



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:30 AM UTC

PDB ID : 6YNZ / pdb_00006ynz
EMDB ID : EMD-10861
Title : Cryo-EM structure of Tetrahymena thermophila mitochondrial ATP synthase
- F1Fo composite tetramer model
Authors : Kock Flygaard, R.; Muhleip, A.; Amunts, A.
Deposited on : 2020-04-14
Resolution : 3.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

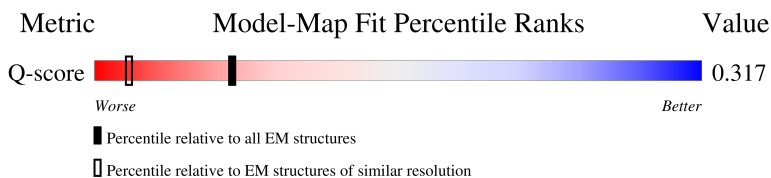
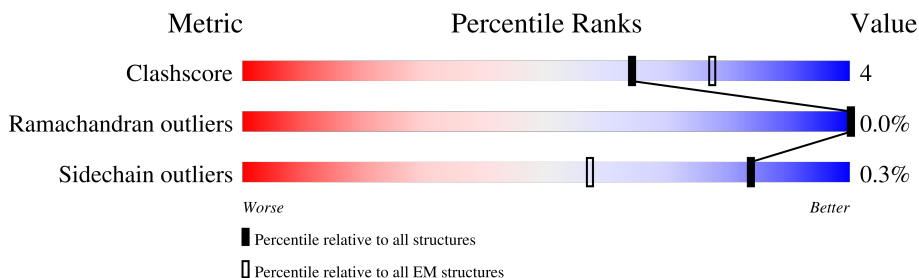
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	A	446	92% 5% .
1	A3	446	91% 6% .
1	a	446	90% 7% .
1	a3	446	91% 6% .

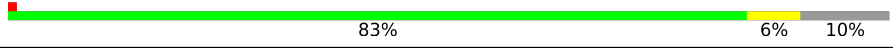
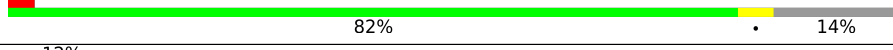
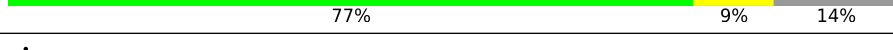
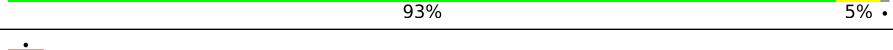
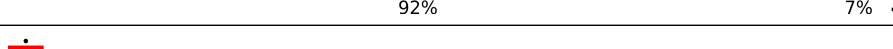
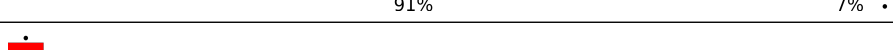
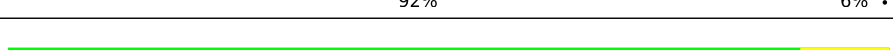
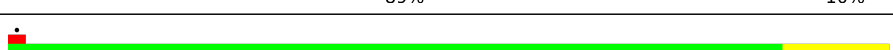
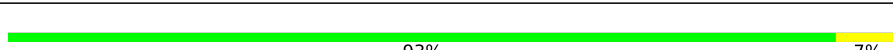
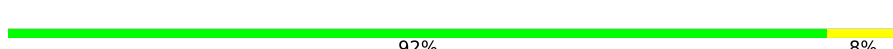
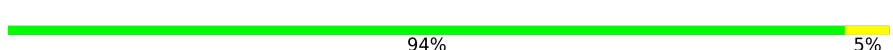
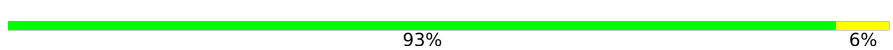
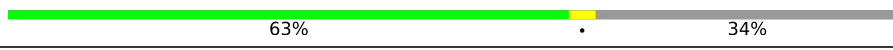
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Mol	Chain	Length	Quality of chain
2	B	381	
2	B3	381	
2	b	381	
2	b3	381	
3	D	234	
3	D3	234	
3	d	234	
3	d3	234	
4	F	204	
4	F3	204	
4	f	204	
4	f3	204	
5	I	209	
5	I3	209	
5	i	209	
5	i3	209	
6	K	179	
6	K3	179	
6	k	179	
6	k3	179	
7	C	100	
7	C3	100	
7	c	100	
7	c3	100	
8	G	286	

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Mol	Chain	Length	Quality of chain
8	G3	286	
8	g	286	
8	g3	286	
9	H	268	
9	H3	268	
9	h	268	
9	h3	268	
10	J	273	
10	J3	273	
10	j	273	
10	j3	273	
11	L	247	
11	L3	247	
11	l	247	
11	l3	247	
12	M	221	
12	M3	221	
12	m	221	
12	m3	221	
13	N	179	
13	N3	179	
13	n	179	
13	n3	179	
14	O	154	
14	O3	154	

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Mol	Chain	Length	Quality of chain
14	o	154	
14	o3	154	
15	P	152	
15	P3	152	
15	p	152	
15	p3	152	
16	Q	152	
16	Q3	152	
16	q	152	
16	q3	152	
17	R	149	
17	R3	149	
17	r	149	
17	r3	149	
18	S	145	
18	S3	145	
18	s	145	
18	s3	145	
19	E	480	
19	E3	480	
19	e	480	
19	e3	480	
20	i1	108	
20	i2	108	
20	i4	108	

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Mol	Chain	Length	Quality of chain
20	i5	108	
21	t	460	
21	t3	460	
22	G1	219	
22	G2	219	
22	G4	219	
22	G5	219	
23	g1	299	
23	g2	299	
23	g4	299	
23	g5	299	
24	A1	546	
24	A2	546	
24	A4	546	
24	A5	546	
24	B1	546	
24	B2	546	
24	B4	546	
24	B5	546	
24	C1	546	
24	C2	546	
24	C4	546	
24	C5	546	
25	D1	497	
25	D2	497	

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Mol	Chain	Length	Quality of chain
25	D4	497	93% 85%10%5%
25	D5	497	94% 84%11%5%
25	E1	497	85% 83%12%5%
25	E2	497	94% 83%11%5%
25	E4	497	94% 84%11%5%
25	E5	497	86% 81%13%5%
25	F1	497	91% 81%13%6%
25	F2	497	91% 82%12%6%
25	F4	497	92% 81%13%6%
25	F5	497	91% 83%11%6%
26	H1	76	9% 83%16%.
26	H2	76	5% 84%14%.
26	H4	76	7% 87%12%.
26	H5	76	9% 80%18%.
26	I1	76	14% 82%17%.
26	I2	76	. 76%22%.
26	I4	76	5% 80%18%.
26	I5	76	14% 82%17%.
26	J1	76	24% 89%9%.
26	J2	76	8% 83%16%.
26	J4	76	8% 84%14%.
26	J5	76	26% 84%14%.
26	K1	76	32% 87%12%.
26	K2	76	13% 86%13%.
26	K4	76	14% 83%16%.

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Mol	Chain	Length	Quality of chain
26	K5	76	
26	L1	76	
26	L2	76	
26	L4	76	
26	L5	76	
26	M1	76	
26	M2	76	
26	M4	76	
26	M5	76	
26	N1	76	
26	N2	76	
26	N4	76	
26	N5	76	
26	O1	76	
26	O2	76	
26	O4	76	
26	O5	76	
26	P1	76	
26	P2	76	
26	P4	76	
26	P5	76	
26	Q1	76	
26	Q2	76	
26	Q4	76	
26	Q5	76	

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Mol	Chain	Length	Quality of chain
27	d1	158	
27	d2	158	
27	d4	158	
27	d5	158	
28	e1	71	
28	e2	71	
28	e4	71	
28	e5	71	

2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 571866 atoms, of which 287810 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 Ymf66.

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		
1	a3	433	Total	C	H	N	O	S	0	0
			7155	2453	3527	526	633	16		
1	A3	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		
2	b3	354	Total	C	H	N	O	S	0	0
			5726	1845	2851	487	531	12		
2	B3	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		
3	d3	206	Total	C	H	N	O	S	0	0
			3274	1065	1598	274	332	5		
3	D3	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		
4	f3	200	Total	C	H	N	O	S	0	0
			3373	1095	1691	299	278	10		
4	F3	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		
5	i3	209	Total	C	H	N	O	S	0	0
			3462	1121	1742	304	285	10		
5	I3	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		
6	k3	179	Total	C	H	N	O	S	0	0
			2902	939	1429	257	266	11		
6	K3	179	Total	C	H	N	O	S	0	0
			2903	939	1430	257	266	11		

- Molecule 7 is a protein called Ymf56.

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		
7	c3	96	Total	C	H	N	O	S	0	0
			1671	565	830	131	143	2		

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Mol	Chain	Residues	Atoms						AltConf	Trace
7	C3	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		
8	g3	256	Total	C	H	N	O	S	0	0
			4338	1474	2118	348	388	10		
8	G3	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		
9	h3	231	Total	C	H	N	O	S	0	0
			3836	1236	1883	361	350	6		
9	H3	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		
10	J	269	Total	C	H	N	O	S	0	0
			4346	1381	2147	406	404	8		
10	j3	269	Total	C	H	N	O	S	0	0
			4346	1381	2147	406	404	8		
10	J3	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	l	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		
11	l3	246	Total	C	H	N	O	S	0	0
			4070	1344	1999	360	361	6		
11	L3	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		
12	m3	221	Total	C	H	N	O	S	0	0
			3696	1205	1835	313	336	7		
12	M3	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		
13	n3	119	Total	C	H	N	O	S	0	0
			1960	655	962	164	173	6		
13	N3	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		
14	o3	99	Total	C	H	N	O	S	0	0
			1599	507	794	145	147	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
14	O3	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		
15	p3	150	Total	C	H	N	O	S	0	0
			2413	788	1196	204	224	1		
15	P3	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		
16	q3	108	Total	C	H	N	O	S	0	0
			1749	556	874	149	169	1		
16	Q3	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		
17	r3	145	Total	C	H	N	O	S	0	0
			2373	776	1180	201	212	4		
17	R3	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		
18	s3	124	Total	C	H	N	O	S	0	0
			2025	648	1009	174	189	5		
18	S3	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		
19	e3	417	Total	C	H	N	O	S	0	0
			6681	2171	3286	602	614	8		
19	E3	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		
20	i5	64	Total	C	H	N	O	S	0	0
			1112	351	556	97	107	1		
20	i4	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		
21	t3	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		
22	G4	188	Total	C	H	N	O	S	0	0
			3000	942	1515	252	287	4		
22	G5	188	Total	C	H	N	O	S	0	0
			3000	942	1515	252	287	4		

- Molecule 23 is a protein called ATP synthase 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		
23	g4	275	Total	C	H	N	O	S	0	0
			4332	1343	2206	373	400	10		
23	g5	275	Total	C	H	N	O	S	0	0
			4332	1343	2206	373	400	10		

- Molecule 24 is a protein called ATP synthase 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		
24	C4	513	Total	C	H	N	O	S	0	0
			7980	2481	4058	685	739	17		
24	B4	511	Total	C	H	N	O	S	0	0
			7934	2469	4030	681	737	17		
24	A4	512	Total	C	H	N	O	S	0	0
			7946	2472	4037	682	738	17		
24	C5	513	Total	C	H	N	O	S	0	0
			7980	2481	4058	685	739	17		

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Mol	Chain	Residues	Atoms						AltConf	Trace
24	B5	511	Total	C	H	N	O	S	0	0
			7934	2469	4030	681	737	17		
24	A5	512	Total	C	H	N	O	S	0	0
			7946	2472	4037	682	738	17		

- Molecule 25 is a protein called ATP synthase 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		
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		
25	D4	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
25	F4	469	Total	C	H	N	O	S	0	0
			7113	2237	3568	610	687	11		
25	E4	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
25	D5	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
25	F5	469	Total	C	H	N	O	S	0	0
			7113	2237	3568	610	687	11		
25	E5	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		

- Molecule 26 is a protein called ATP synthase F0 subunit 9.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	P1	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	O1	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	N1	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
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
26	K2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	J2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	I2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	H2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	Q2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	P4	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	O4	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	N4	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	M4	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	L4	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	K4	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	J4	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	I4	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	H4	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	Q4	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	P5	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	O5	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	N5	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	M5	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	L5	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	K5	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	J5	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	I5	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	H5	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	Q5	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0

- 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		
27	d4	134	Total	C	H	N	O	S	0	0
			2144	674	1082	185	200	3		

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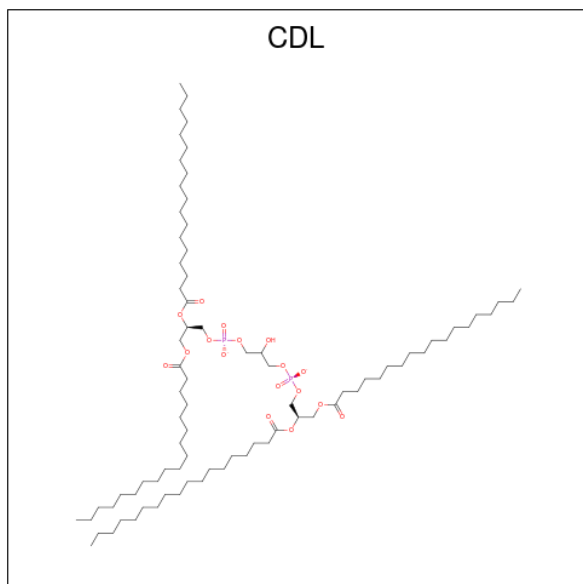
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Mol	Chain	Residues	Atoms						AltConf	Trace
27	d5	134	Total	C	H	N	O	S	0	0
			2144	674	1082	185	200	3		

- 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		
28	e4	68	Total	C	H	N	O	S	0	0
			1096	347	559	94	95	1		
28	e5	68	Total	C	H	N	O	S	0	0
			1096	347	559	94	95	1		

- Molecule 29 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms					AltConf
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	

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Mol	Chain	Residues	Atoms					AltConf
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	k	1	Total 256	C 81	H 156	O 17	P 2	0
29	g	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
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	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

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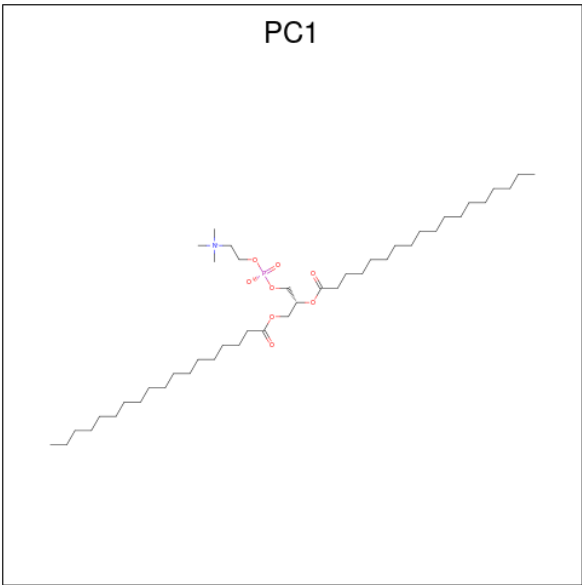
Mol	Chain	Residues	Atoms					AltConf
29	J	1	Total 256	C 81	H 156	O 17	P 2	0
29	J	1	Total 256	C 81	H 156	O 17	P 2	0
29	L	1	Total 256	C 81	H 156	O 17	P 2	0
29	L	1	Total 256	C 81	H 156	O 17	P 2	0
29	P	1	Total 256	C 81	H 156	O 17	P 2	0
29	a3	1	Total 256	C 81	H 156	O 17	P 2	0
29	a3	1	Total 256	C 81	H 156	O 17	P 2	0
29	b3	1	Total 256	C 81	H 156	O 17	P 2	0
29	f3	1	Total 256	C 81	H 156	O 17	P 2	0
29	f3	1	Total 256	C 81	H 156	O 17	P 2	0
29	f3	1	Total 256	C 81	H 156	O 17	P 2	0
29	f3	1	Total 256	C 81	H 156	O 17	P 2	0
29	i3	1	Total 256	C 81	H 156	O 17	P 2	0
29	i3	1	Total 256	C 81	H 156	O 17	P 2	0
29	k3	1	Total 256	C 81	H 156	O 17	P 2	0
29	g3	1	Total 256	C 81	H 156	O 17	P 2	0
29	j3	1	Total 256	C 81	H 156	O 17	P 2	0
29	j3	1	Total 256	C 81	H 156	O 17	P 2	0
29	l3	1	Total 256	C 81	H 156	O 17	P 2	0
29	l3	1	Total 256	C 81	H 156	O 17	P 2	0
29	p3	1	Total 256	C 81	H 156	O 17	P 2	0
29	A3	1	Total 256	C 81	H 156	O 17	P 2	0

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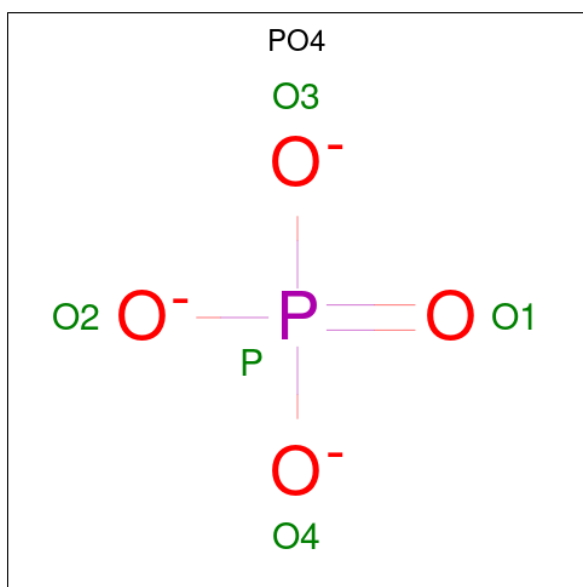
Mol	Chain	Residues	Atoms					AltConf
29	B3	1	Total 256	C 81	H 156	O 17	P 2	0
29	B3	1	Total 256	C 81	H 156	O 17	P 2	0
29	B3	1	Total 256	C 81	H 156	O 17	P 2	0
29	B3	1	Total 256	C 81	H 156	O 17	P 2	0
29	F3	1	Total 256	C 81	H 156	O 17	P 2	0
29	I3	1	Total 256	C 81	H 156	O 17	P 2	0
29	I3	1	Total 256	C 81	H 156	O 17	P 2	0
29	I3	1	Total 256	C 81	H 156	O 17	P 2	0
29	K3	1	Total 256	C 81	H 156	O 17	P 2	0
29	K3	1	Total 256	C 81	H 156	O 17	P 2	0
29	J3	1	Total 256	C 81	H 156	O 17	P 2	0
29	J3	1	Total 256	C 81	H 156	O 17	P 2	0
29	L3	1	Total 256	C 81	H 156	O 17	P 2	0
29	P3	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: C₄₄H₈₈NO₈P).



