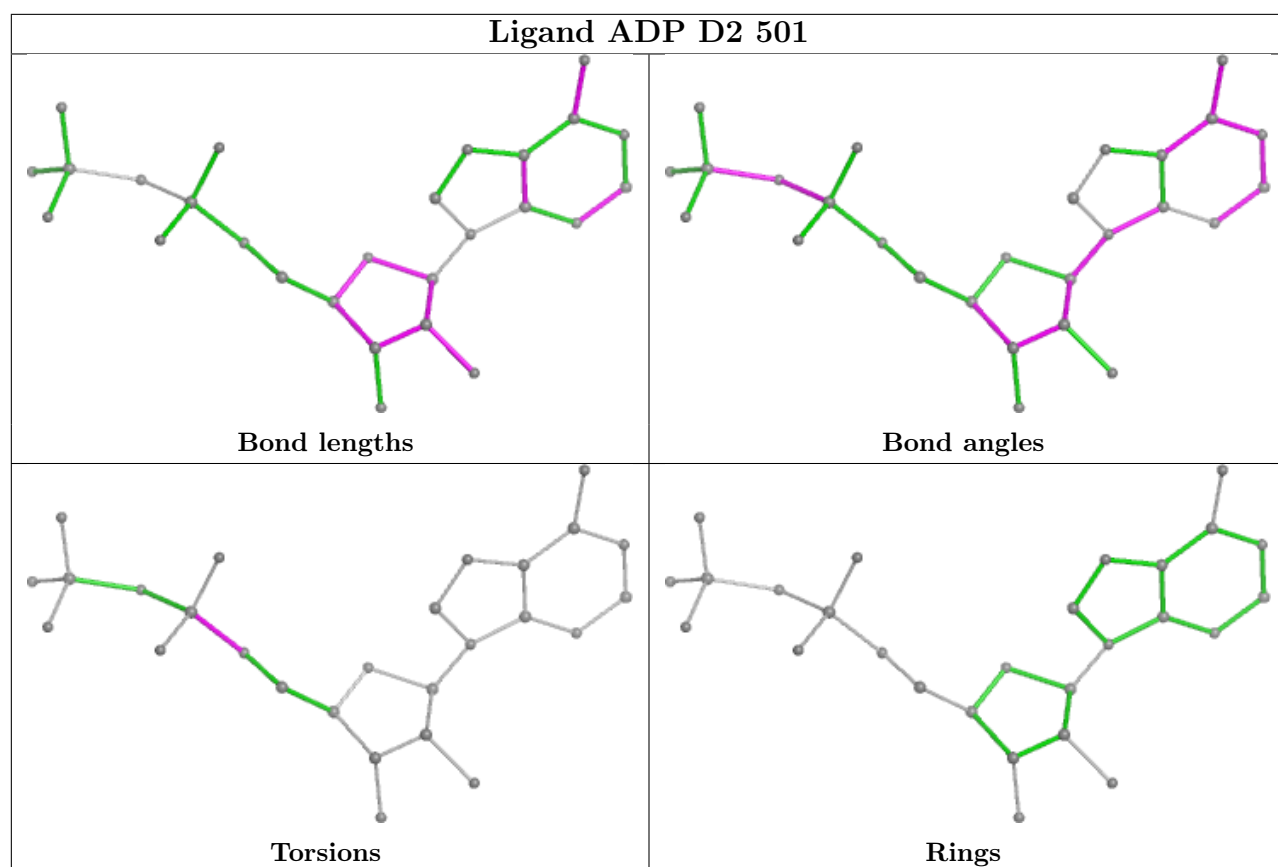


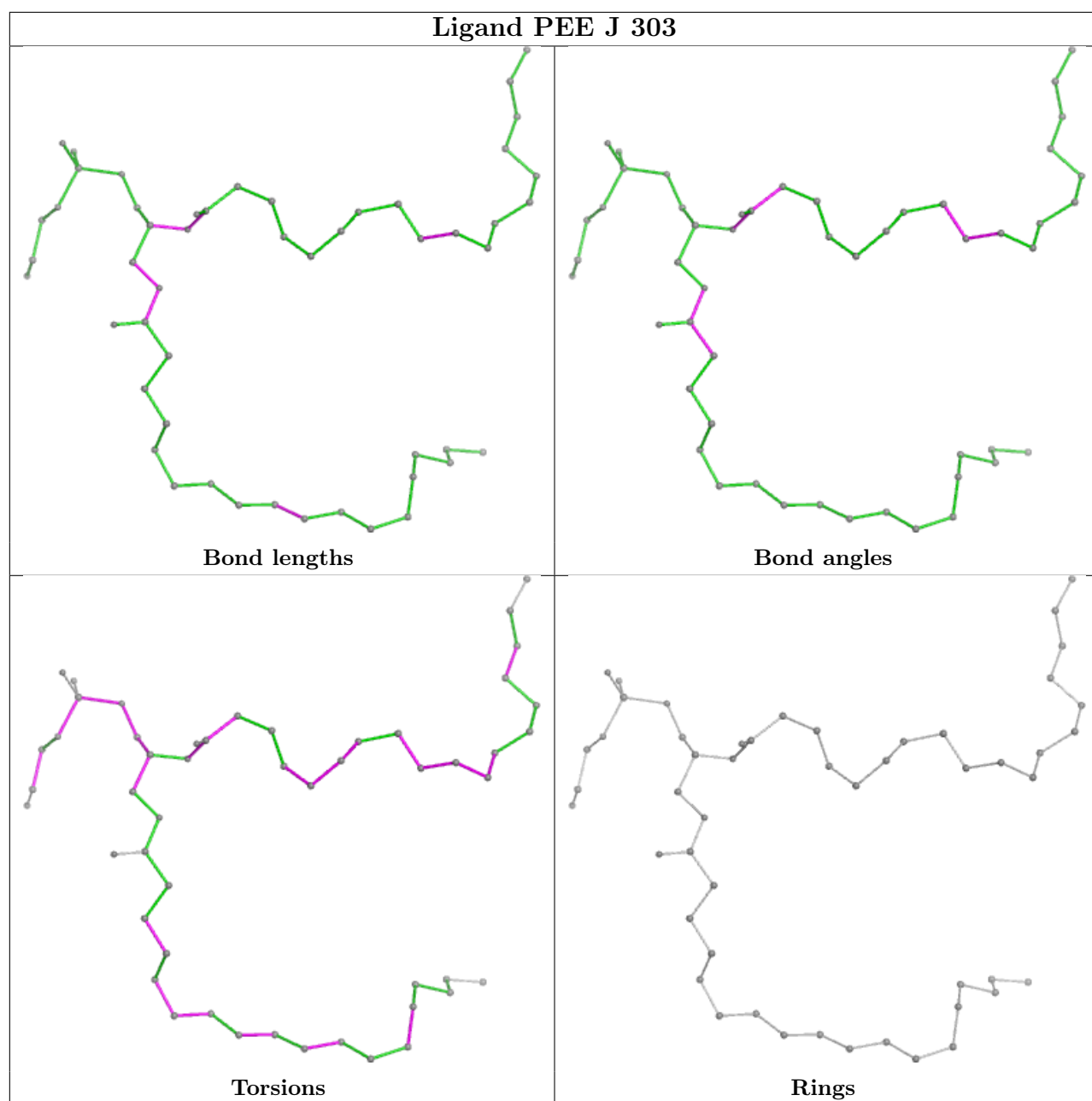