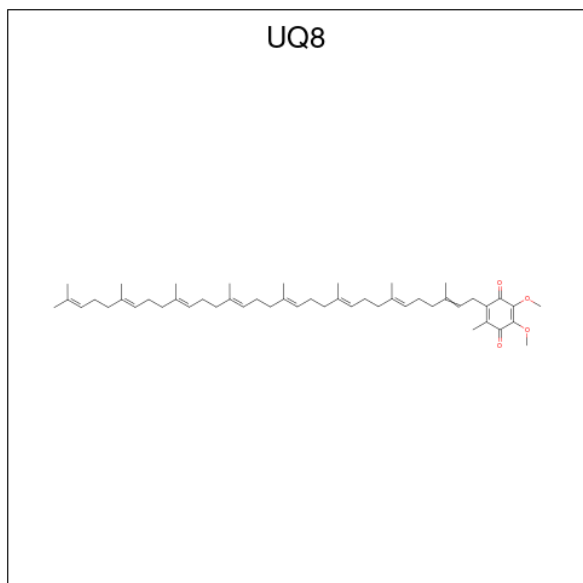
Mol	Chain	Residues	Atoms						AltConf
30	d	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	g	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	g	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	D	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	G	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	G	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	d3	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	g3	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	g3	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	D3	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	G3	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	G3	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

- Molecule 31 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



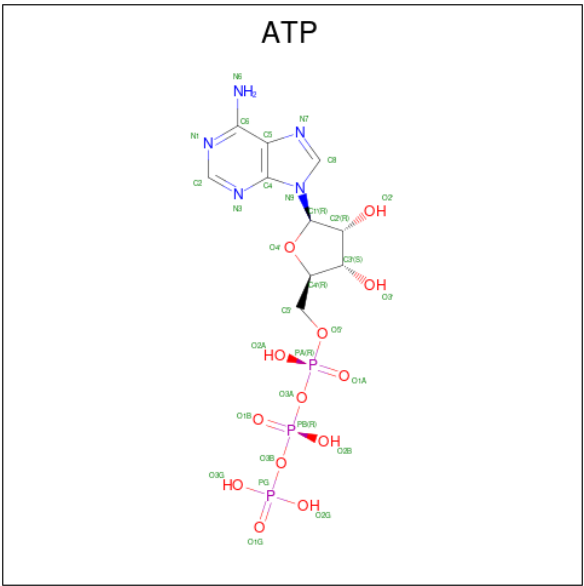
Mol	Chain	Residues	Atoms			AltConf
31	f	1	Total	O	P	0
			5	4	1	
31	F	1	Total	O	P	0
			5	4	1	
31	f3	1	Total	O	P	0
			5	4	1	
31	F3	1	Total	O	P	0
			5	4	1	

- Molecule 32 is Ubiquinone-8 (CCD ID: UQ8) (formula: C₄₉H₇₄O₄).



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	
32	i3	1	Total	C	H	O	0
			127	49	74	4	
32	I3	1	Total	C	H	O	0
			127	49	74	4	

- Molecule 33 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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Mol	Chain	Residues	Atoms						AltConf
33	g3	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	G3	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	C4	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	B4	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	A4	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	C5	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	B5	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	A5	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	

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

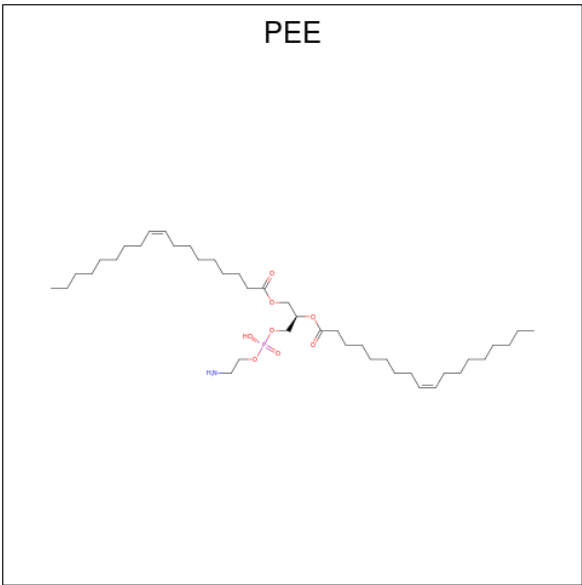
Mol	Chain	Residues	Atoms		AltConf
34	g	1	Total	Mg	0
			1	1	
34	G	1	Total	Mg	0
			1	1	
34	C1	1	Total	Mg	0
			1	1	
34	D1	1	Total	Mg	0
			1	1	
34	B1	1	Total	Mg	0
			1	1	
34	A1	1	Total	Mg	0
			1	1	
34	E1	1	Total	Mg	0
			1	1	
34	C2	1	Total	Mg	0
			1	1	
34	D2	1	Total	Mg	0
			1	1	
34	B2	1	Total	Mg	0
			1	1	
34	A2	1	Total	Mg	0
			1	1	

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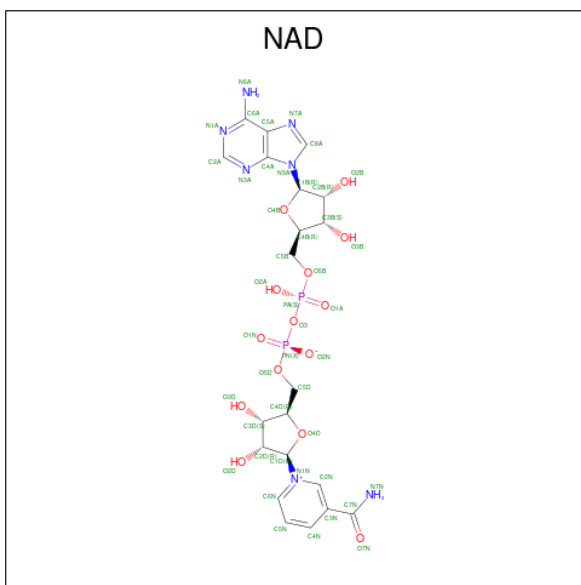
Mol	Chain	Residues	Atoms		AltConf
34	E2	1	Total 1	Mg 1	0
34	g3	1	Total 1	Mg 1	0
34	G3	1	Total 1	Mg 1	0
34	C4	1	Total 1	Mg 1	0
34	D4	1	Total 1	Mg 1	0
34	B4	1	Total 1	Mg 1	0
34	A4	1	Total 1	Mg 1	0
34	E4	1	Total 1	Mg 1	0
34	C5	1	Total 1	Mg 1	0
34	D5	1	Total 1	Mg 1	0
34	B5	1	Total 1	Mg 1	0
34	A5	1	Total 1	Mg 1	0
34	E5	1	Total 1	Mg 1	0

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



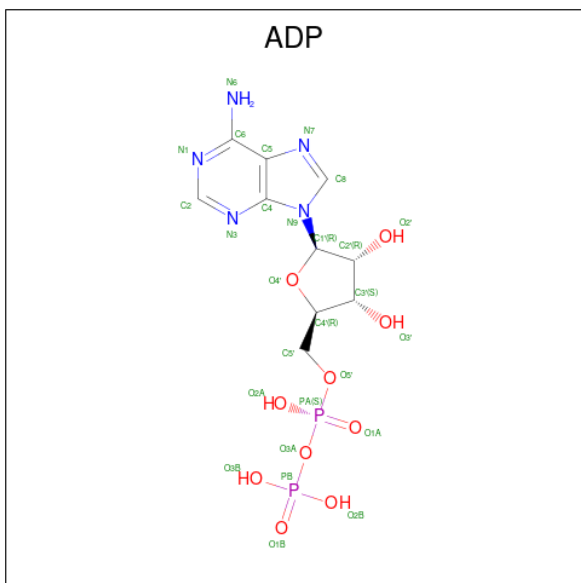
Mol	Chain	Residues	Atoms						AltConf
35	m	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
35	A	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	
35	J	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
35	L	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	
35	a3	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	
35	j3	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
35	l3	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	
35	L3	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

- Molecule 36 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms						AltConf
36	e	1	Total 70	C 21	H 26	N 7	O 14	P 2	0
36	E	1	Total 70	C 21	H 26	N 7	O 14	P 2	0
36	e3	1	Total 70	C 21	H 26	N 7	O 14	P 2	0
36	E3	1	Total 70	C 21	H 26	N 7	O 14	P 2	0

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

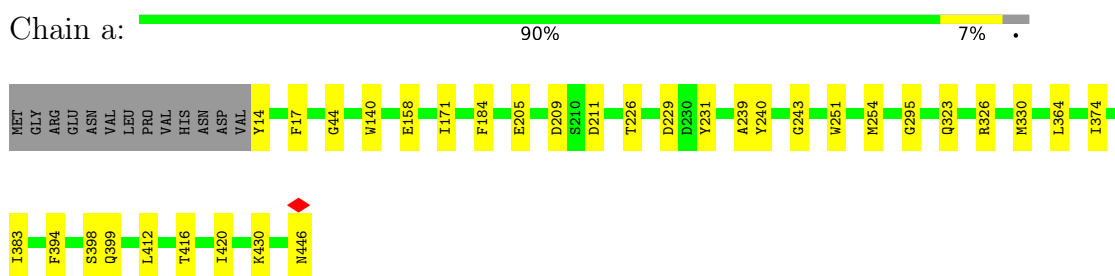


Mol	Chain	Residues	Atoms						AltConf
37	D1	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
37	B1	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
37	D2	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
37	B2	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
37	D4	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
37	B4	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
37	D5	1	Total 38	C 10	H 11	N 5	O 10	P 2	0
37	B5	1	Total 38	C 10	H 11	N 5	O 10	P 2	0

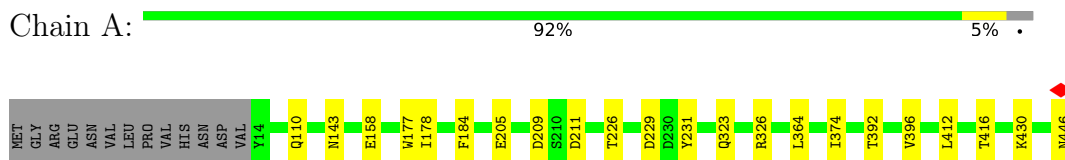
3 Residue-property plots [i](#)

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.

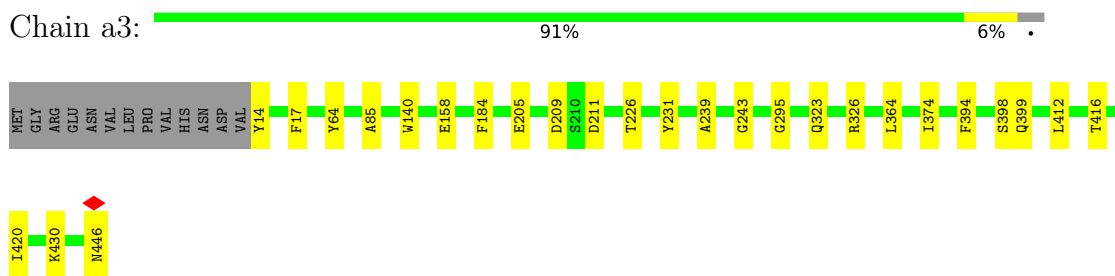
- Molecule 1: Ymf66



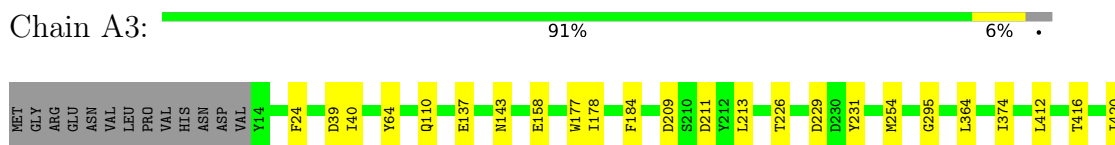
- Molecule 1: Ymf66



- Molecule 1: Ymf66

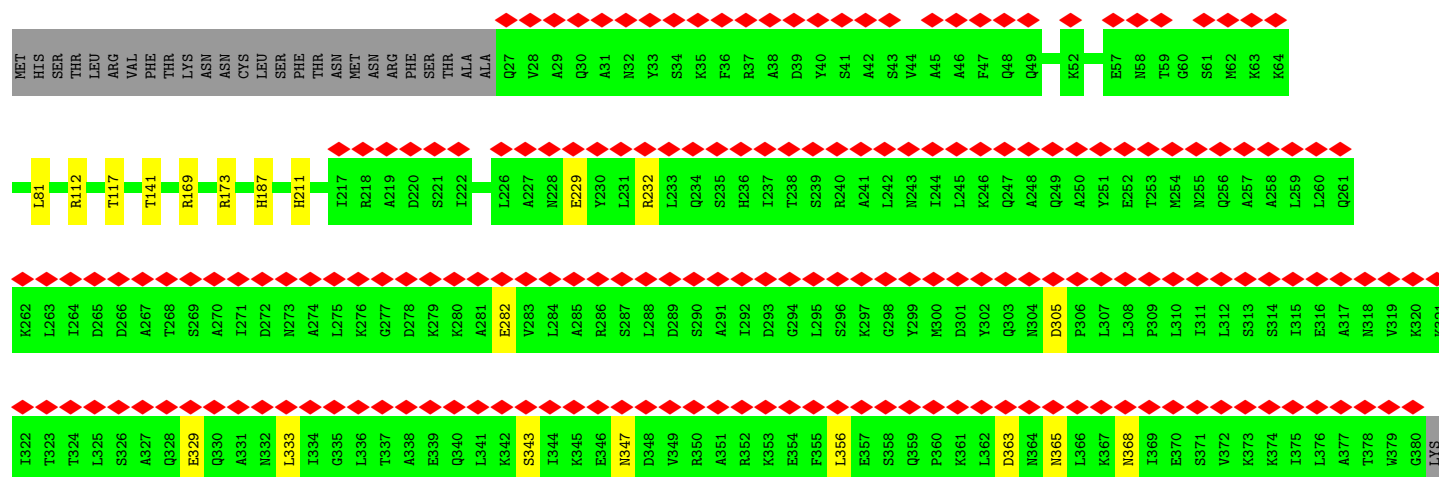
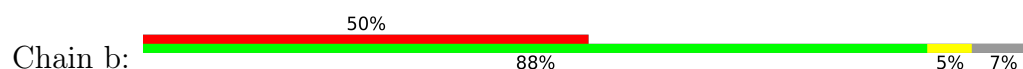


- Molecule 1: Ymf66

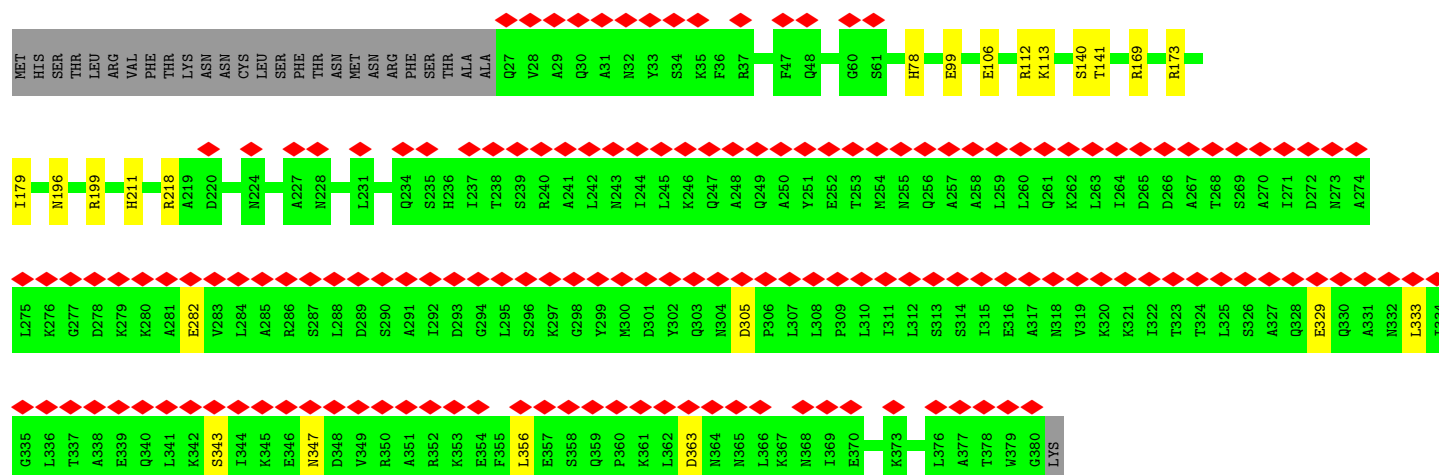
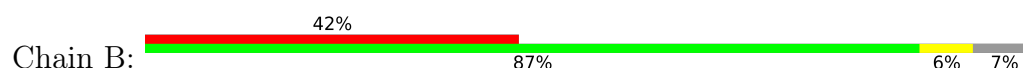




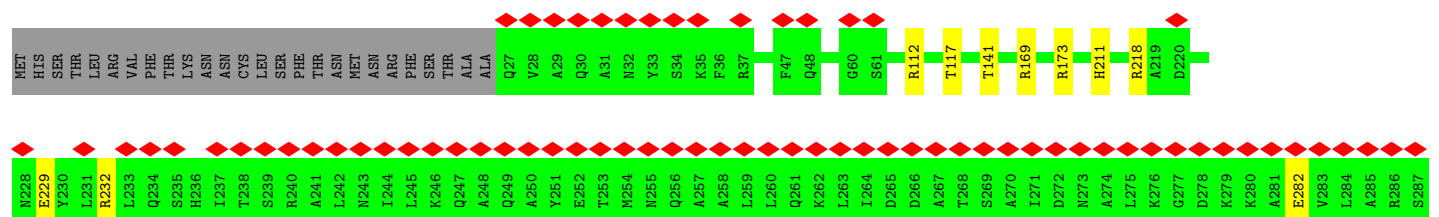
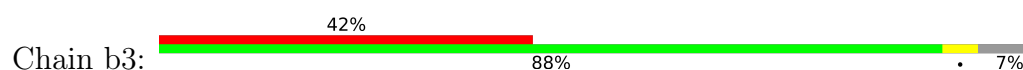
• Molecule 2: subunit b

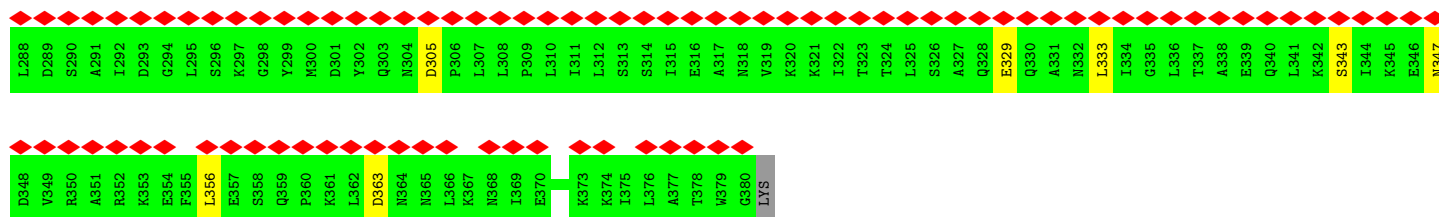


• Molecule 2: subunit b

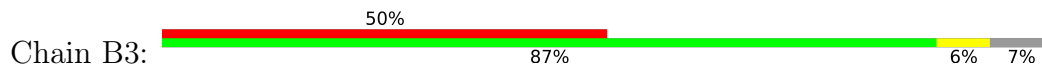


• Molecule 2: subunit b

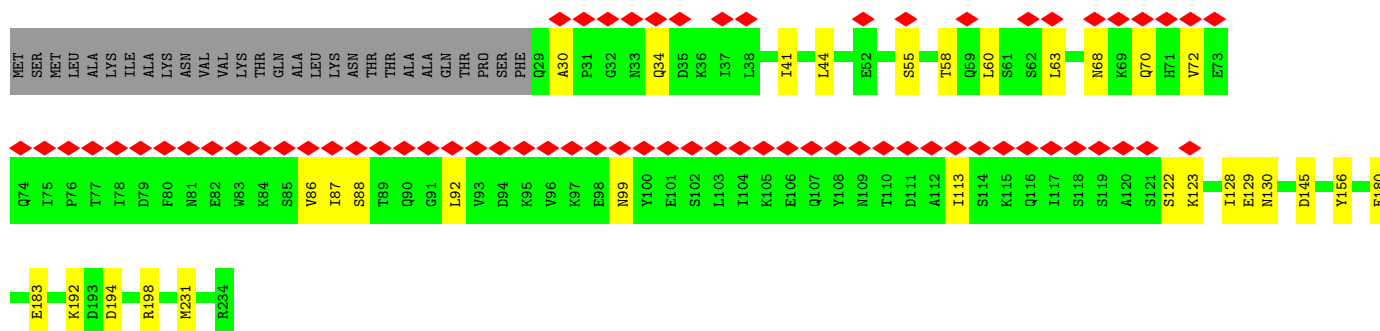
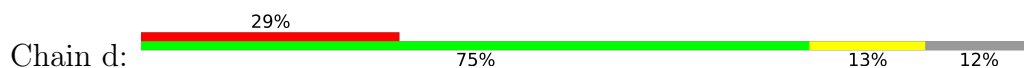




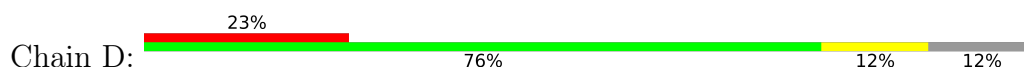
- Molecule 2: subunit b

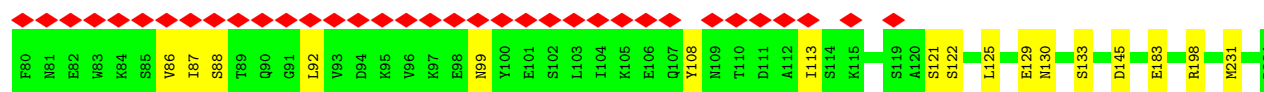


- Molecule 3: subunit d

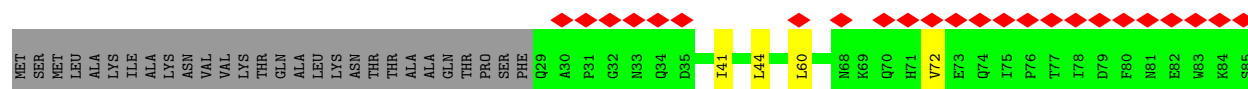
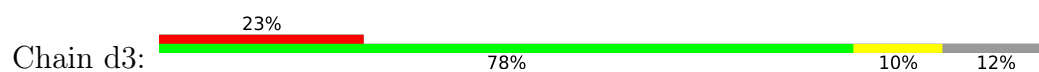


- Molecule 3: subunit d

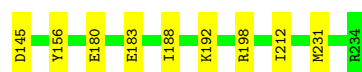
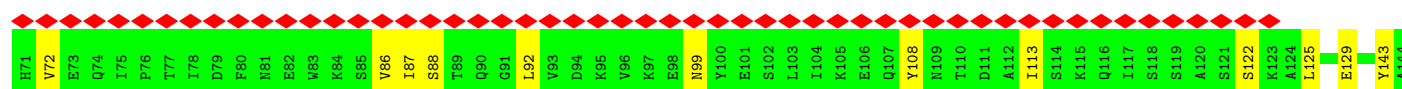
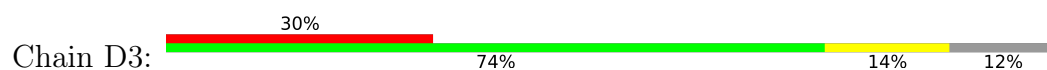




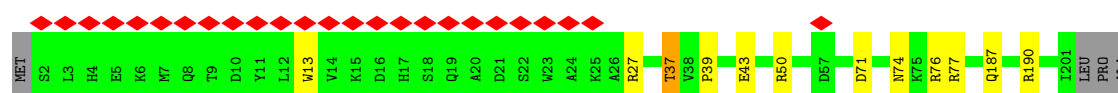
- Molecule 3: subunit d



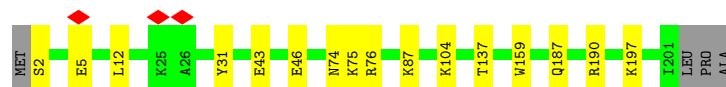
- Molecule 3: subunit d



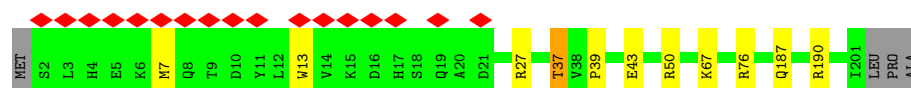
- Molecule 4: subunit f



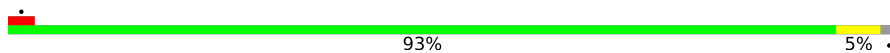
- Molecule 4: subunit f

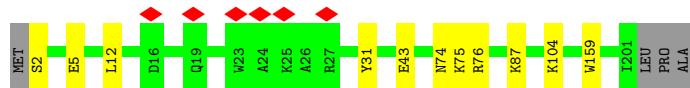


- Molecule 4: subunit f



- Molecule 4: subunit f

Chain F3:  93% 5%



- Molecule 5: subunit i/j

Chain i:  91% 9%

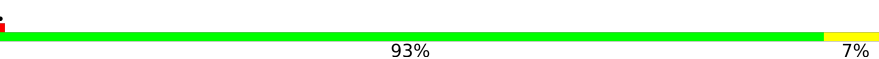


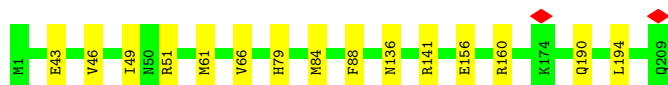
- Molecule 5: subunit i/j

Chain I:  90% 10%



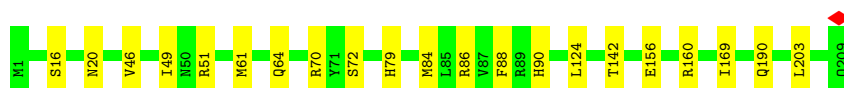
- Molecule 5: subunit i/j

Chain i3:  93% 7%

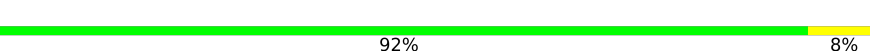


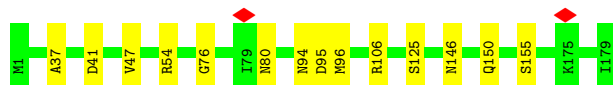
- Molecule 5: subunit i/j

Chain I3:  90% 10%

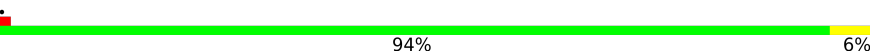


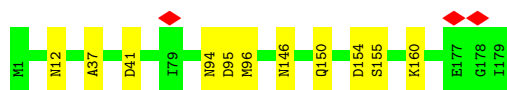
- Molecule 6: subunit k

Chain k:  92% 8%



- Molecule 6: subunit k

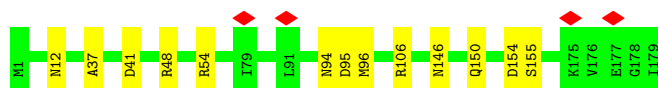
Chain K:  94% 6%



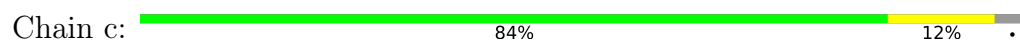
- Molecule 6: subunit k



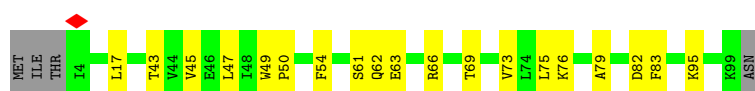
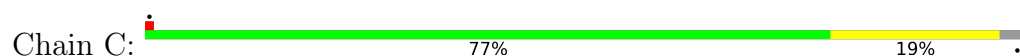
- Molecule 6: subunit k



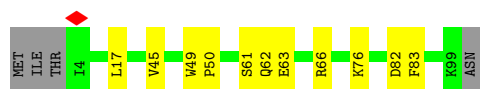
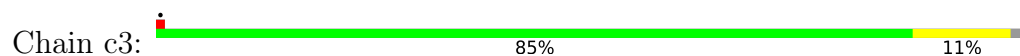
- Molecule 7: Ymf56



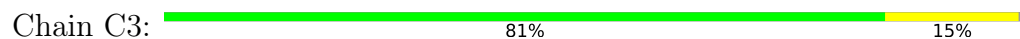
- Molecule 7: Ymf56



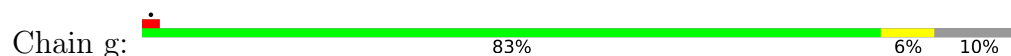
- Molecule 7: Ymf56

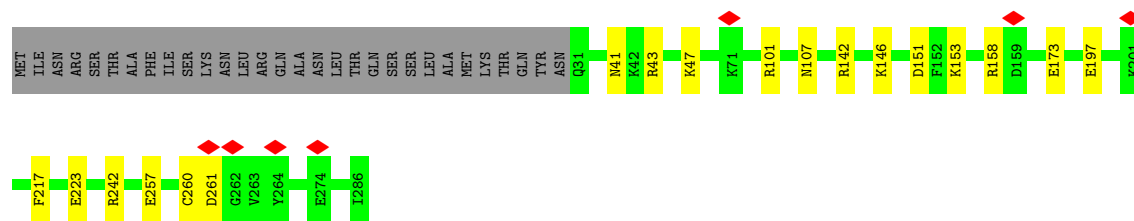


- Molecule 7: Ymf56

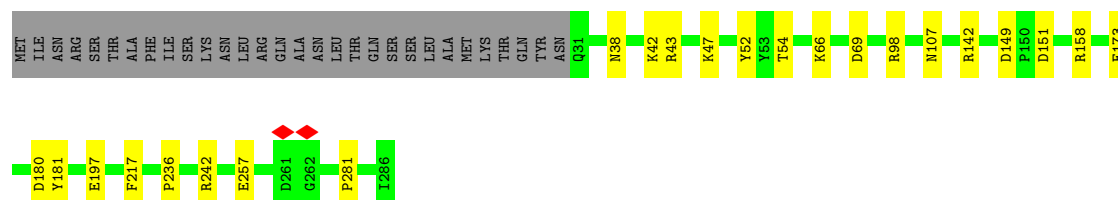
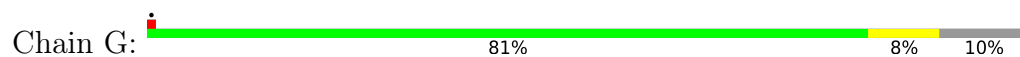


- Molecule 8: ATPTT3

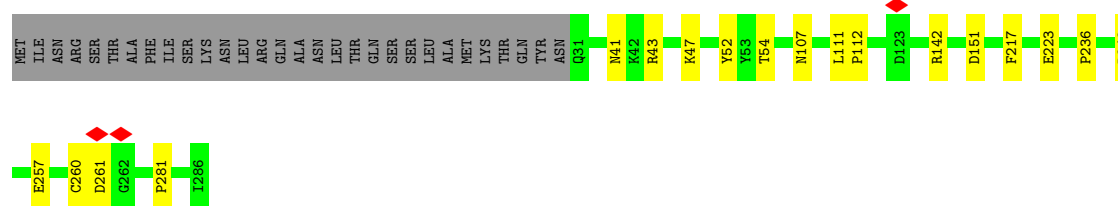
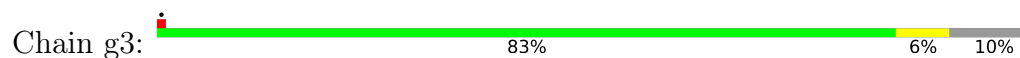




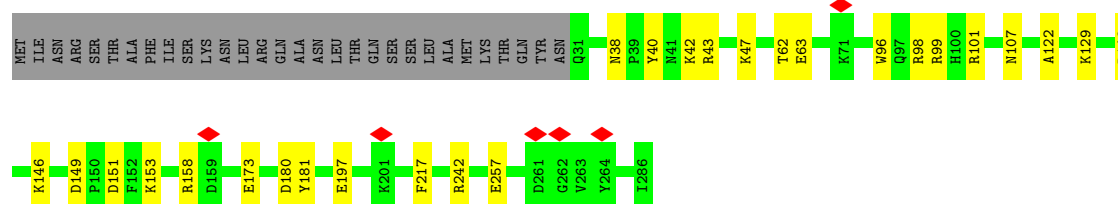
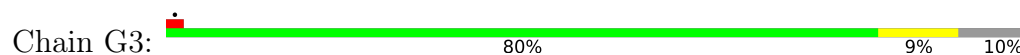
• Molecule 8: ATPTT3



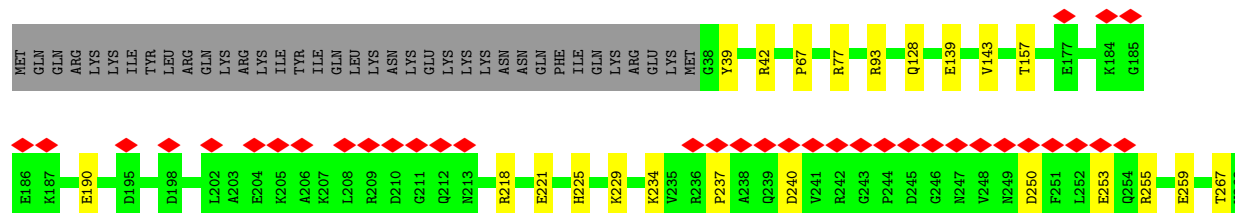
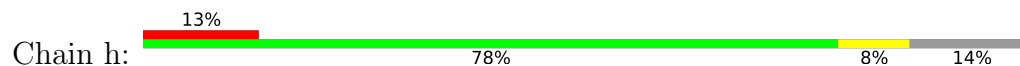
• Molecule 8: ATPTT3