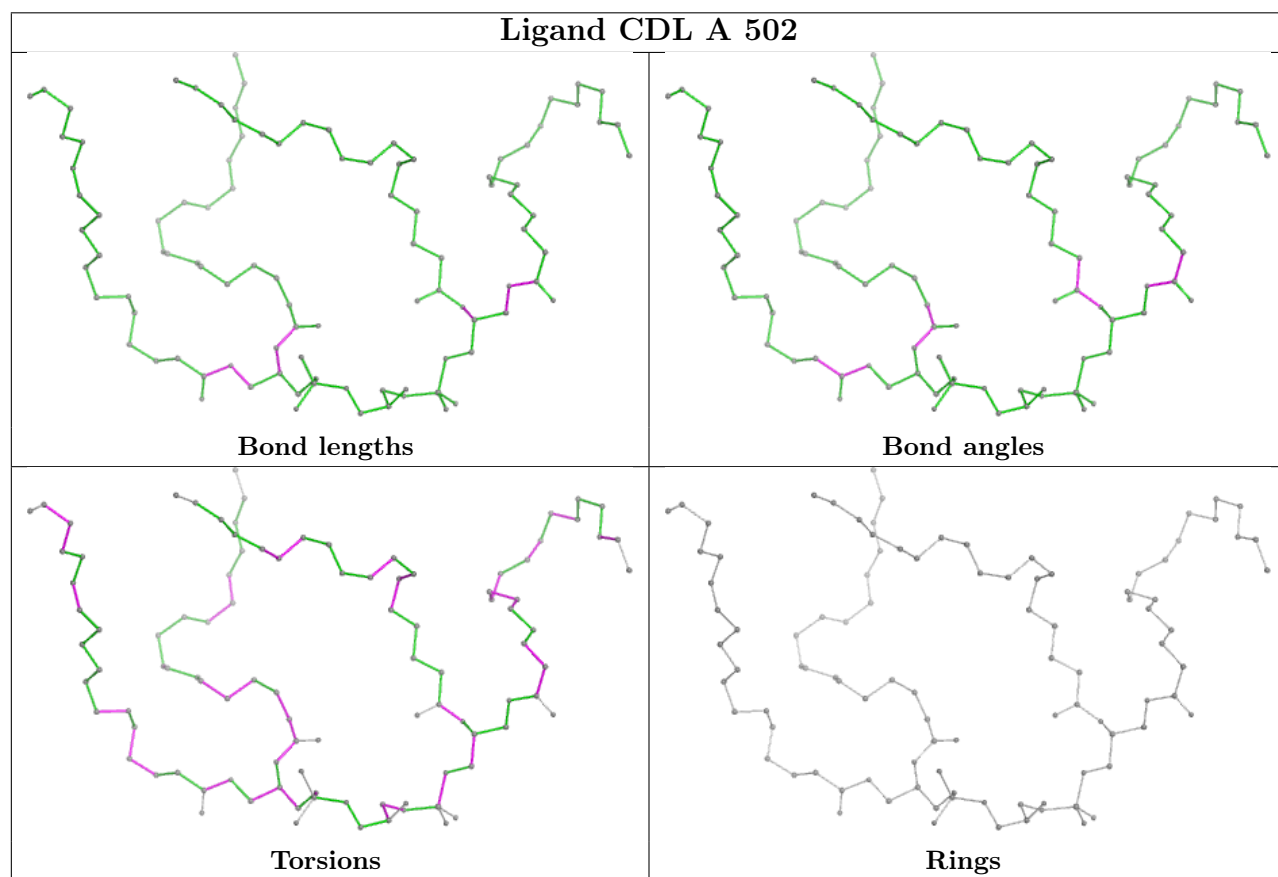
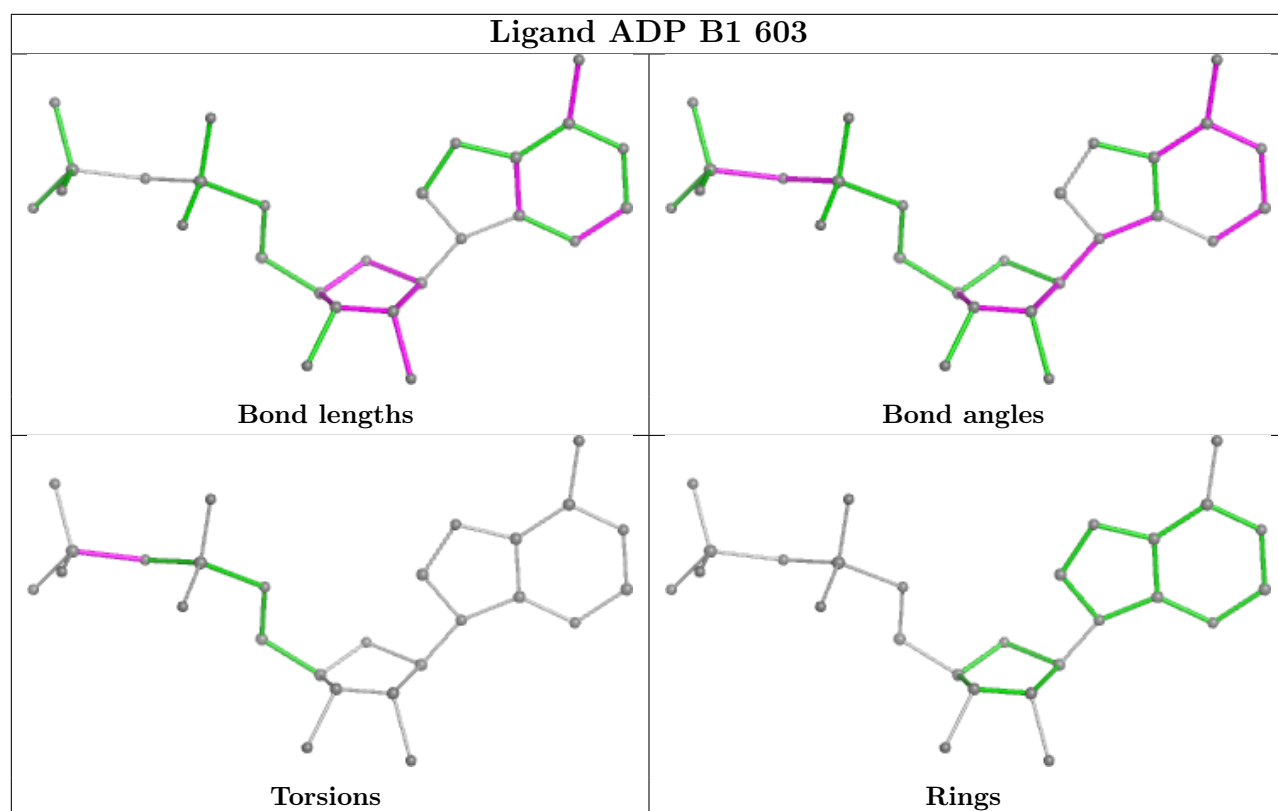