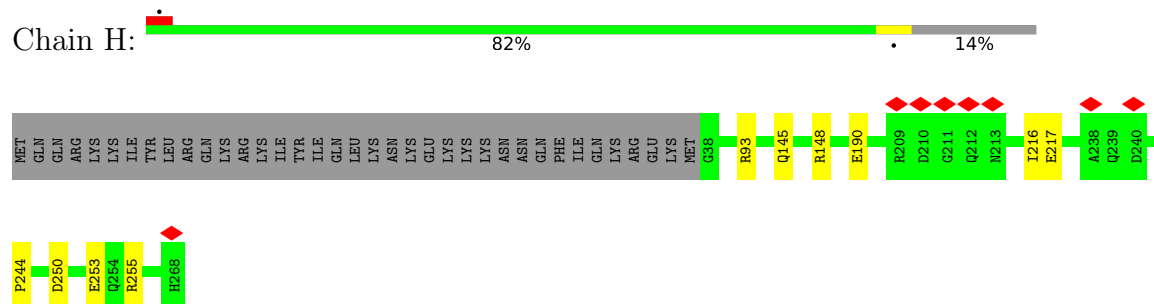
• Molecule 8: ATPTT3



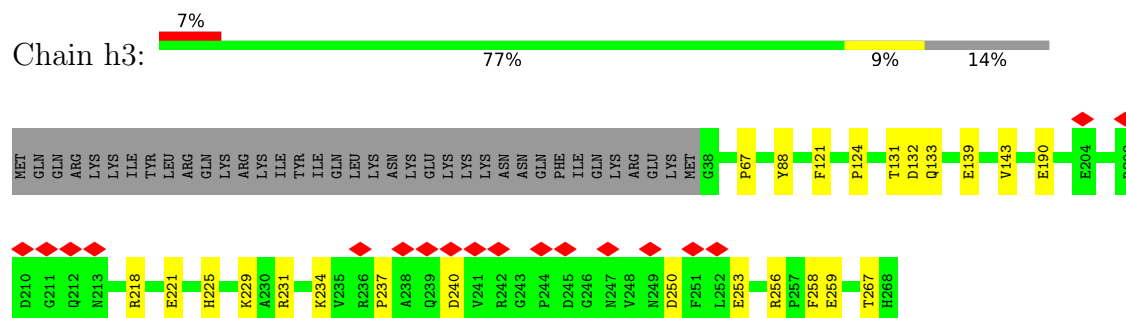
• Molecule 9: ATPTT4



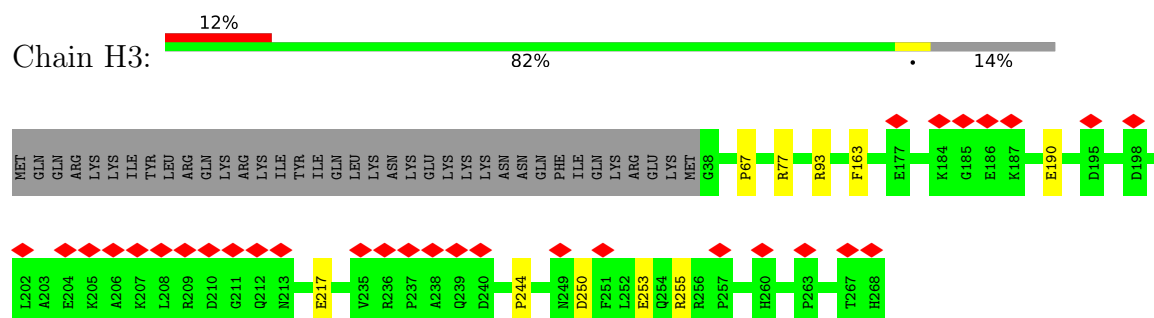
- Molecule 9: ATPTT4



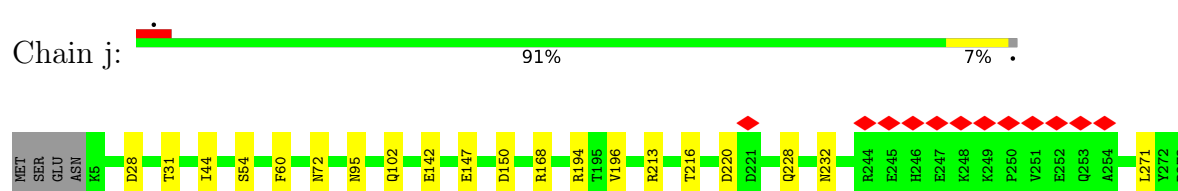
- Molecule 9: ATPTT4



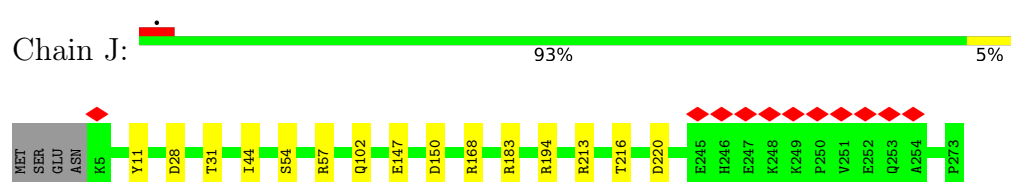
- Molecule 9: ATPTT4



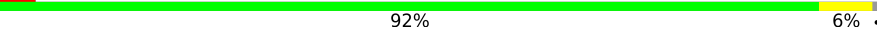
- Molecule 10: ATPTT5



- Molecule 10: ATPTT5



- Molecule 10: ATPTT5

Chain j3:  92% 6%



• Molecule 10: ATPPT5

Chain J3:  92% 7%



• Molecule 11: ATPPT6

Chain l:  89% 11%



• Molecule 11: ATPPT6

Chain L:  89% 10%



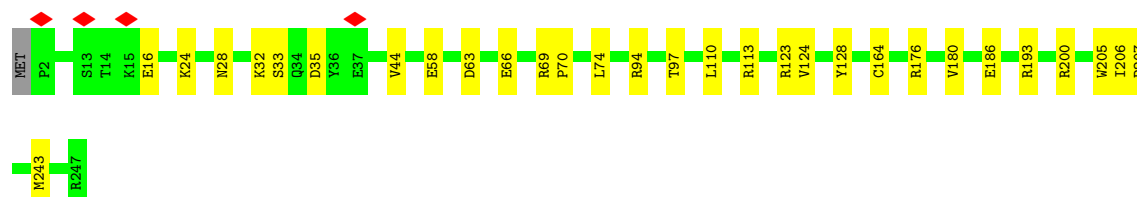
• Molecule 11: ATPPT6

Chain l3:  89% 10%

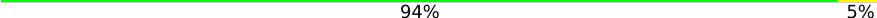


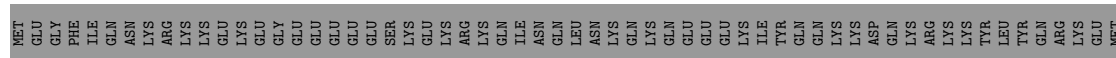
• Molecule 11: ATPPT6

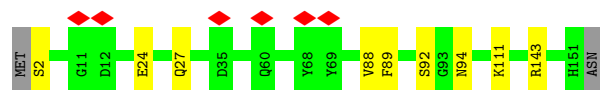
Chain L3:  87% 12%



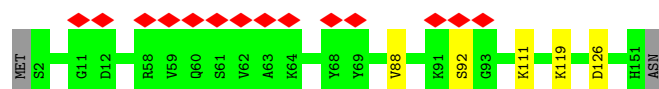
• Molecule 12: ATPPT7

Chain m:  94% 5%

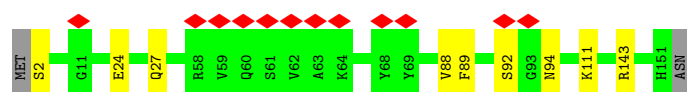




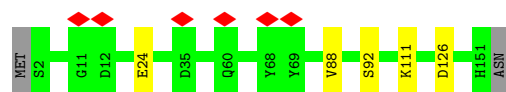
• Molecule 15: ATPTT10



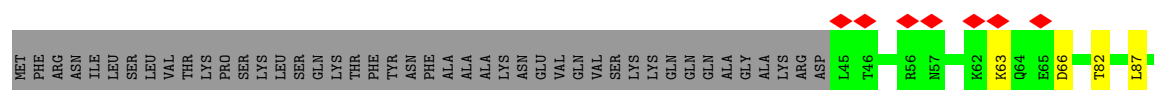
• Molecule 15: ATPTT10



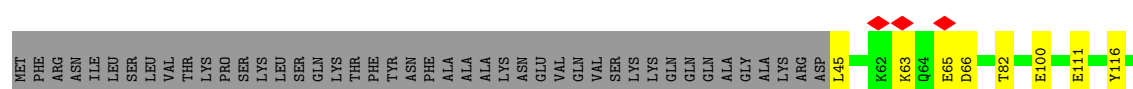
• Molecule 15: ATPTT10



• Molecule 16: ATPTT11

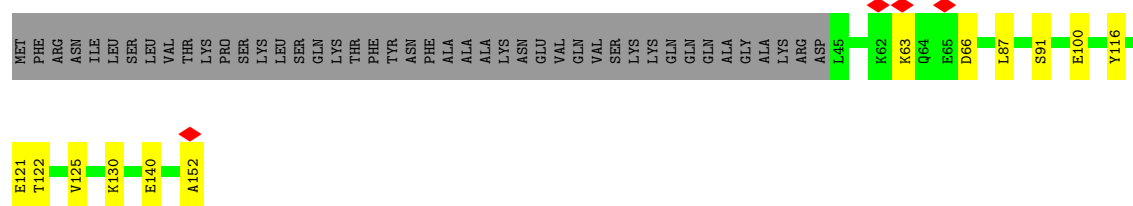


• Molecule 16: ATPTT11



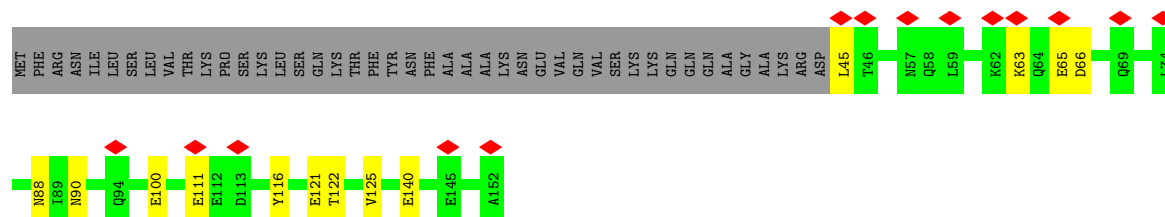
• Molecule 16: ATPTT11

Chain q3: 



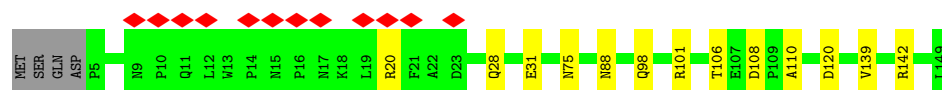
• Molecule 16: ATPPTT11

Chain Q3: 



• Molecule 17: ATPPTT12

Chain r: 



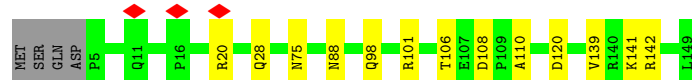
• Molecule 17: ATPPTT12

Chain R: 



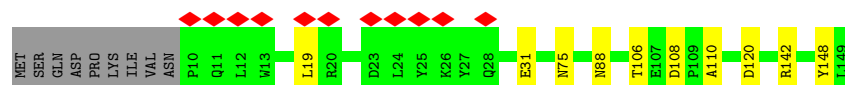
• Molecule 17: ATPPTT12

Chain r3: 

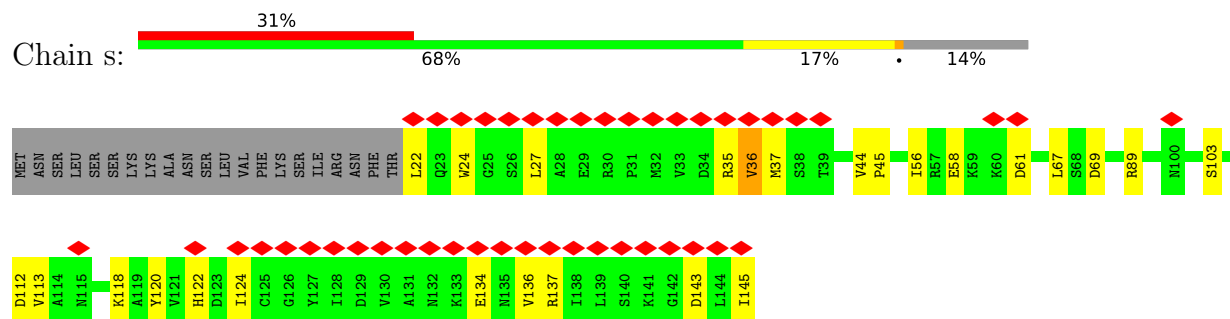


• Molecule 17: ATPPTT12

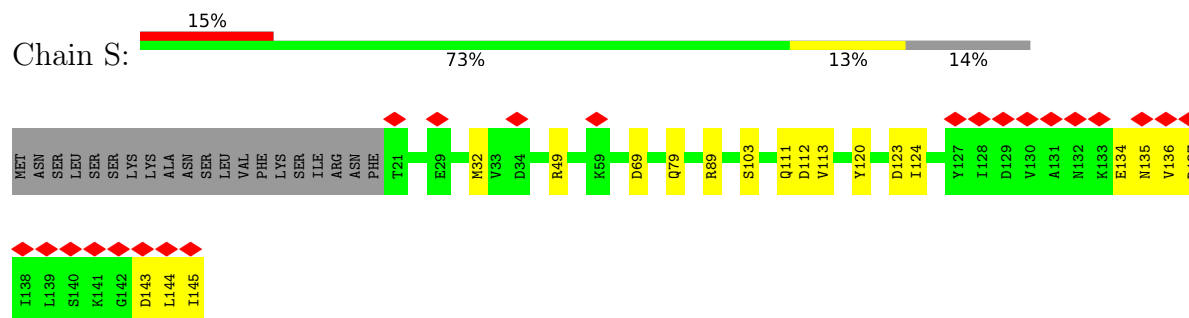
Chain R3: 



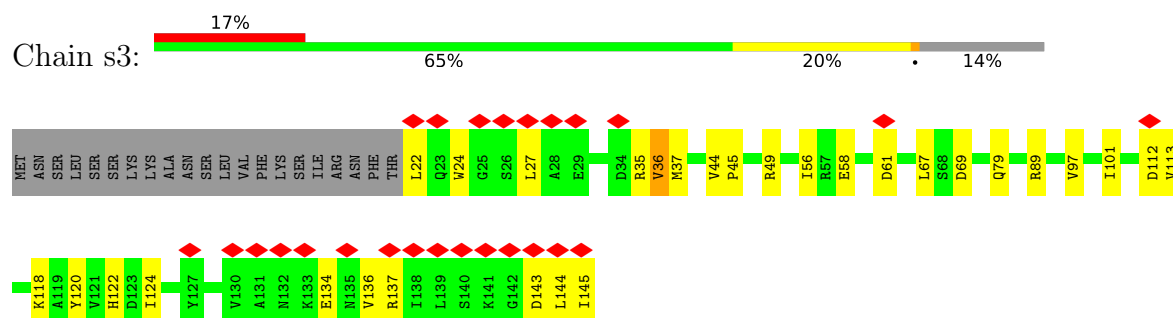
● Molecule 18: ATPTT13



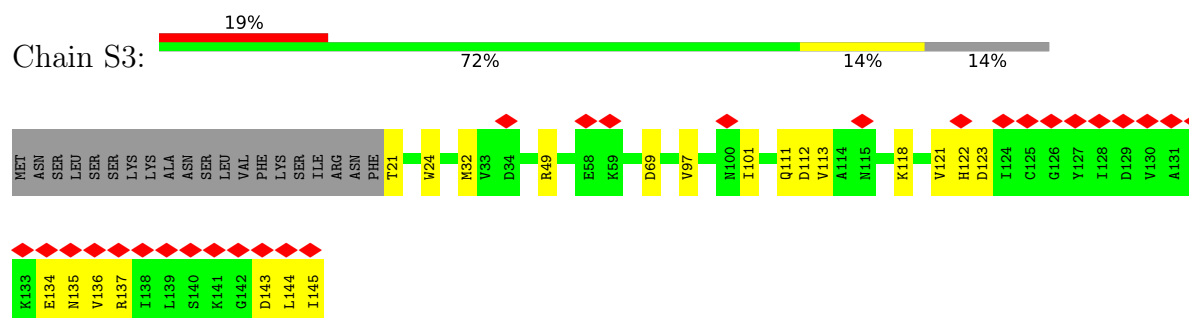
● Molecule 18: ATPTT13



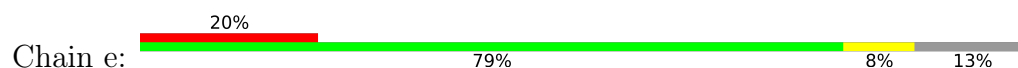
● Molecule 18: ATPTT13

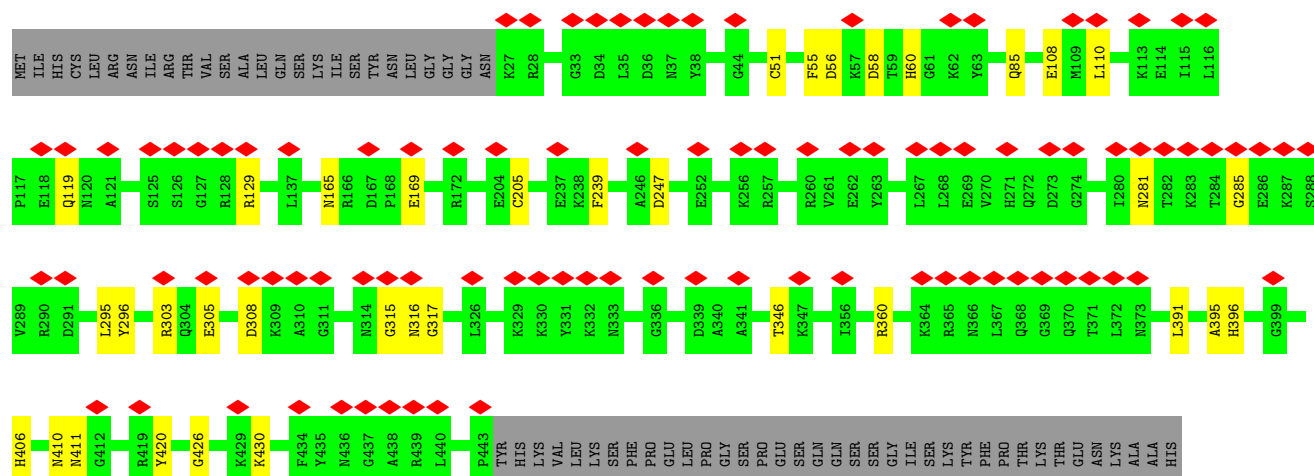


● Molecule 18: ATPTT13

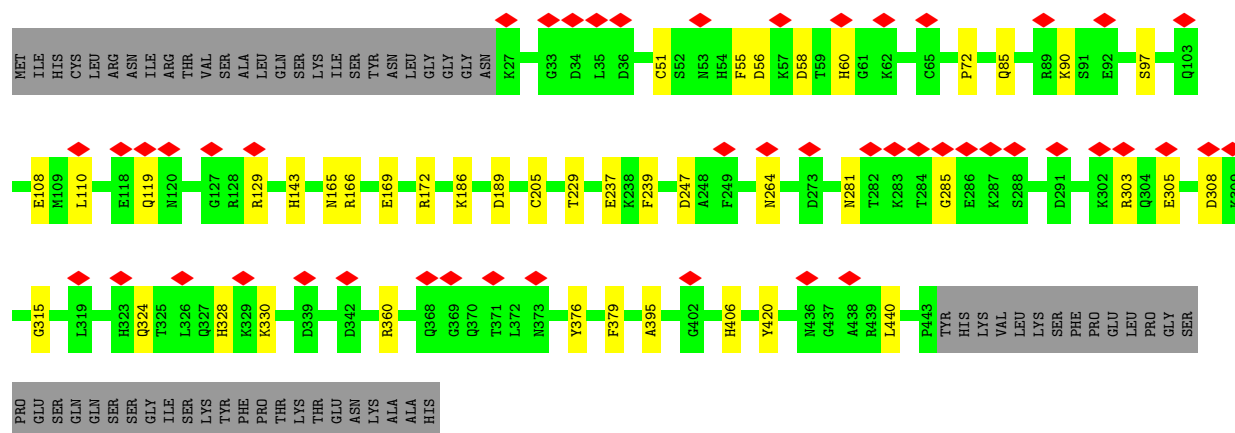
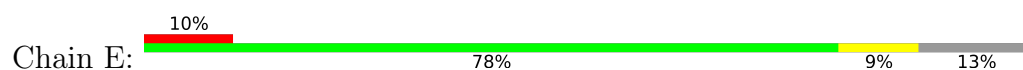


● Molecule 19: ATPTT1

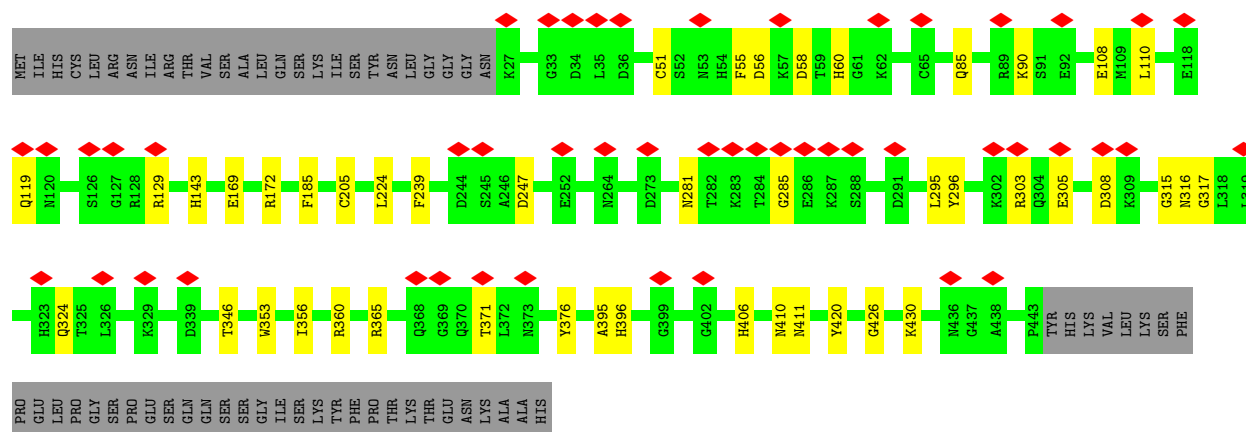
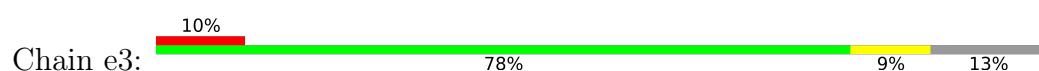




• Molecule 19: ATPPT1

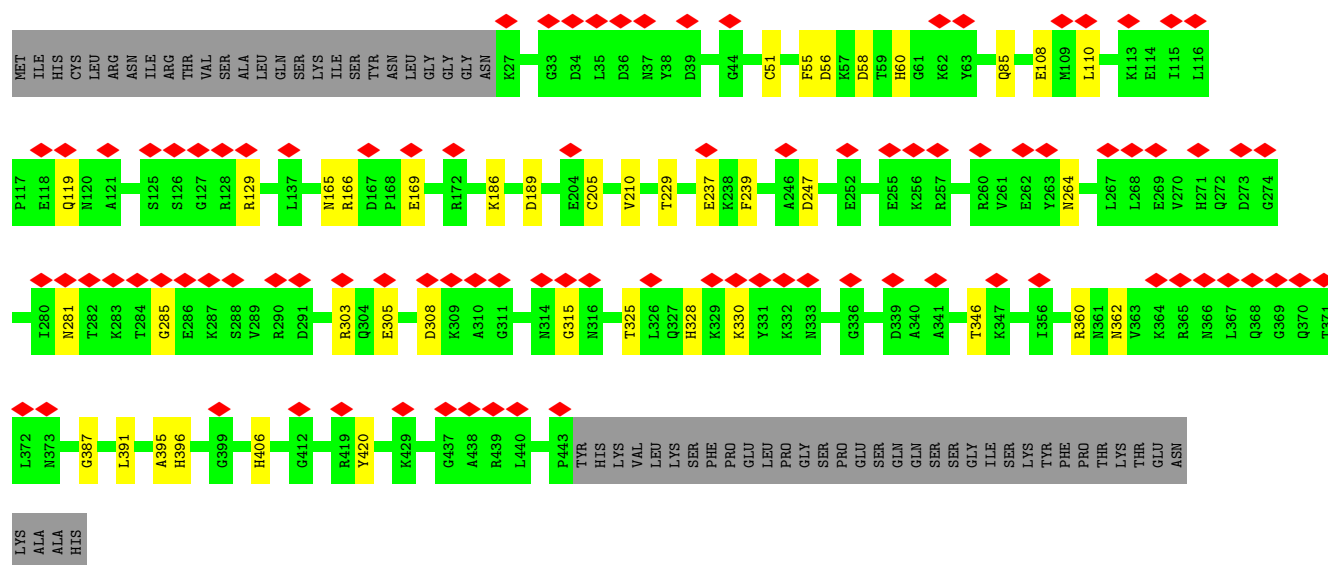


• Molecule 19: ATPPT1



• Molecule 19: ATPPT1

Chain E3: 



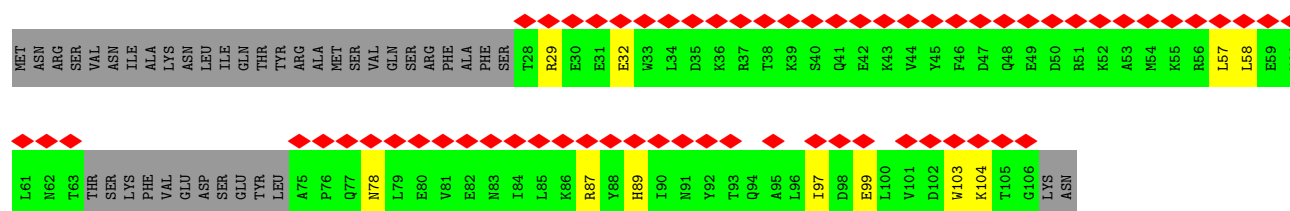
• Molecule 20: Inhibitor of F1 (IF1)

Chain i2: 



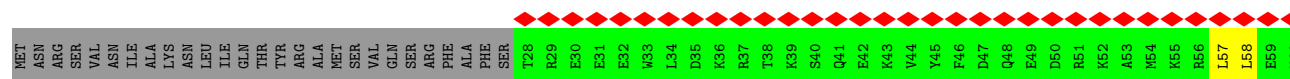
• Molecule 20: Inhibitor of F1 (IF1)

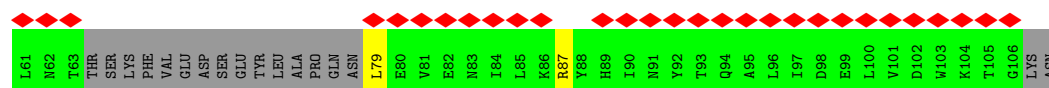
Chain i1: 



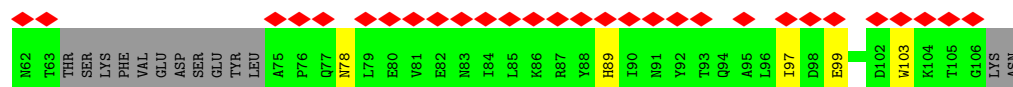
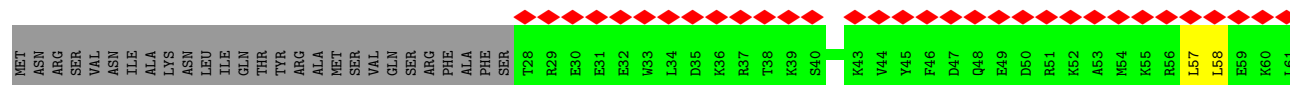
• Molecule 20: Inhibitor of F1 (IF1)

Chain i5: 

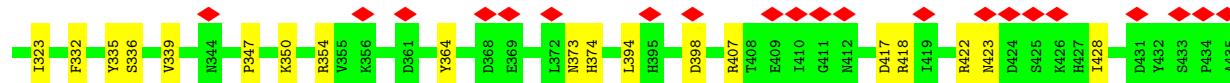
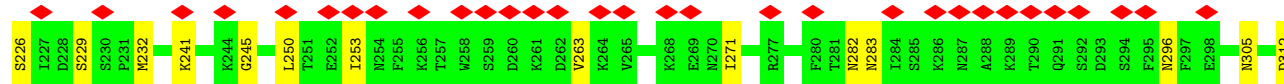
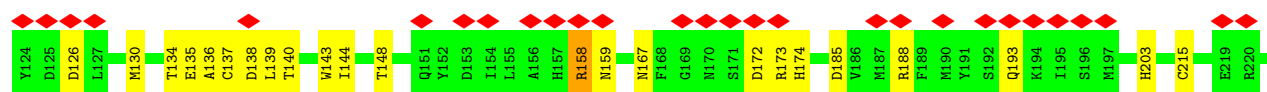
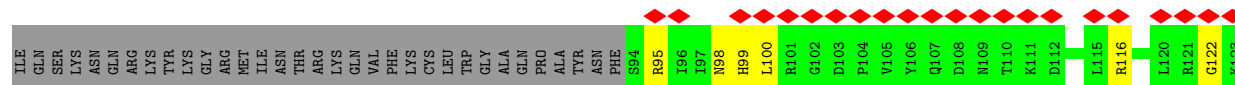
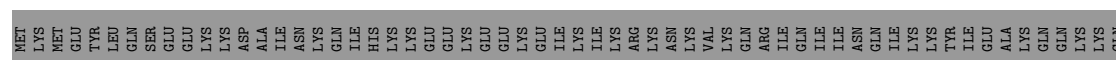




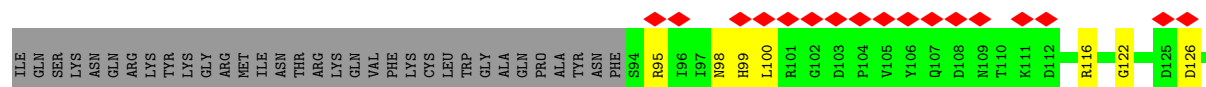
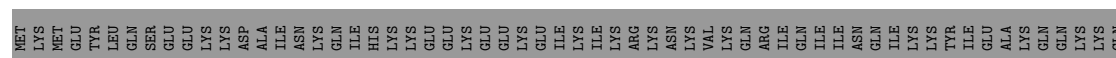
• Molecule 20: Inhibitor of F1 (IF1)

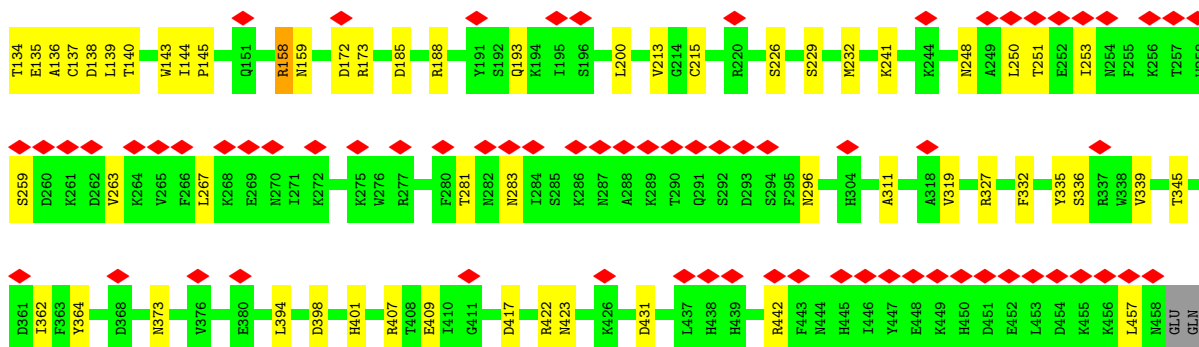


• Molecule 21: ATPPTT2

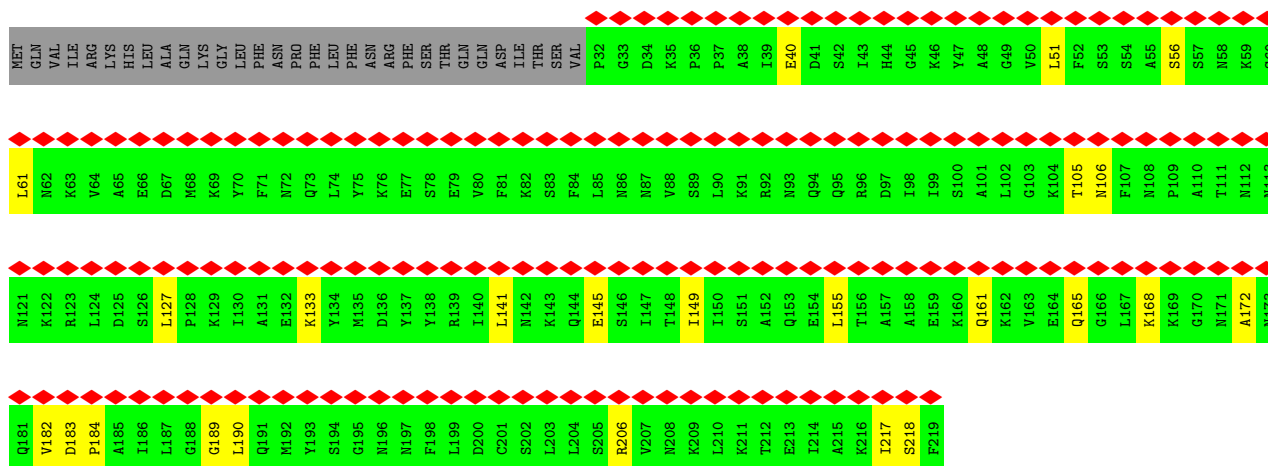
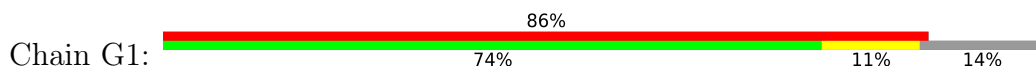


• Molecule 21: ATPPTT2

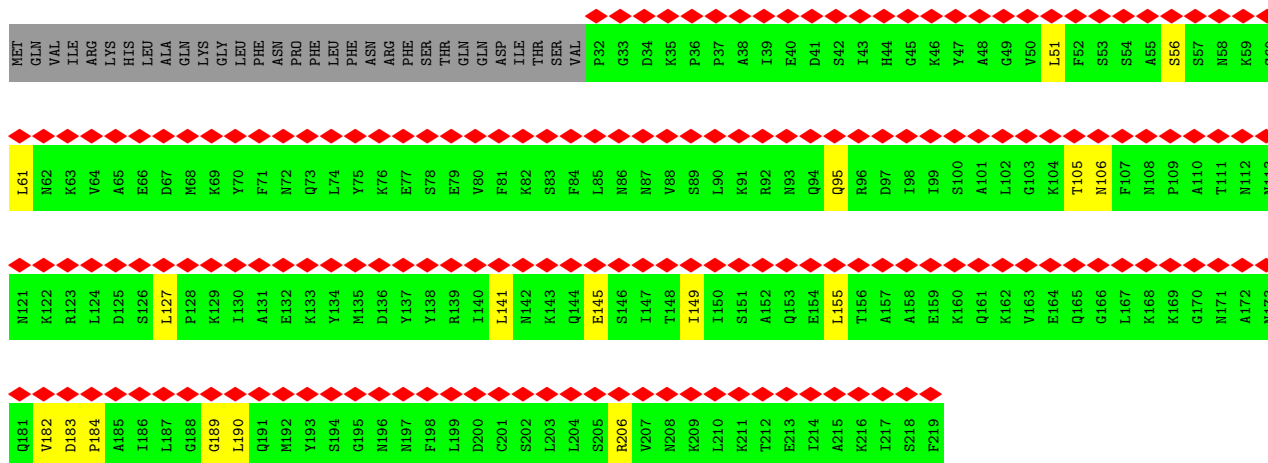
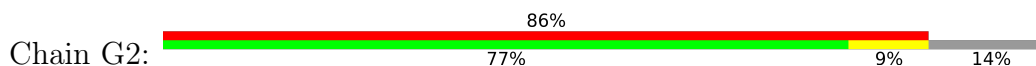




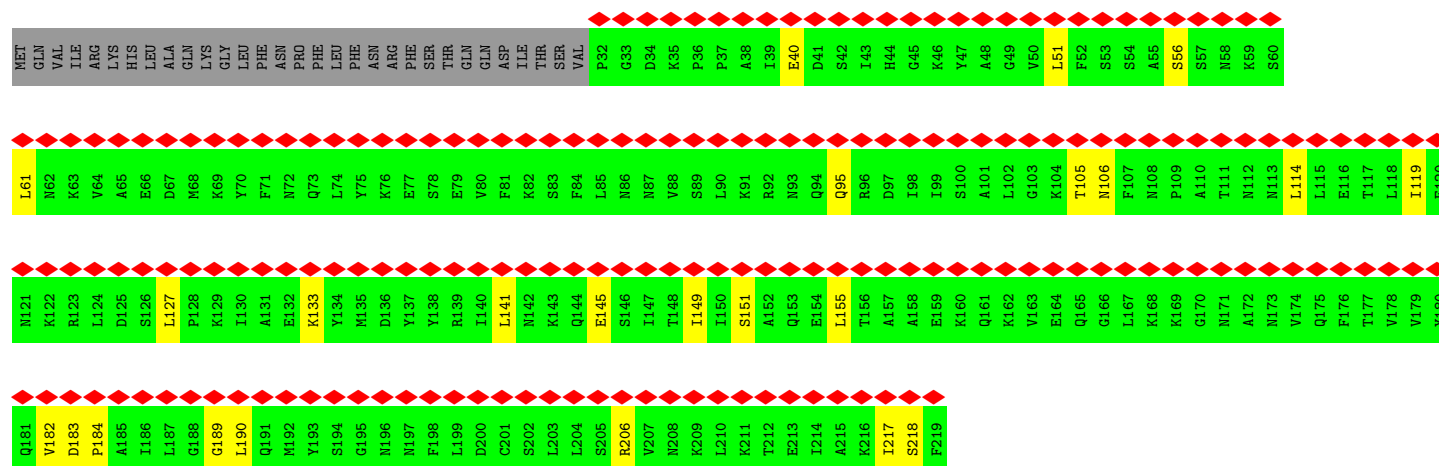
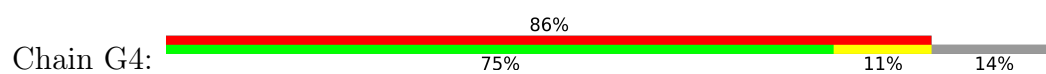
• Molecule 22: Oligomycin sensitivity-conferring protein (OSCP)