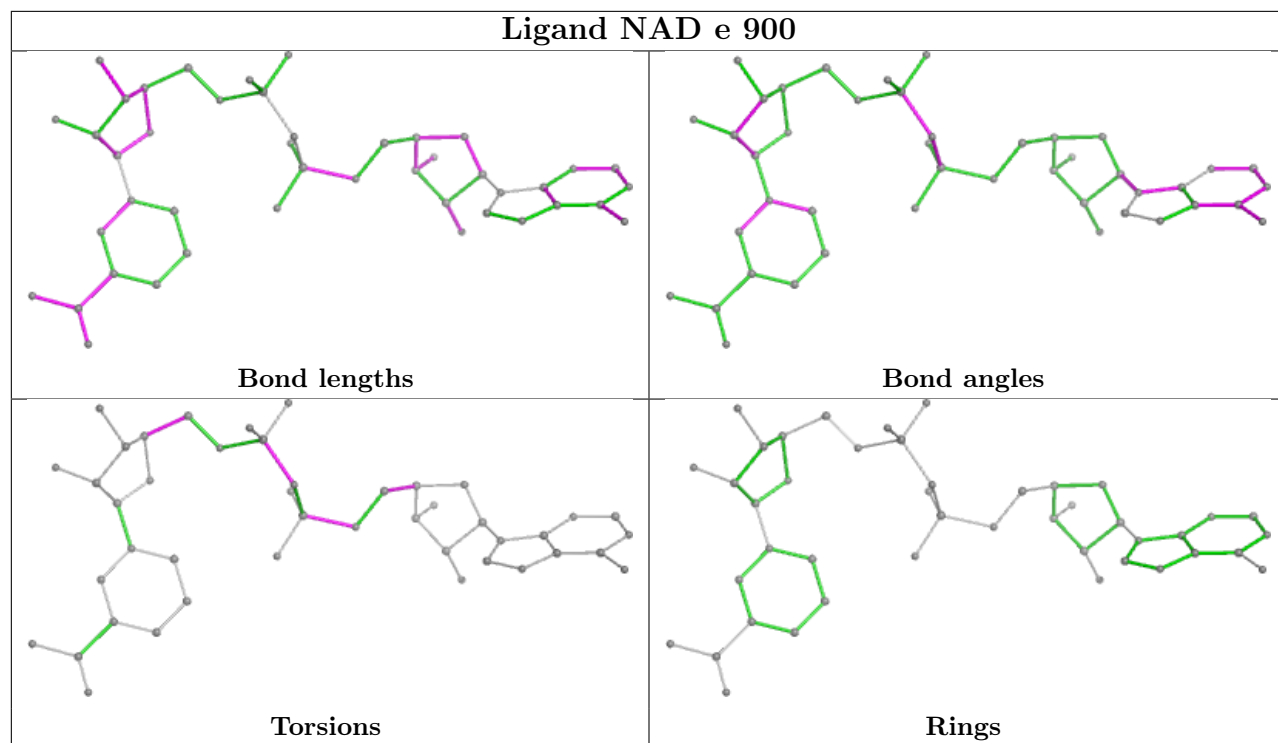




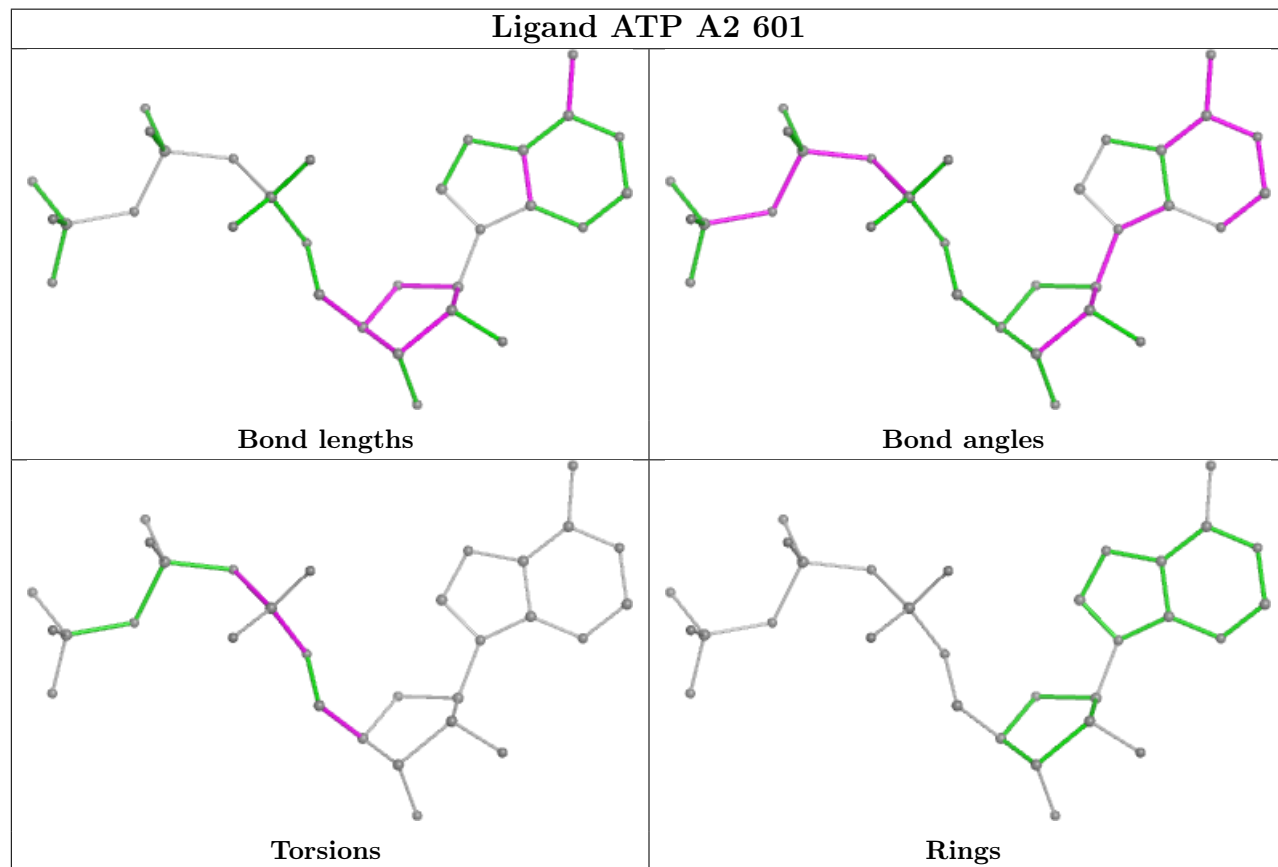




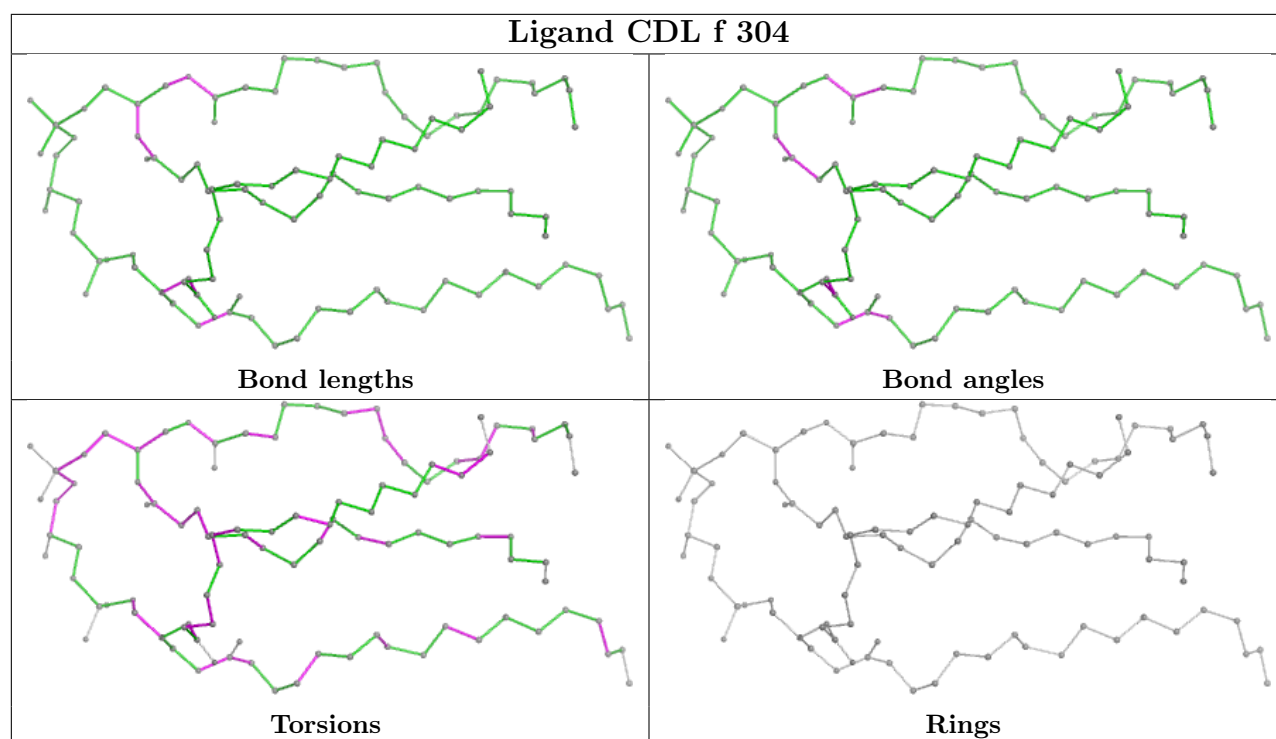
## Ligand NAD e 900

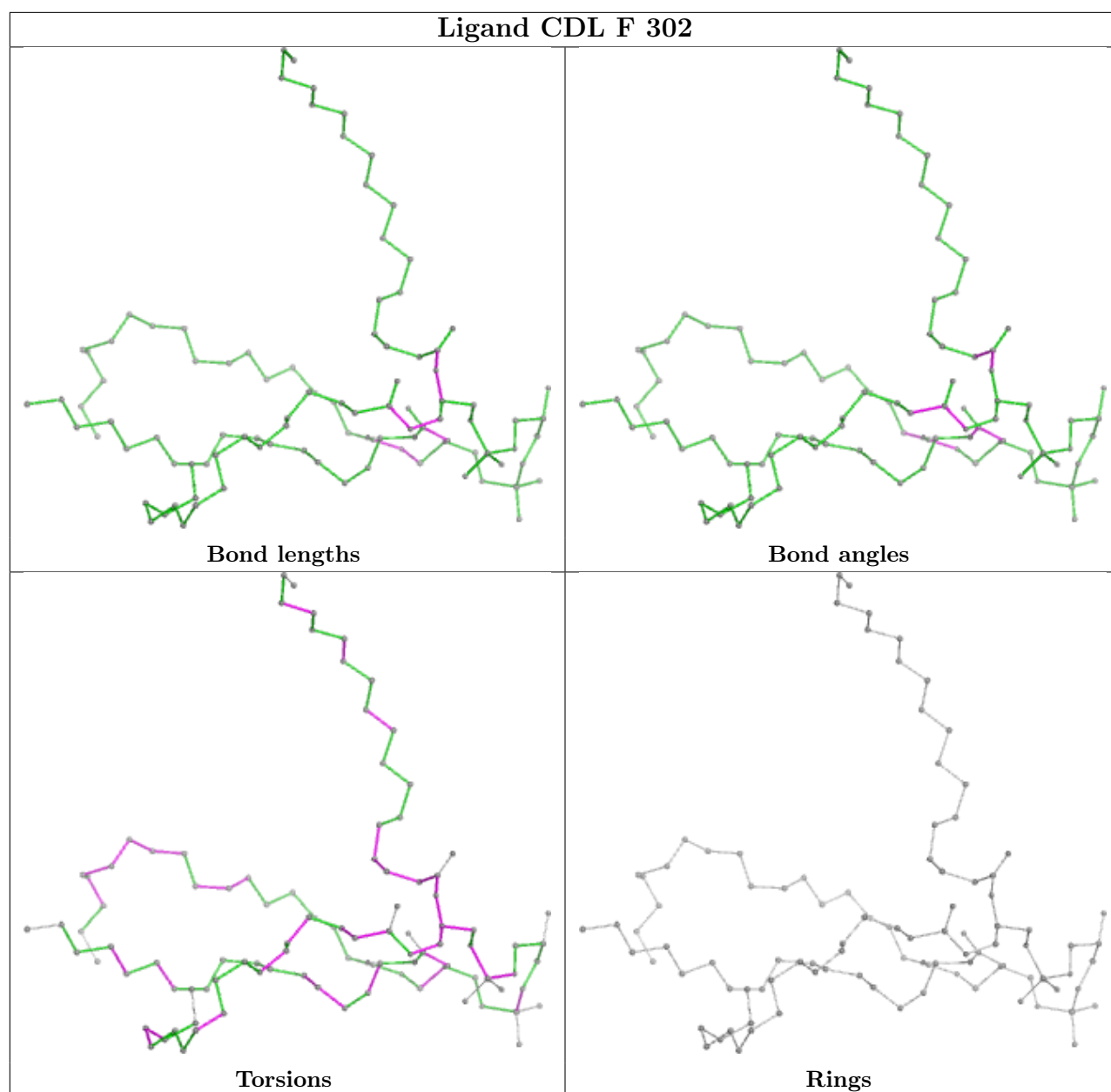


## Ligand ATP A2 601









## 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.

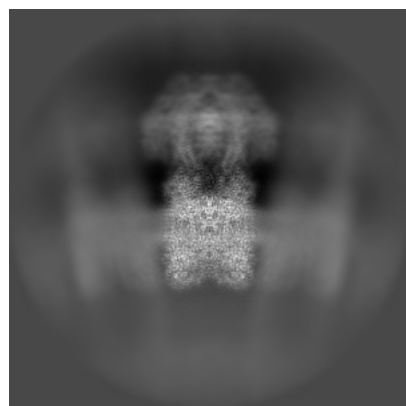
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10860. These allow visual inspection of the internal detail of the map and identification of artifacts.