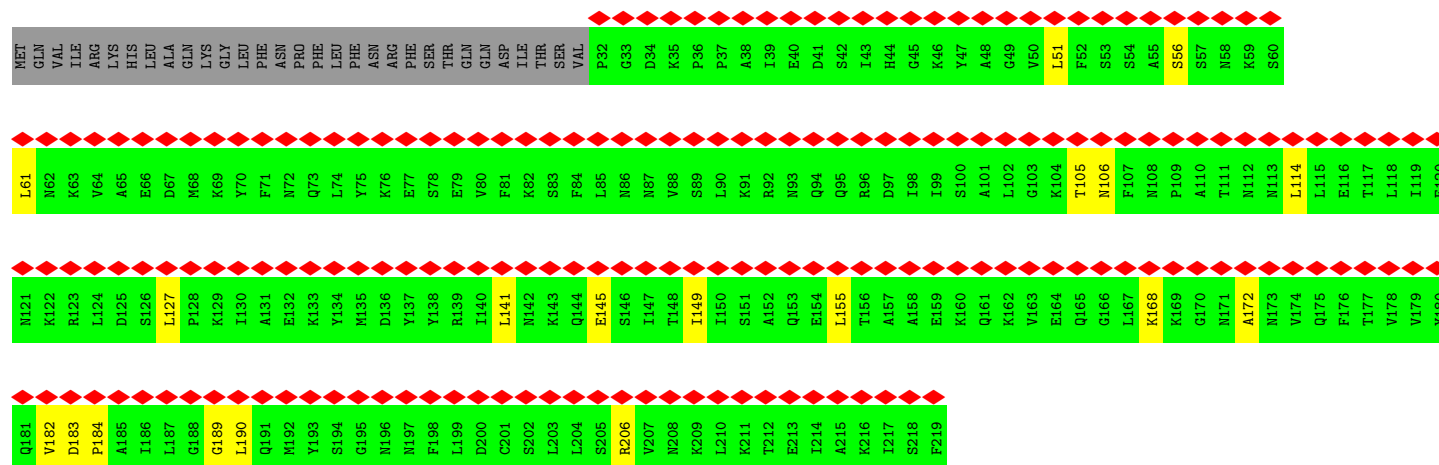
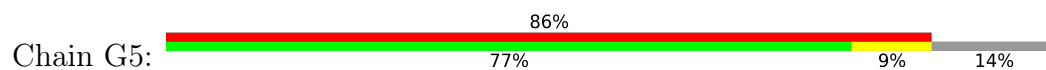
• Molecule 22: Oligomycin sensitivity-conferring protein (OSCP)



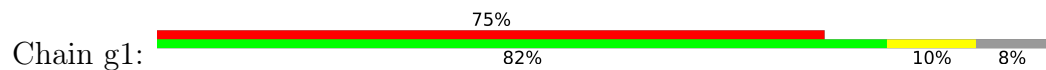
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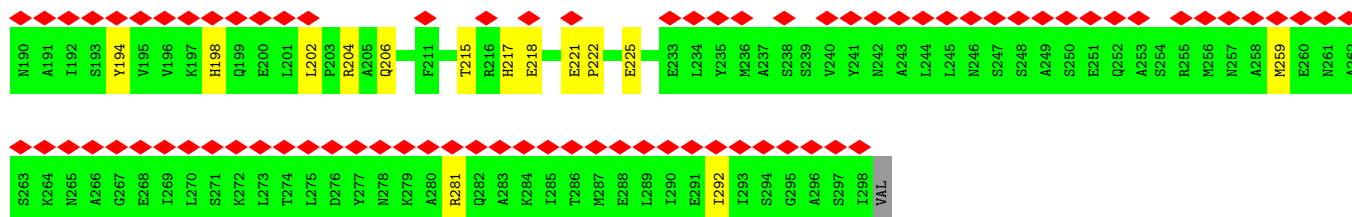


• Molecule 22: Oligomycin sensitivity-conferring protein (OSCP)

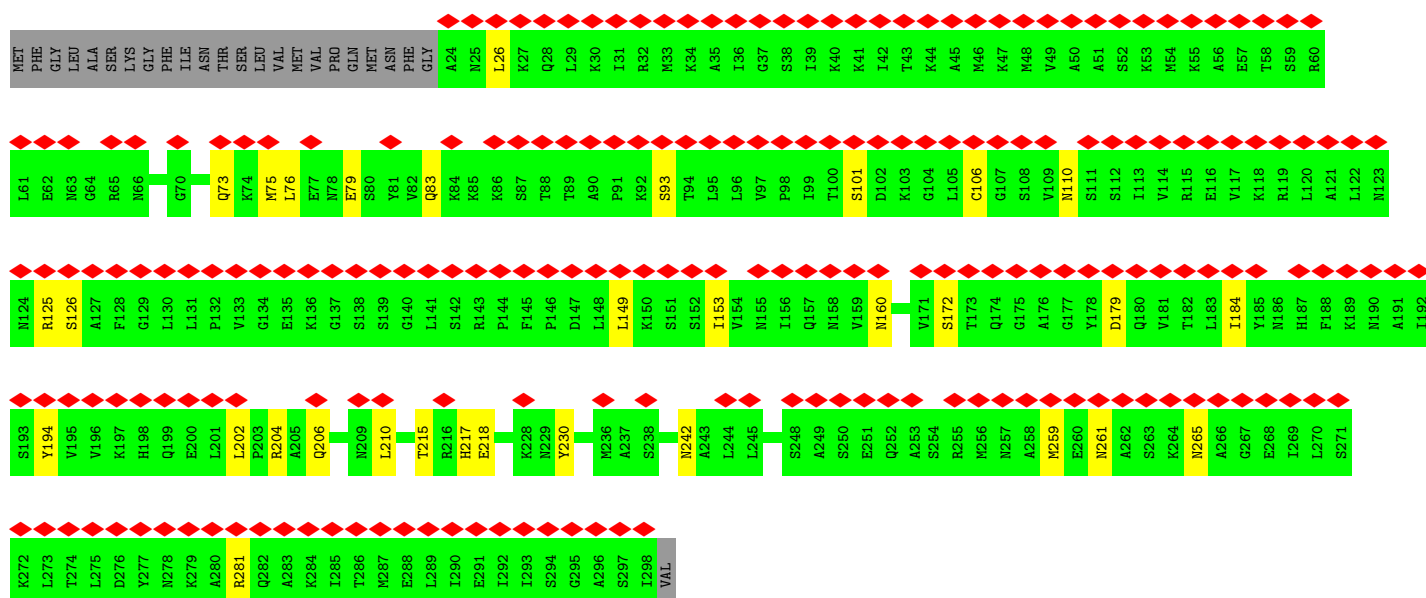
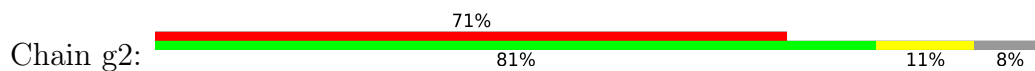


• Molecule 23: ATP synthase subunit gamma

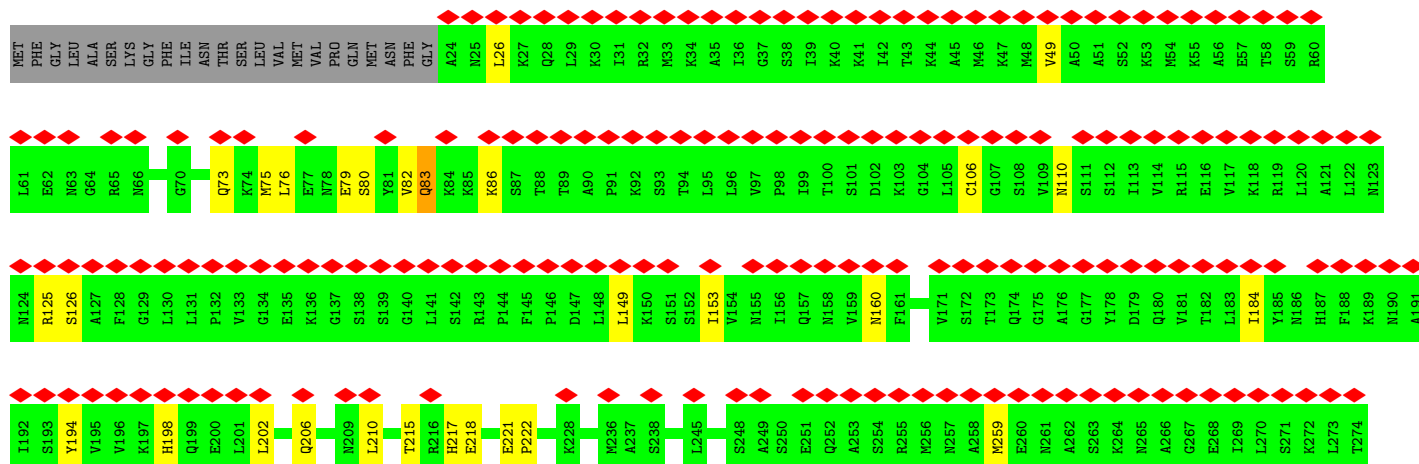
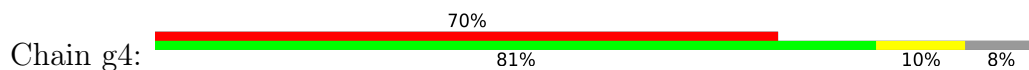


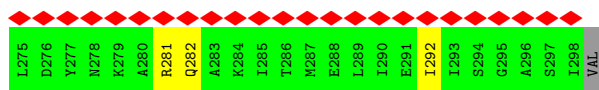


• Molecule 23: ATP synthase subunit gamma

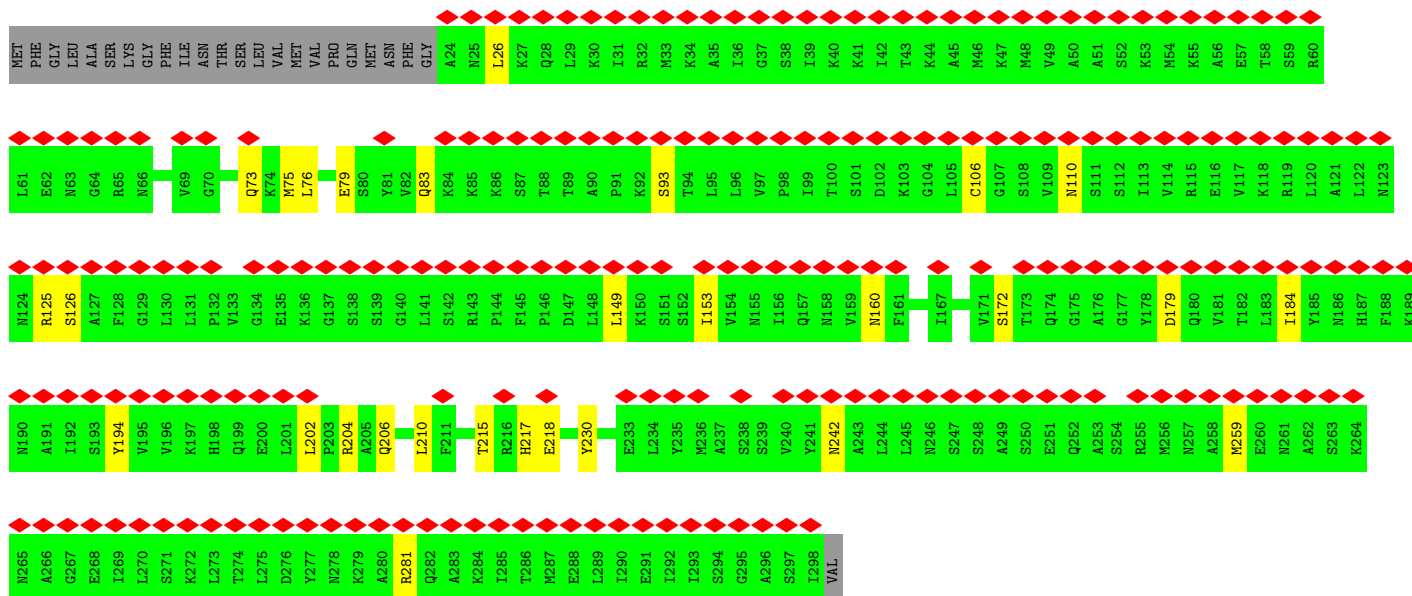
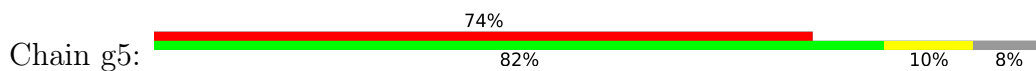


• Molecule 23: ATP synthase subunit gamma

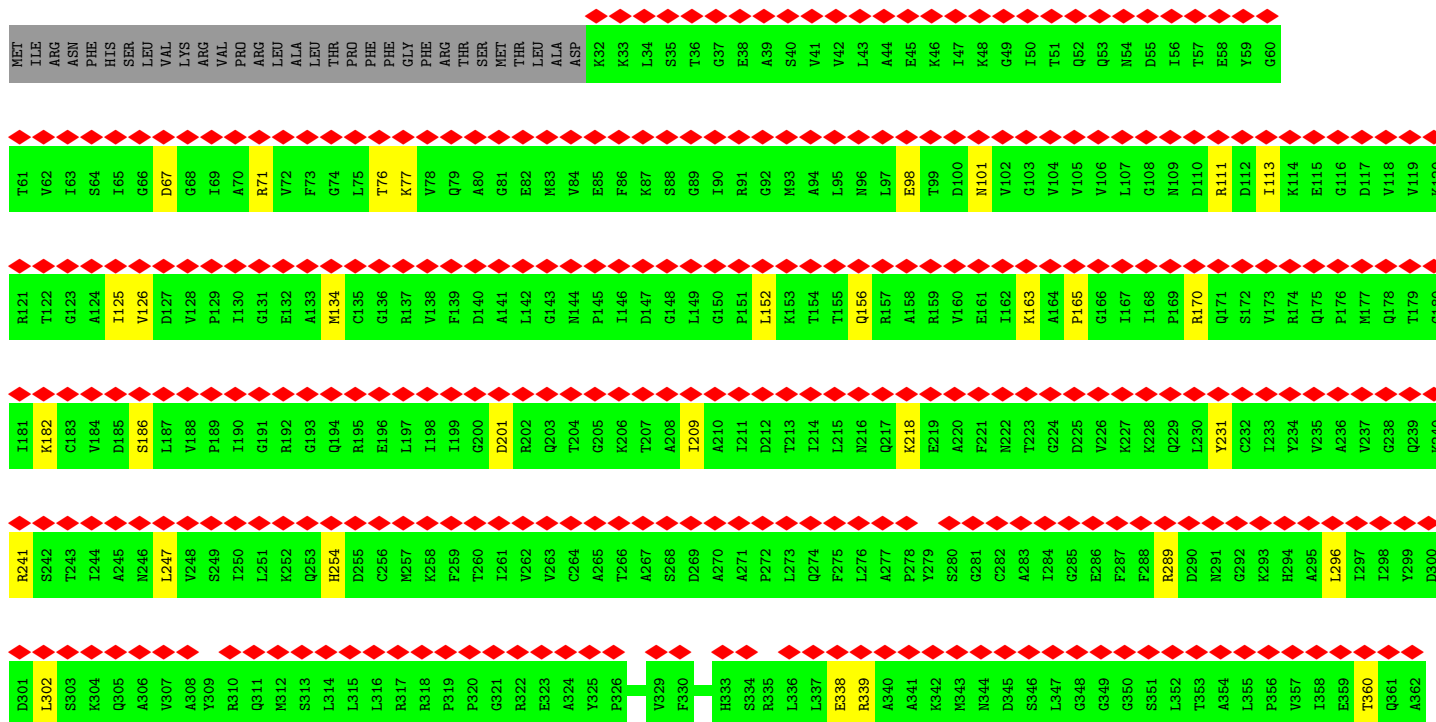
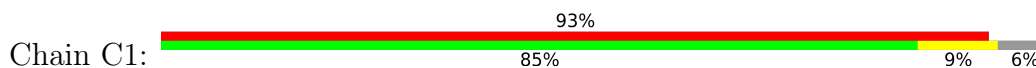