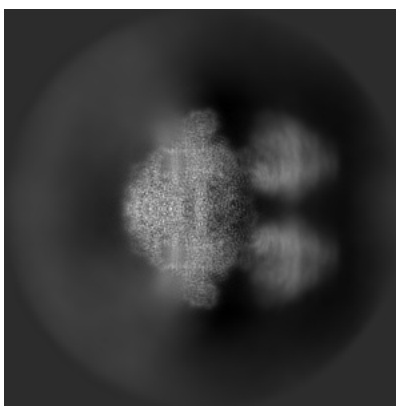
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

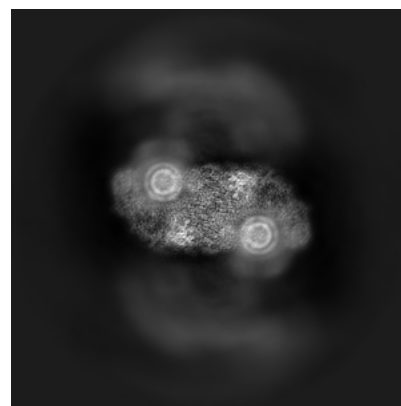
#### 6.1.1 Primary map



X

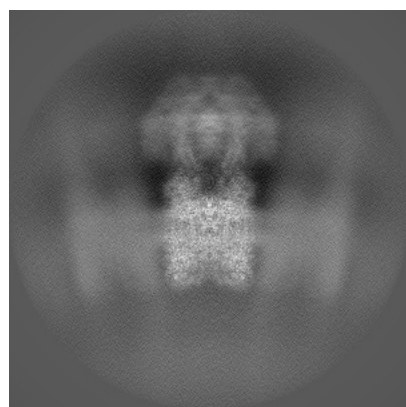


Y

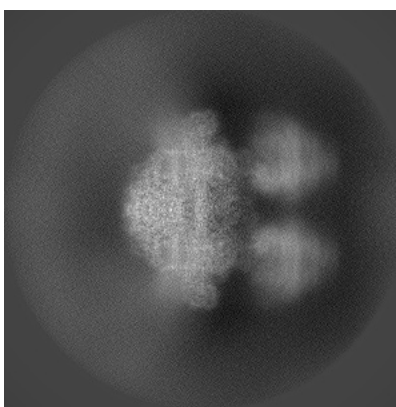


Z

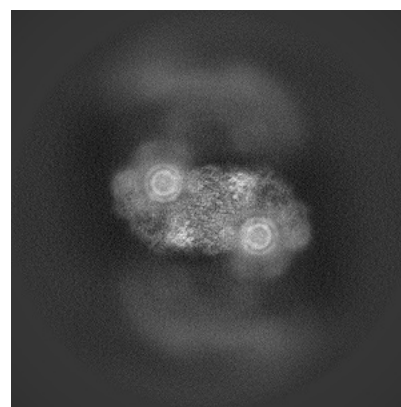
#### 6.1.2 Raw map



X



Y

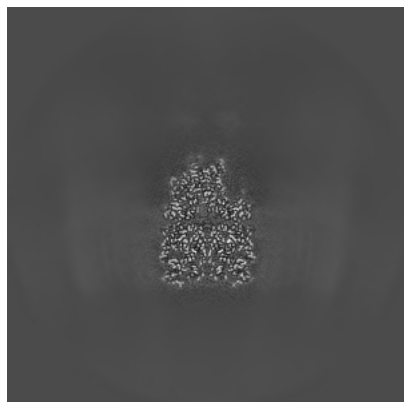


Z

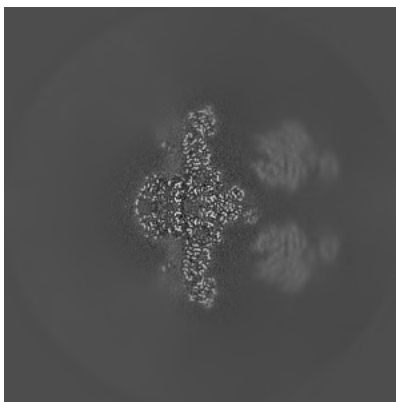
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 300

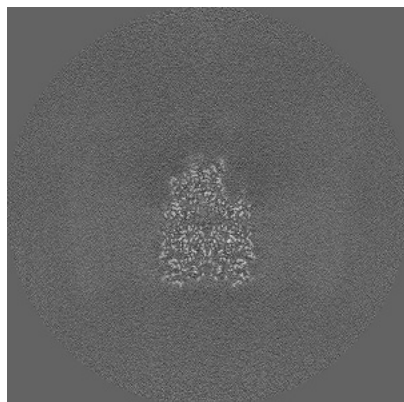


Y Index: 300

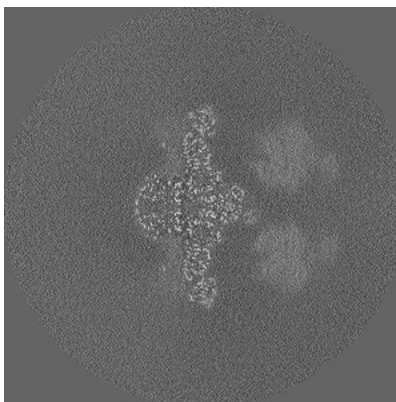


Z Index: 300

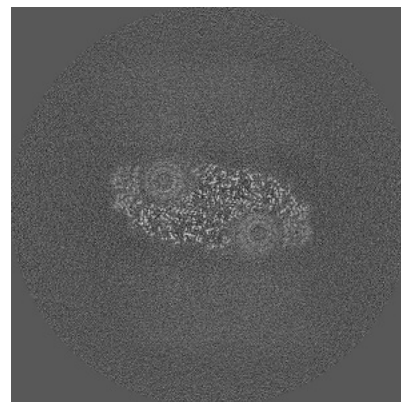
### 6.2.2 Raw map



X Index: 300



Y Index: 300

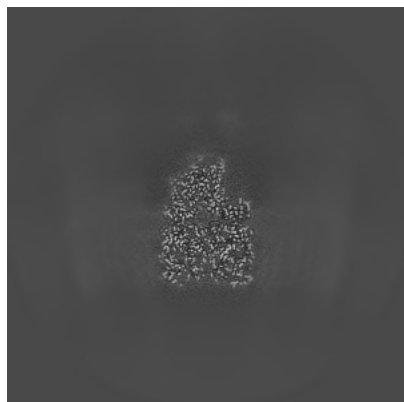


Z Index: 300

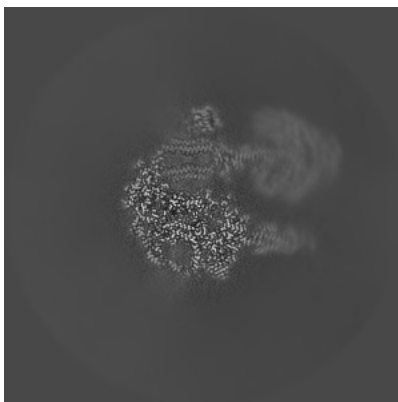
The images above show central slices of the map in three orthogonal directions.

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

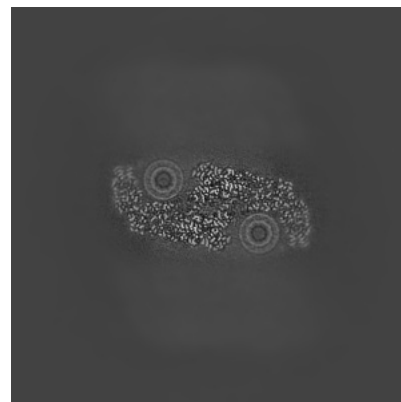
### 6.3.1 Primary map



X Index: 298

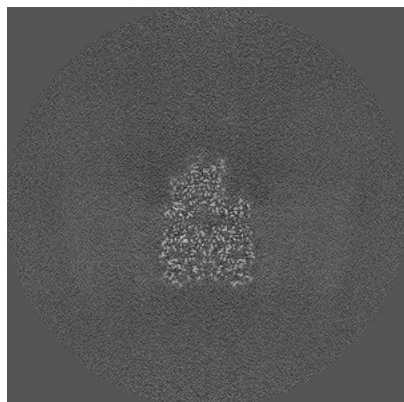


Y Index: 258

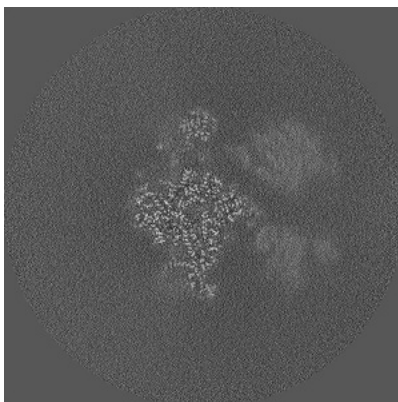


Z Index: 292

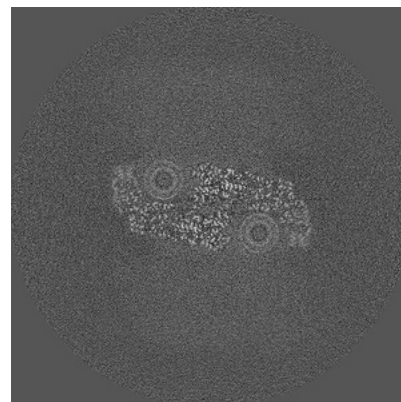
### 6.3.2 Raw map



X Index: 299



Y Index: 290

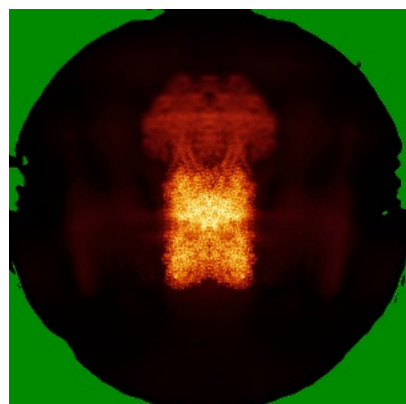


Z Index: 292

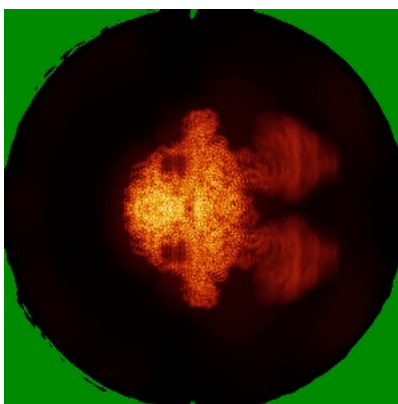
The images above show the largest variance slices of the map in three orthogonal directions.

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

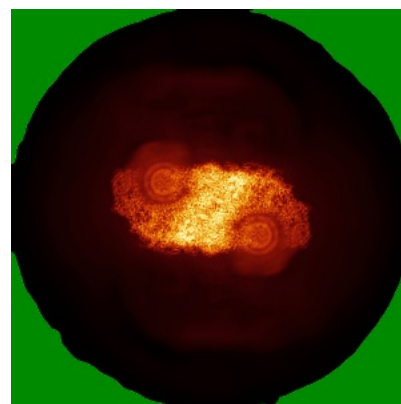
### 6.4.1 Primary map



X

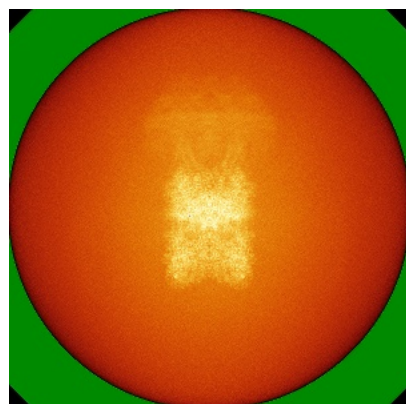


Y

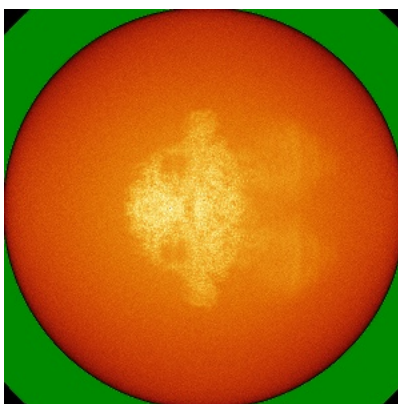


Z

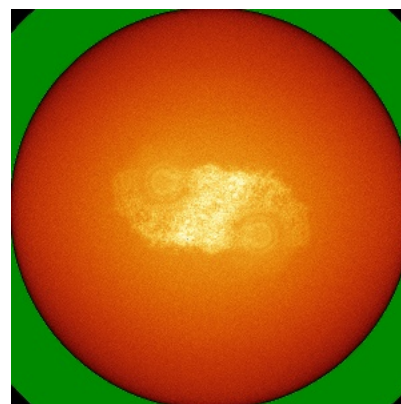
### 6.4.2 Raw map



X



Y



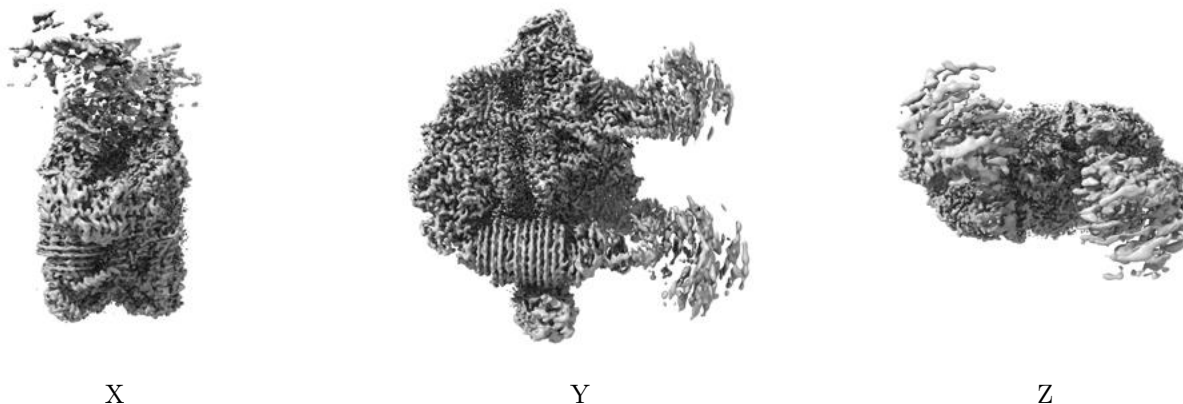
Z

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



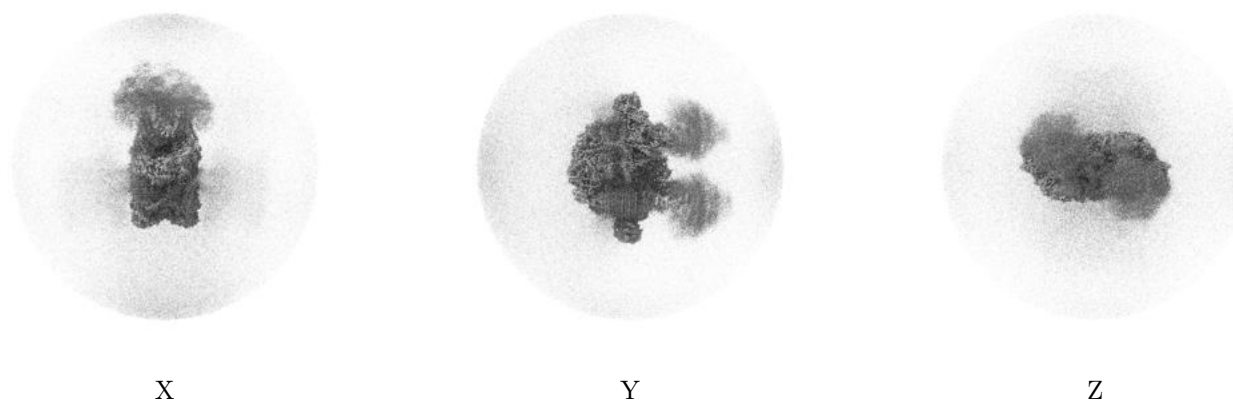
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

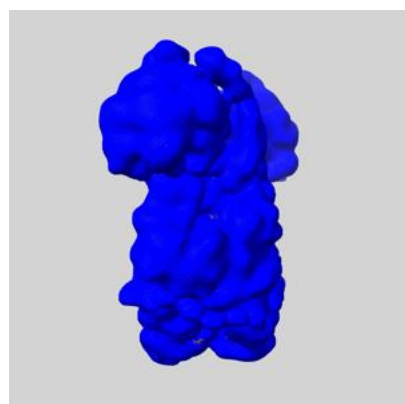
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

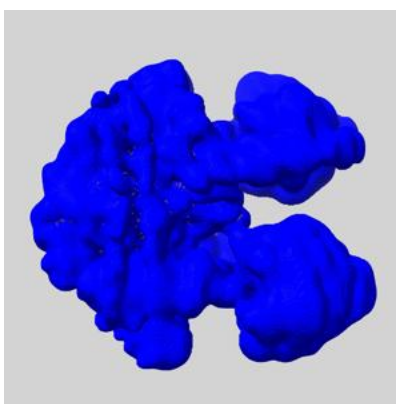
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

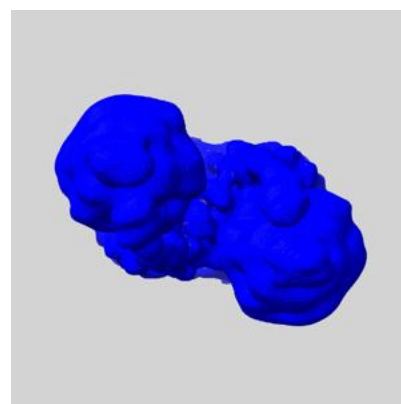
### 6.6.1 emd\_10860\_msk\_1.map [i](#)