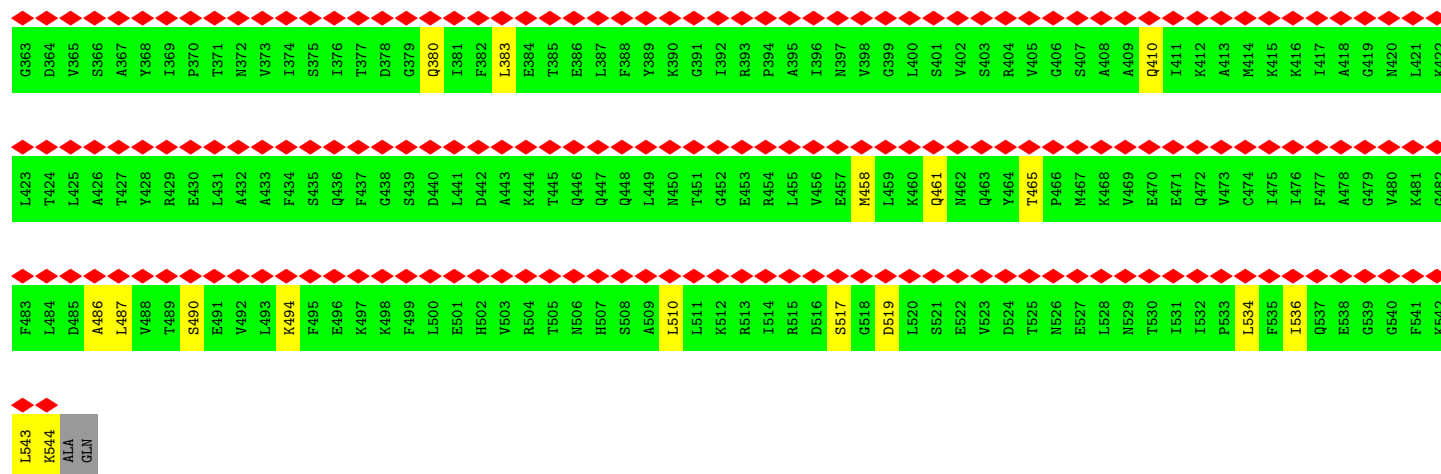


• Molecule 23: ATP synthase subunit gamma

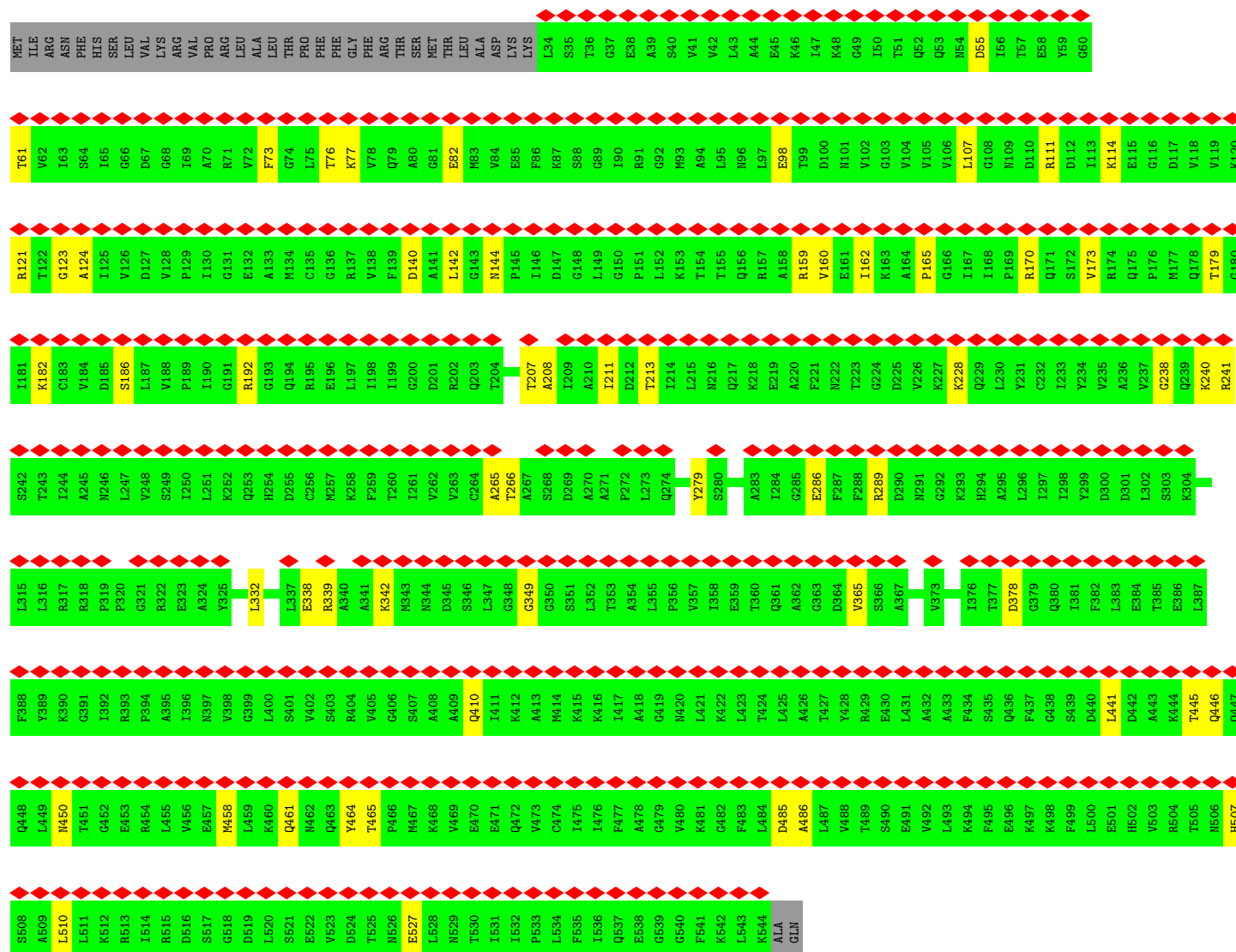
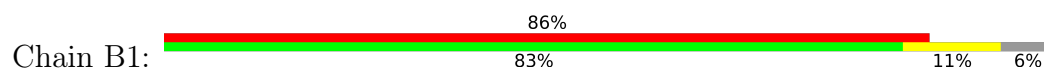


• Molecule 24: ATP synthase subunit alpha



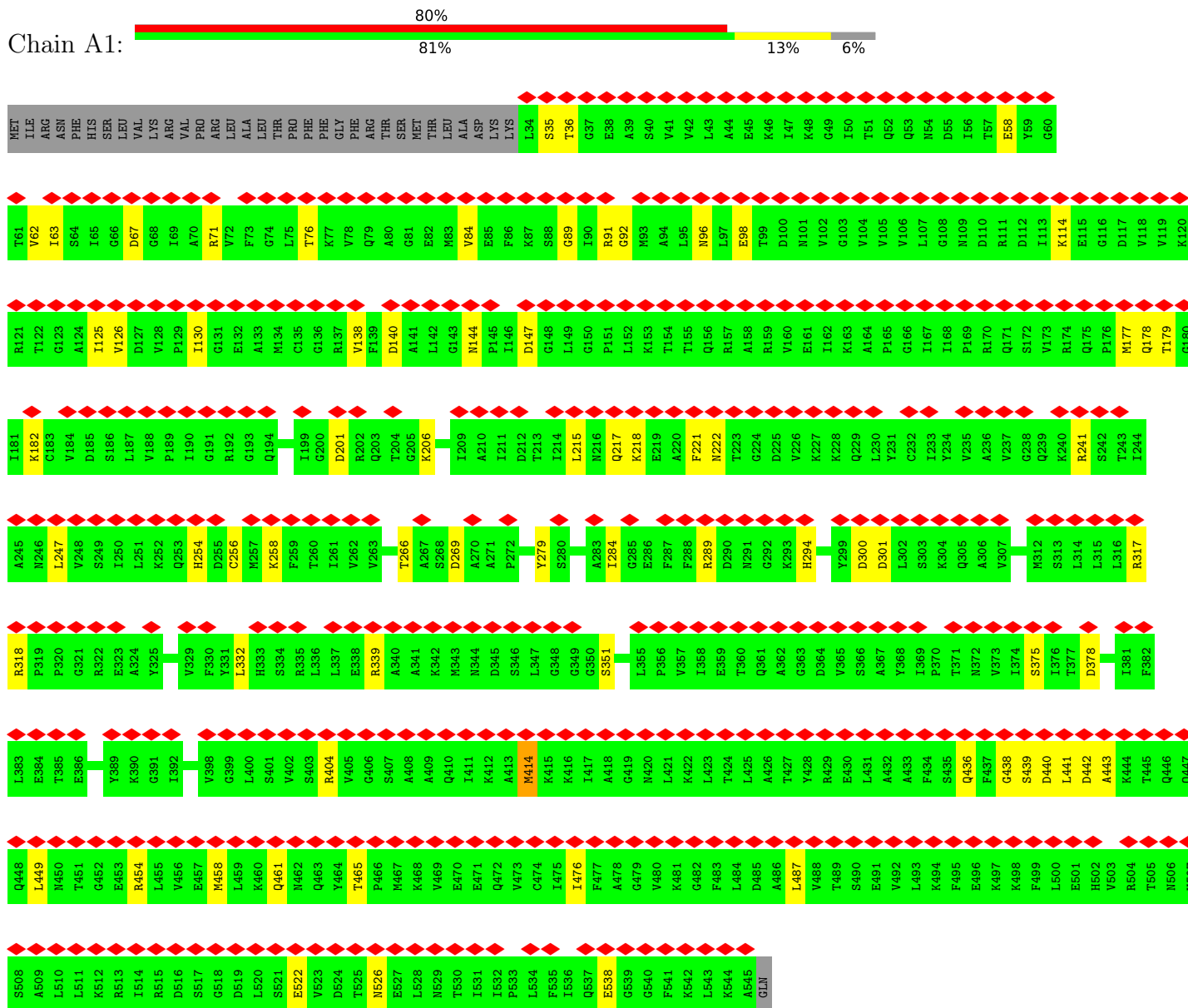


• Molecule 24: ATP synthase subunit alpha



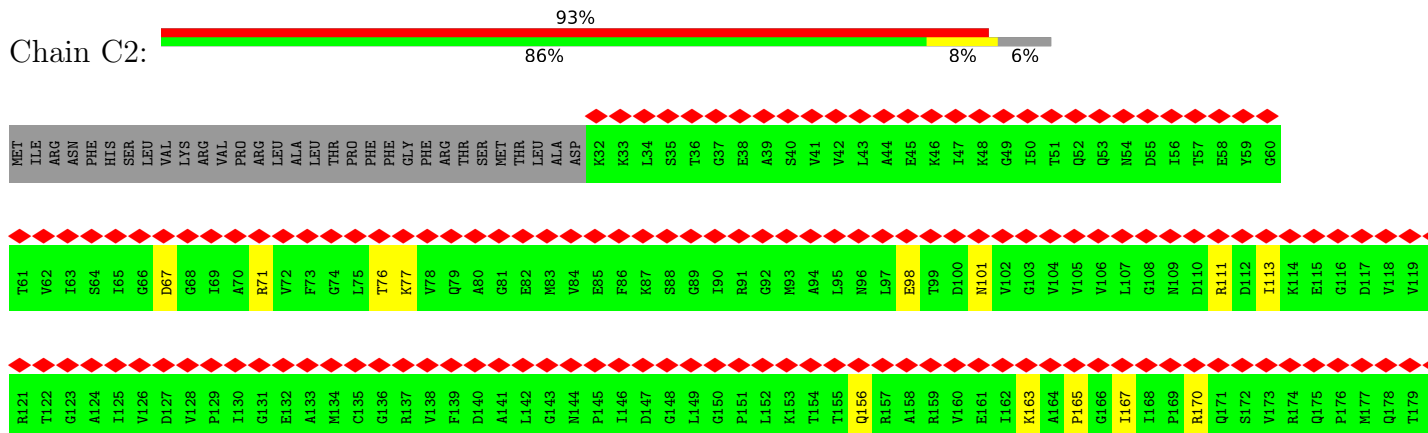
● Molecule 24: ATP synthase subunit alpha

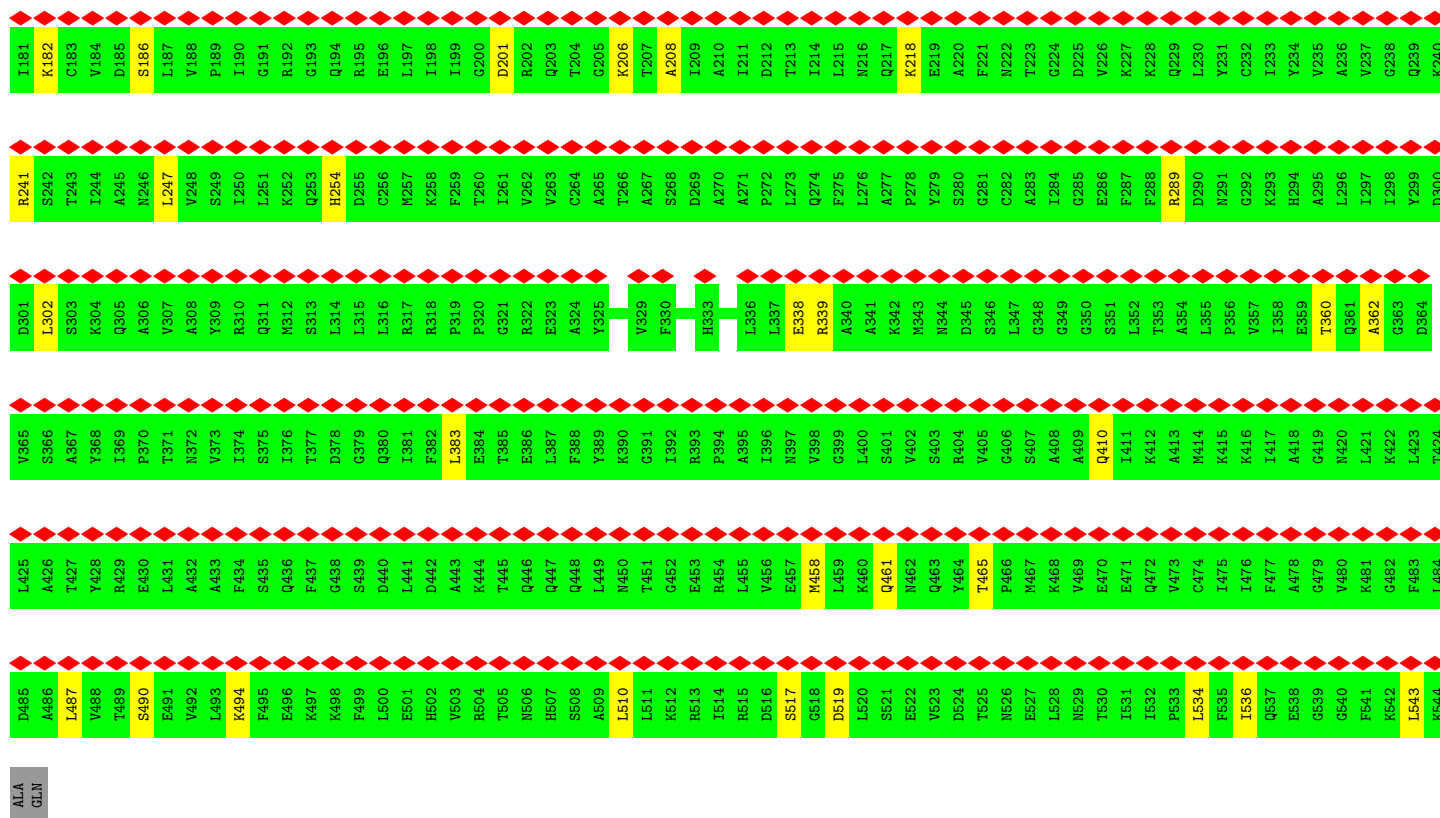
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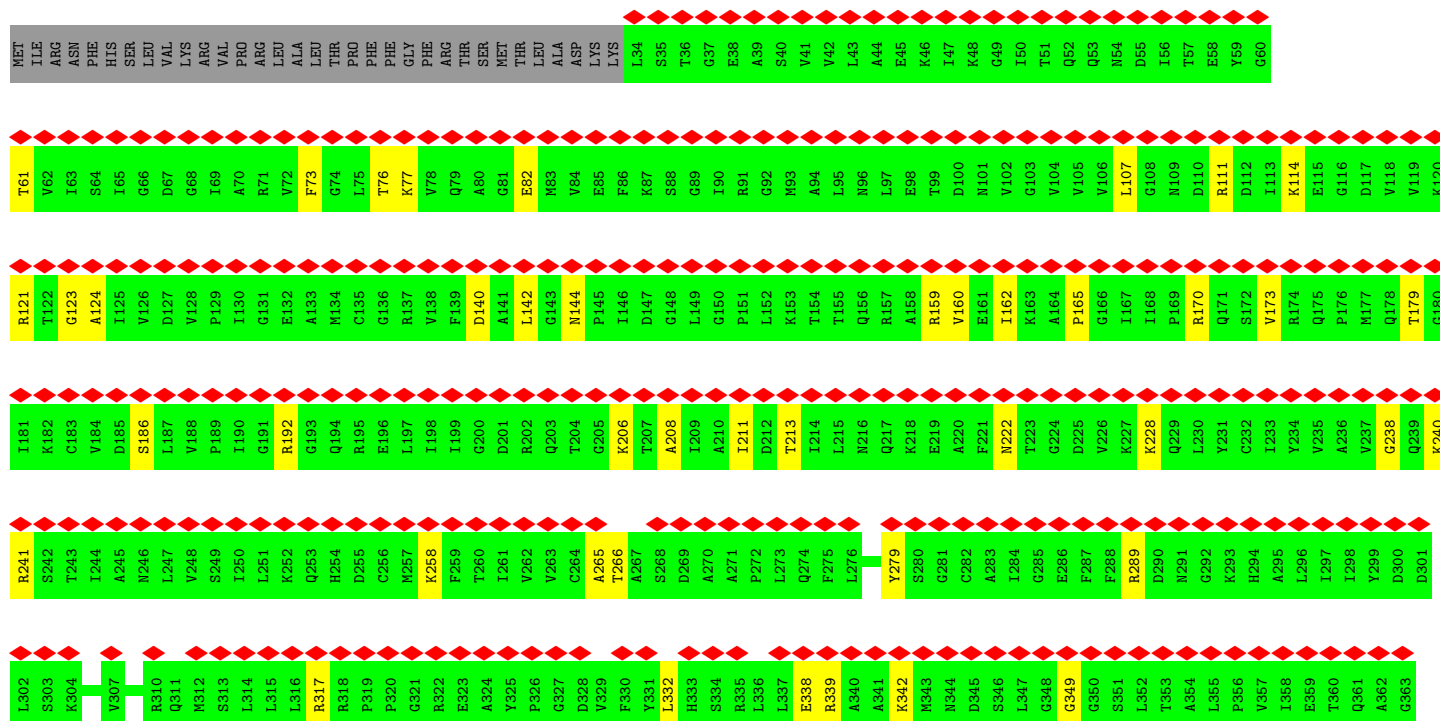
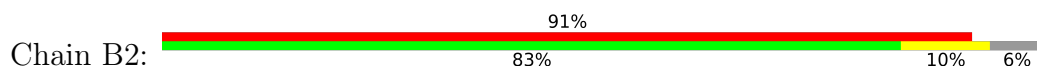
● Molecule 24: ATP synthase subunit alpha