X



Y



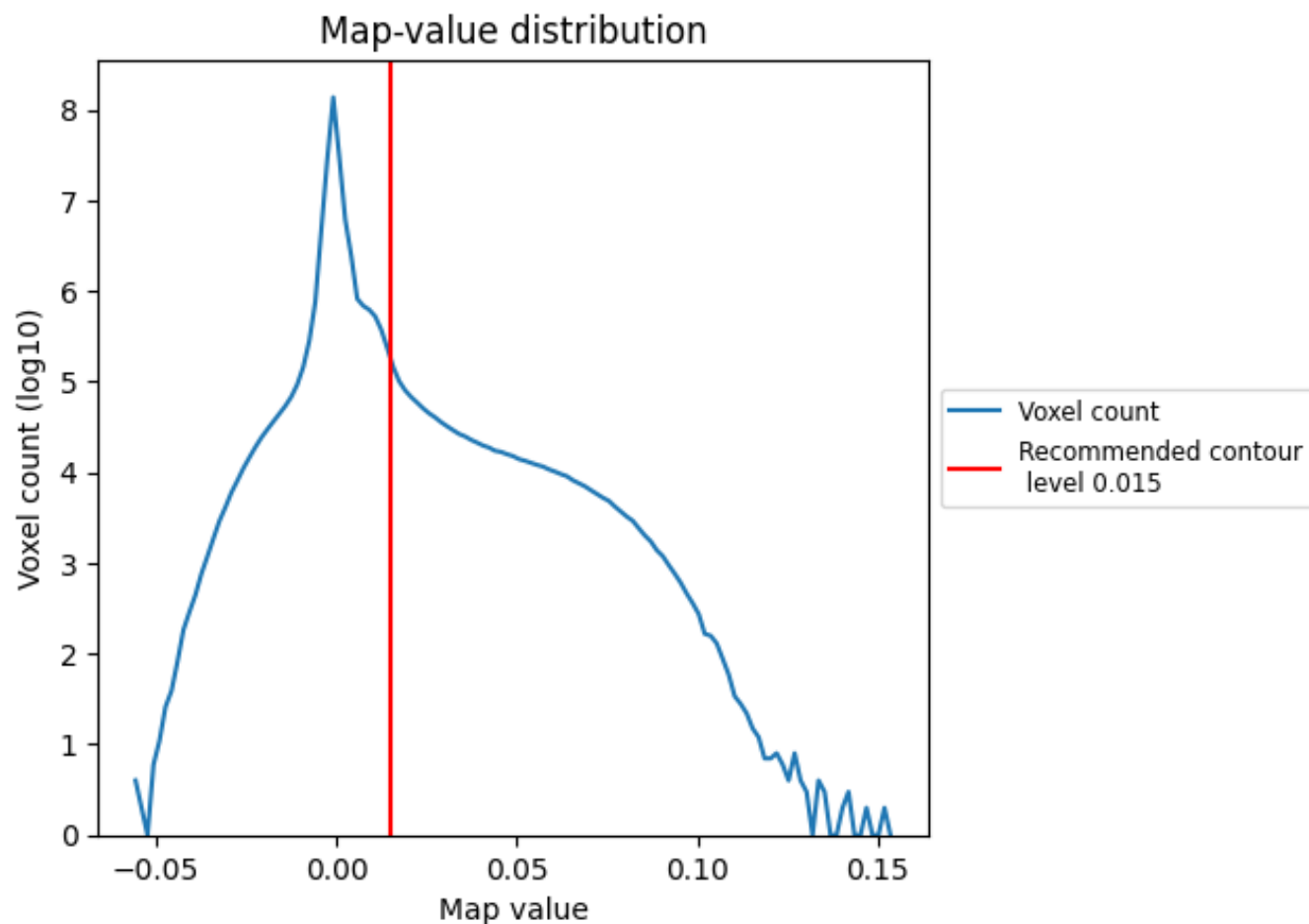
Z



## 7 Map analysis [i](#)

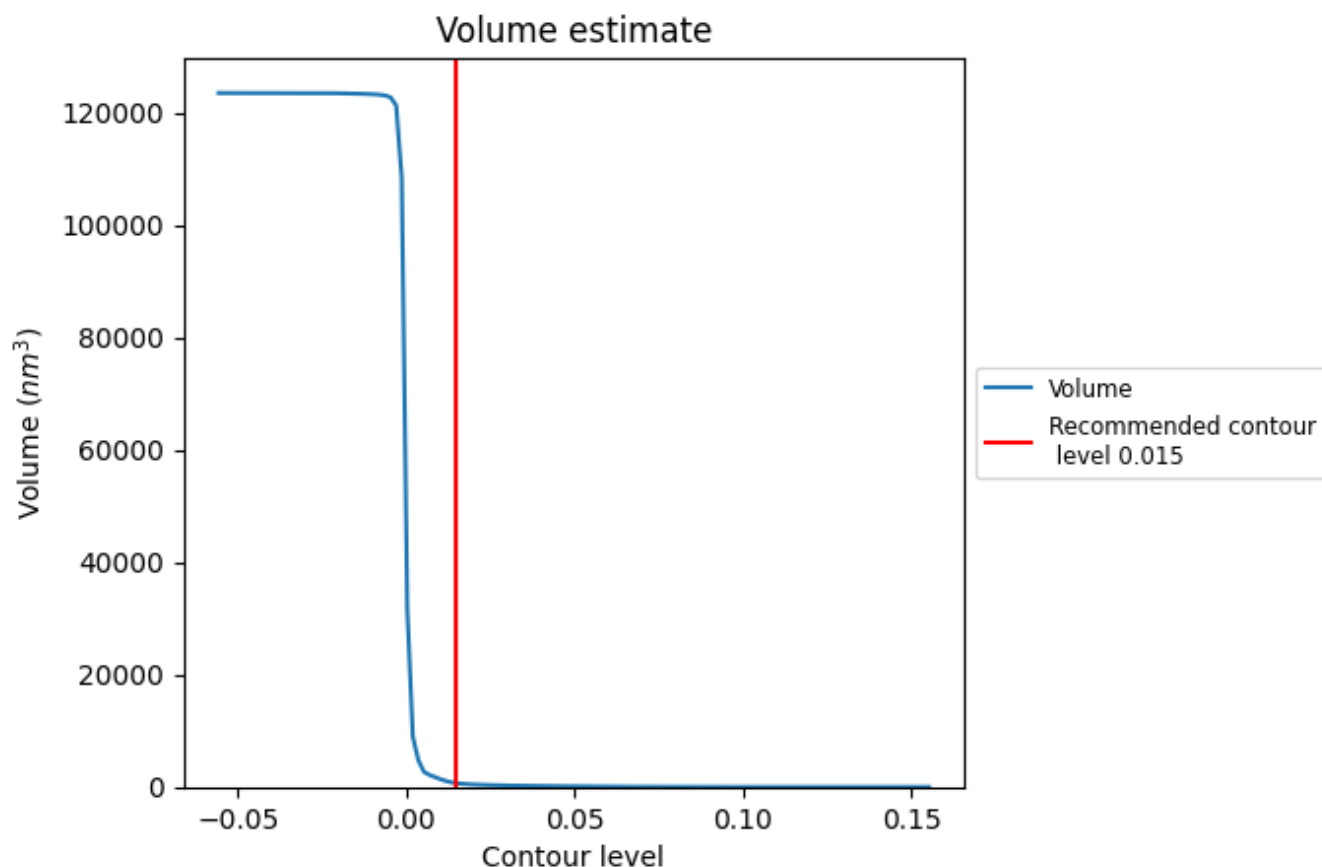
This section contains the results of statistical analysis of the map.

### 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.

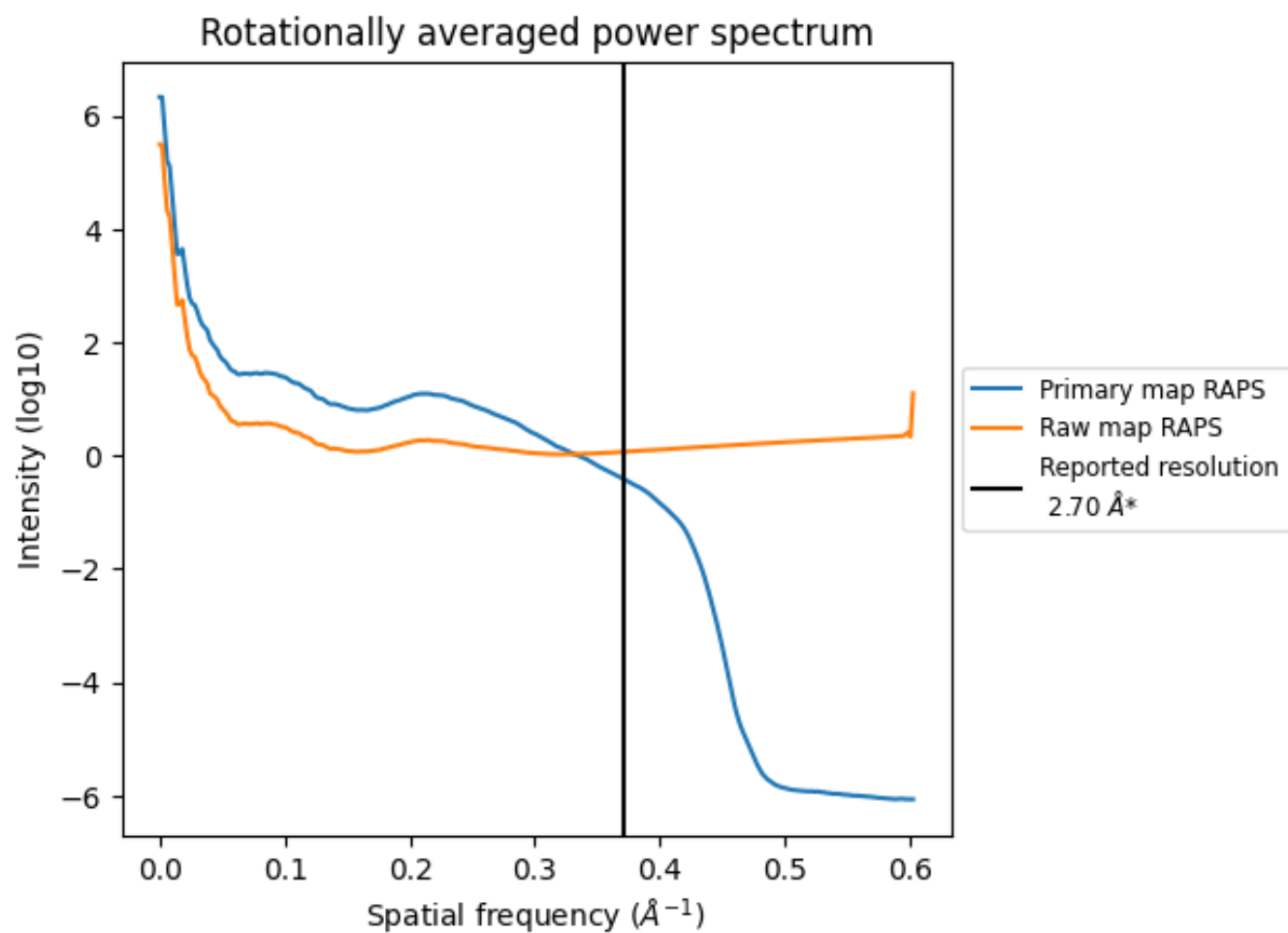
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 665  $\text{nm}^3$ ; this corresponds to an approximate mass of 600 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

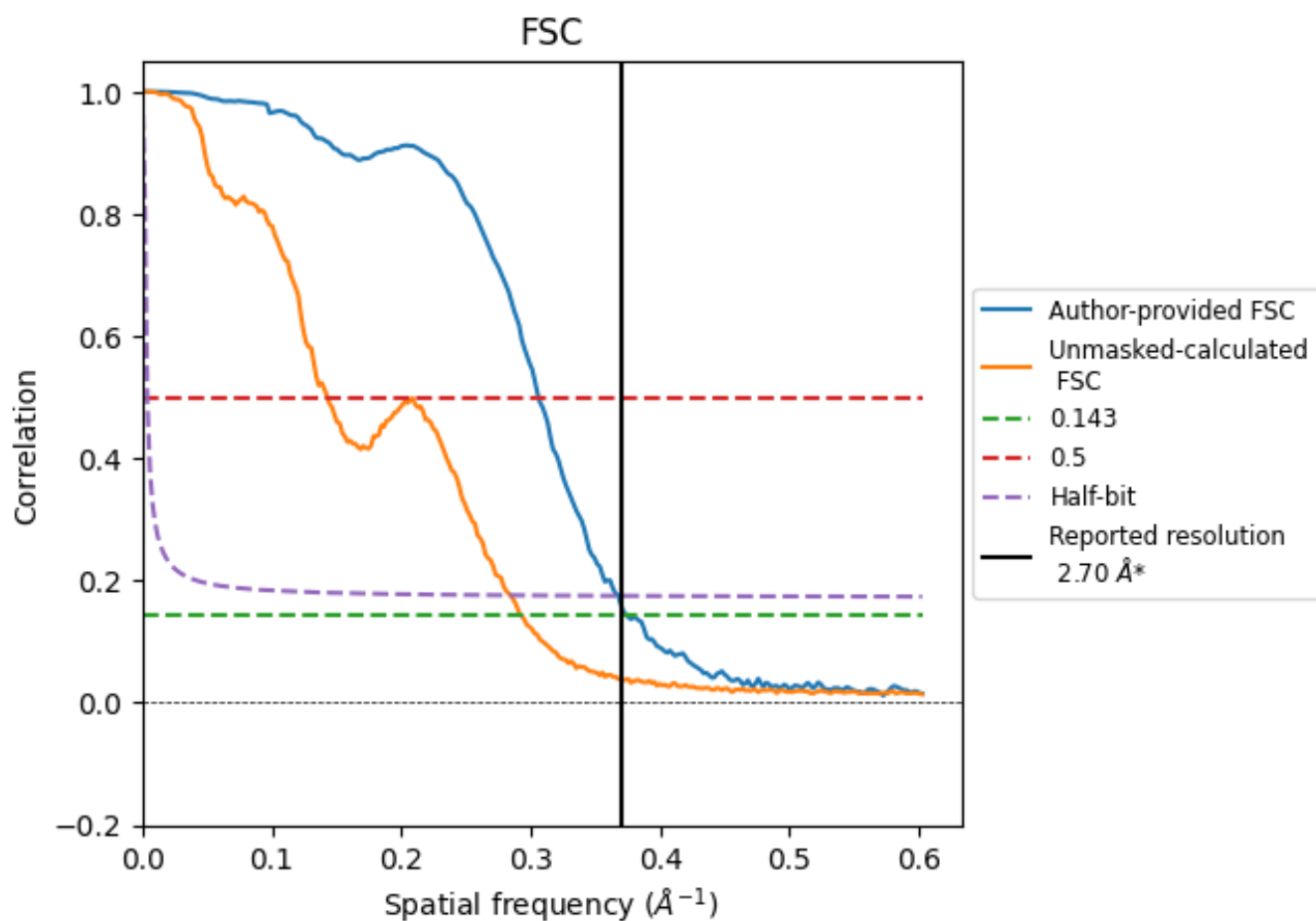


\*Reported resolution corresponds to spatial frequency of 0.370 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.370  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

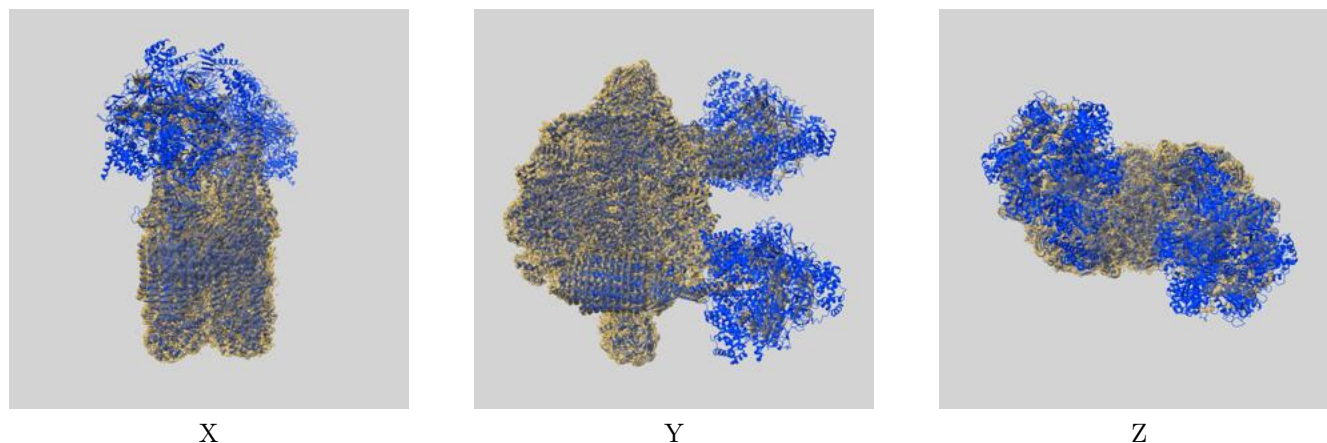
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.67	3.27	2.72
Unmasked-calculated*	3.42	7.00	3.52

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 2.7 by more than 10 %

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

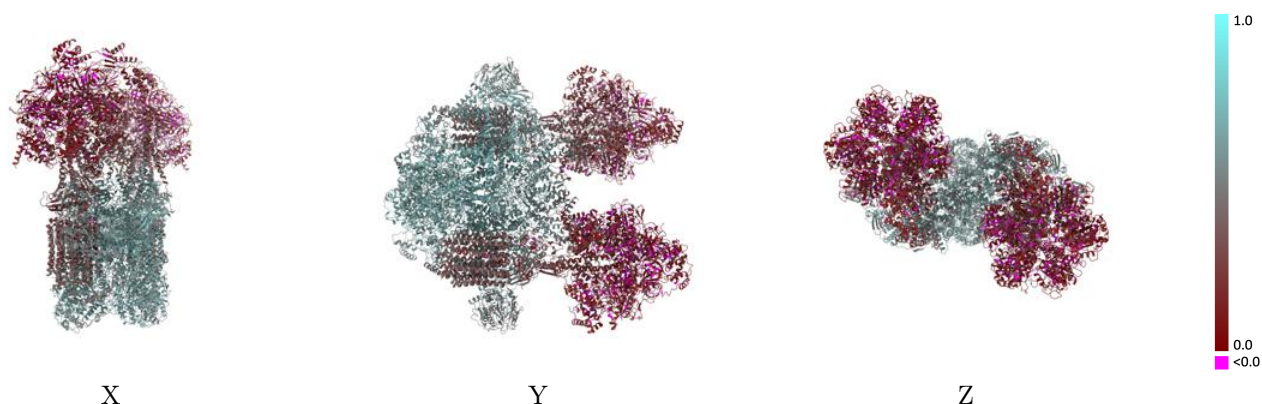
This section contains information regarding the fit between EMDB map EMD-10860 and PDB model 6YNY. Per-residue inclusion information can be found in section [3](#) on page [21](#).

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



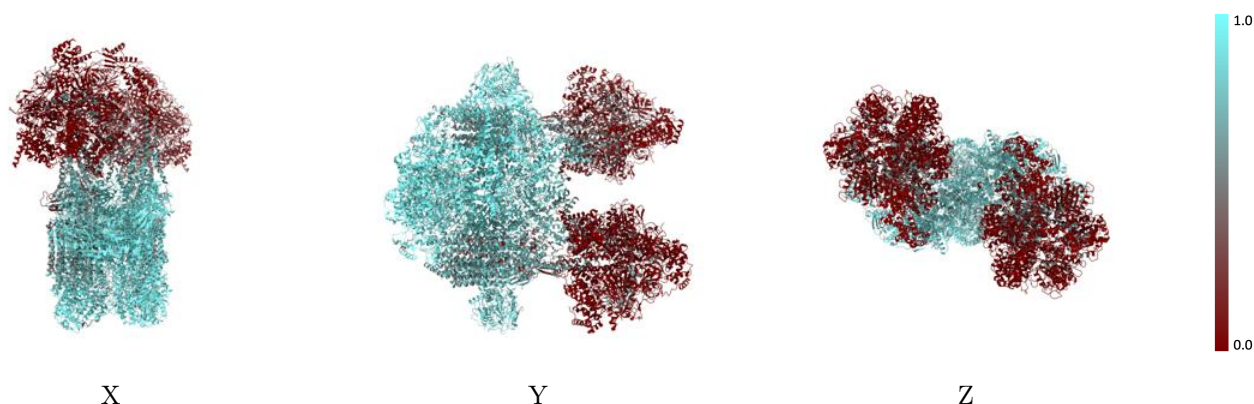
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



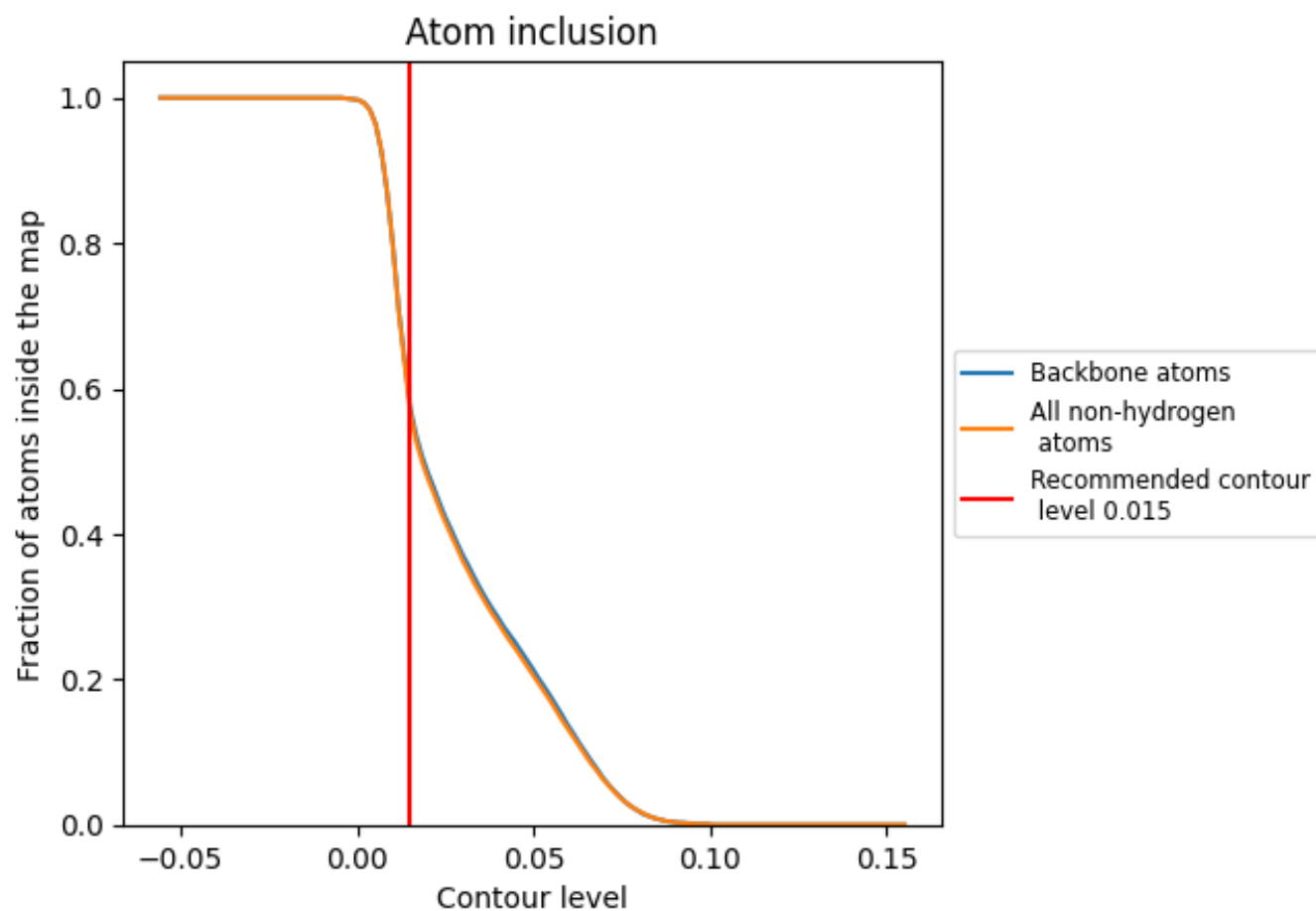
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 58% of all backbone atoms, 57% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5700	 0.4030
A	 0.9540	 0.6410
A1	 0.2440	 0.2160
A2	 0.2050	 0.2000
B	 0.6040	 0.4500
B1	 0.0900	 0.1260
B2	 0.0880	 0.1250
C	 0.9740	 0.6530
C1	 0.0270	 0.1220
C2	 0.0250	 0.1070
D	 0.7480	 0.5130
D1	 0.0540	 0.1330
D2	 0.0470	 0.1300
E	 0.8520	 0.5130
E1	 0.1000	 0.1640
E2	 0.0830	 0.1510
F	 0.9580	 0.6580
F1	 0.0490	 0.1230
F2	 0.0600	 0.1210
G	 0.9160	 0.6040
G1	 0.0000	 0.1260
G2	 0.0000	 0.1340
H	 0.9270	 0.6200
H1	 0.7570	 0.4040
H2	 0.7100	 0.3980
I	 0.9040	 0.6100
I1	 0.6830	 0.3880
I2	 0.6740	 0.3670
J	 0.8810	 0.5980
J1	 0.6960	 0.3790
J2	 0.6760	 0.3790
K	 0.8500	 0.5560
K1	 0.6670	 0.3780
K2	 0.6150	 0.3680
L	 0.9210	 0.6280













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Chain	Atom inclusion	Q-score
L1	 0.6490	 0.3630
L2	 0.6260	 0.3660
M	 0.9690	 0.6440
M1	 0.6940	 0.3700
M2	 0.6640	 0.3670
N	 0.9660	 0.6470
N1	 0.7030	 0.3780
N2	 0.6910	 0.3690
O	 0.9430	 0.6110
O1	 0.6920	 0.3810
O2	 0.6820	 0.3750
P	 0.8320	 0.5540
P1	 0.7010	 0.3740
P2	 0.6960	 0.3710
Q	 0.9260	 0.6100
Q1	 0.7320	 0.3910
Q2	 0.7170	 0.3900
R	 0.9470	 0.6320
S	 0.8480	 0.5740
a	 0.9430	 0.6340
b	 0.6110	 0.4510
c	 0.9790	 0.6570
d	 0.7490	 0.5210
d1	 0.4870	 0.3030
d2	 0.4570	 0.2940
e	 0.8560	 0.5170
e1	 0.5150	 0.3110
e2	 0.4530	 0.2710
f	 0.9220	 0.6320
g	 0.9180	 0.6060
g1	 0.4620	 0.3030
g2	 0.4180	 0.2790
h	 0.9400	 0.6270
i	 0.9140	 0.6180
i1	 0.4320	 0.3210
i2	 0.3790	 0.3130
j	 0.8840	 0.6010
k	 0.8440	 0.5500
l	 0.9270	 0.6260
m	 0.9650	 0.6410
n	 0.9610	 0.6460
o	 0.9370	 0.6100

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Chain	Atom inclusion	Q-score
p	 0.8330	 0.5540
q	 0.9290	 0.6130
r	 0.9380	 0.6240
s	 0.8440	 0.5570
t	 0.9280	 0.6170