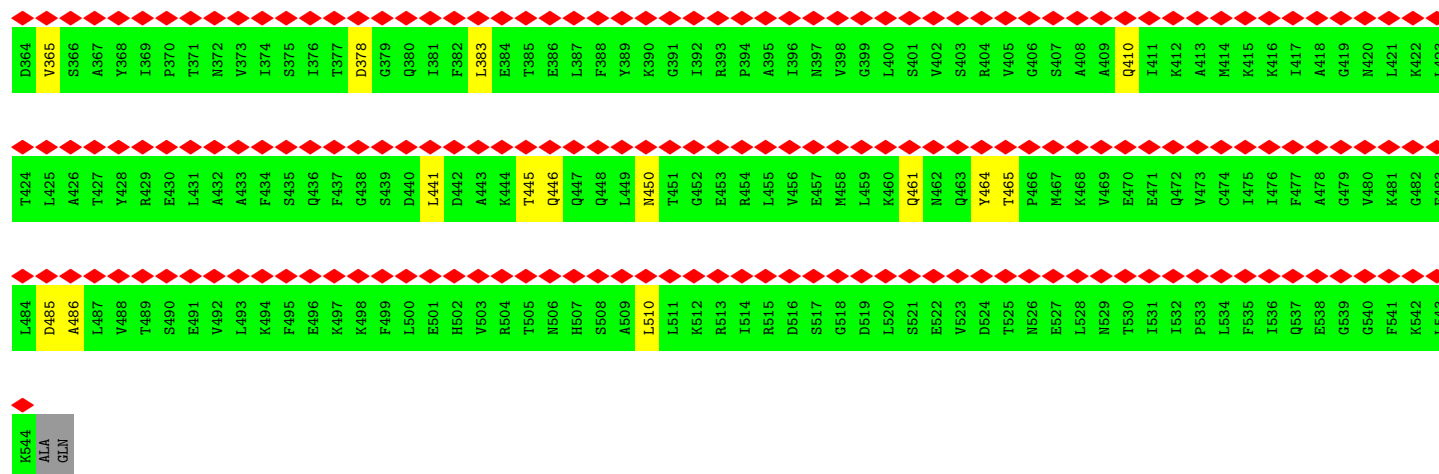
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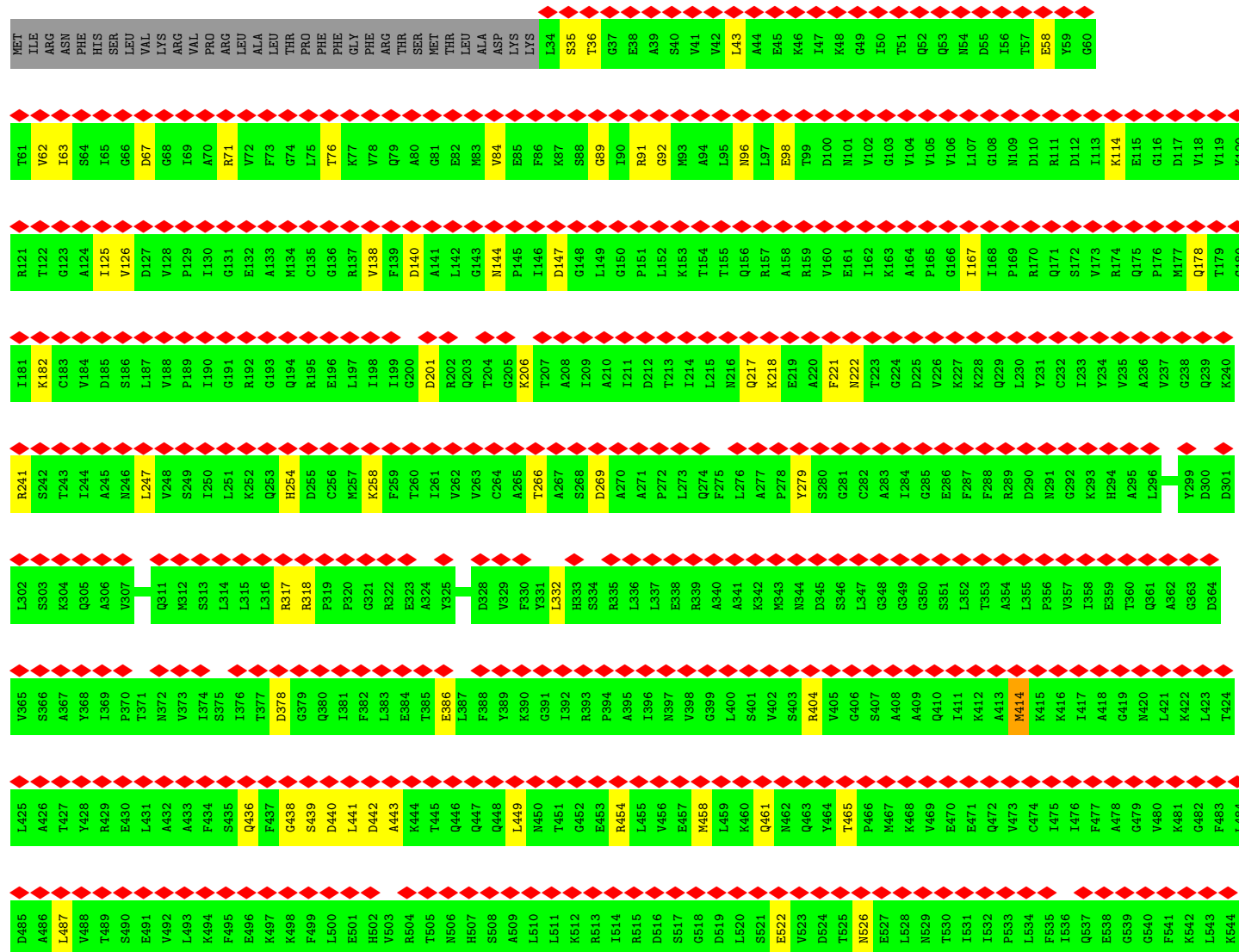
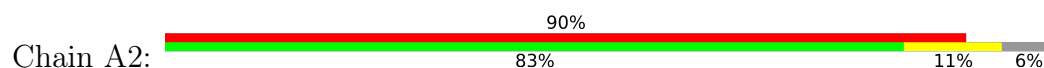


• Molecule 24: ATP synthase subunit alpha



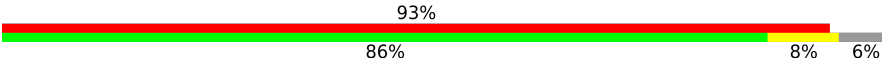


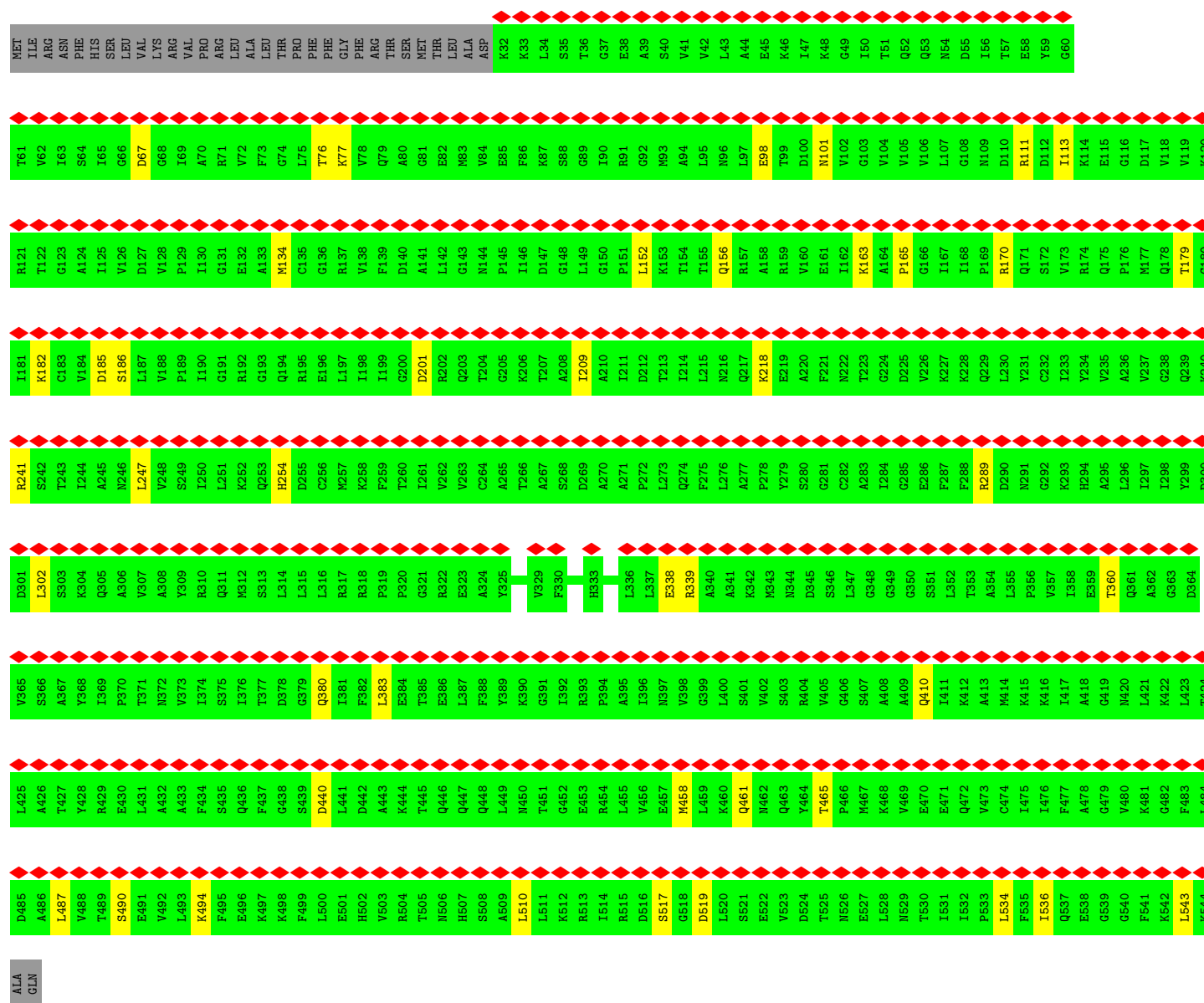
• Molecule 24: ATP synthase subunit alpha



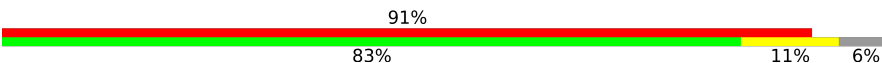


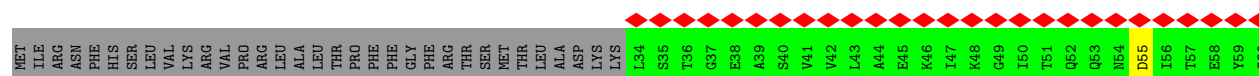
• Molecule 24: ATP synthase subunit alpha

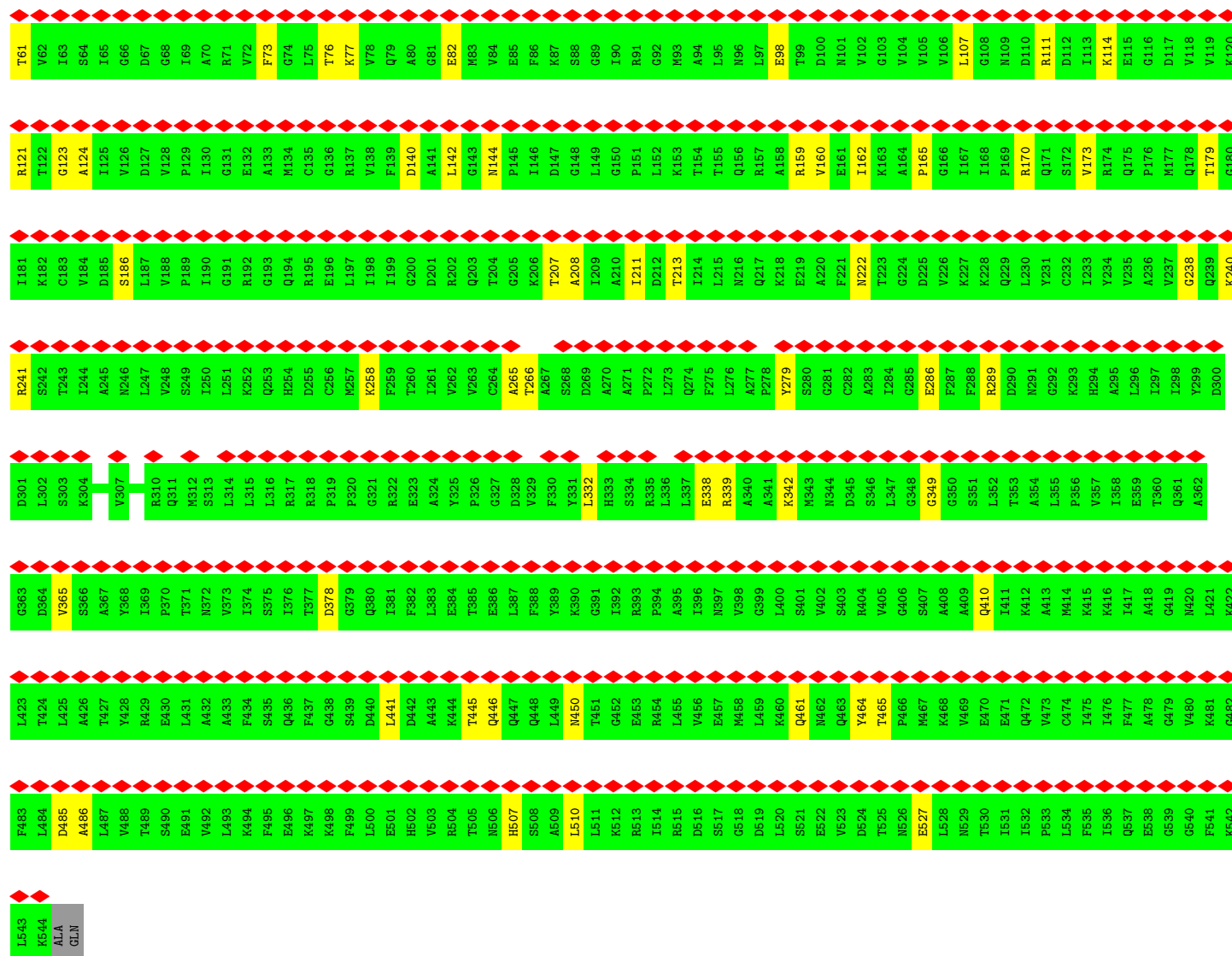
Chain C4: 



• Molecule 24: ATP synthase subunit alpha

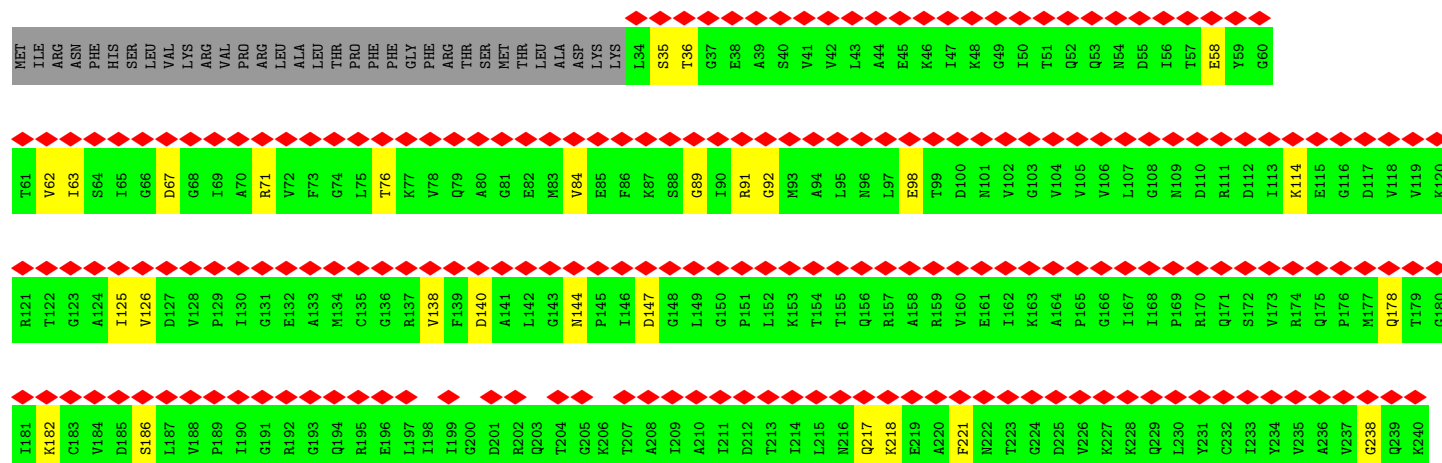
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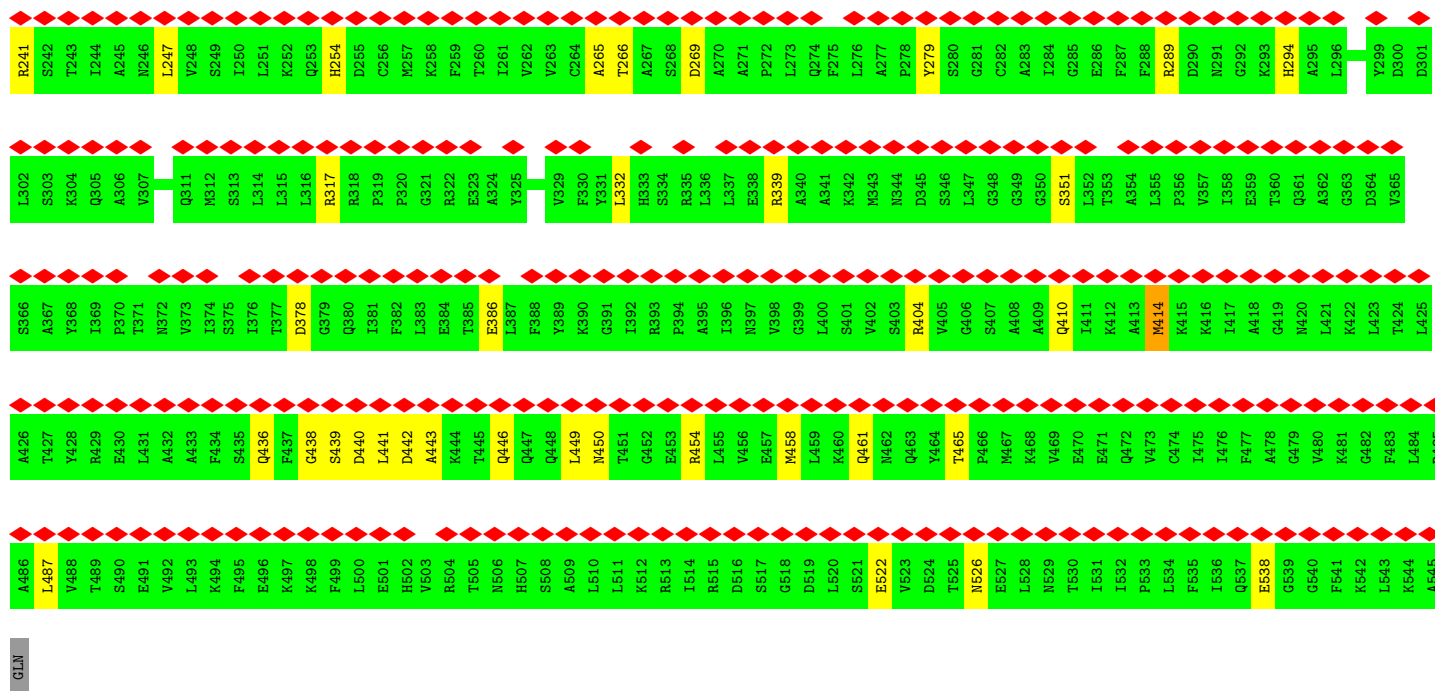




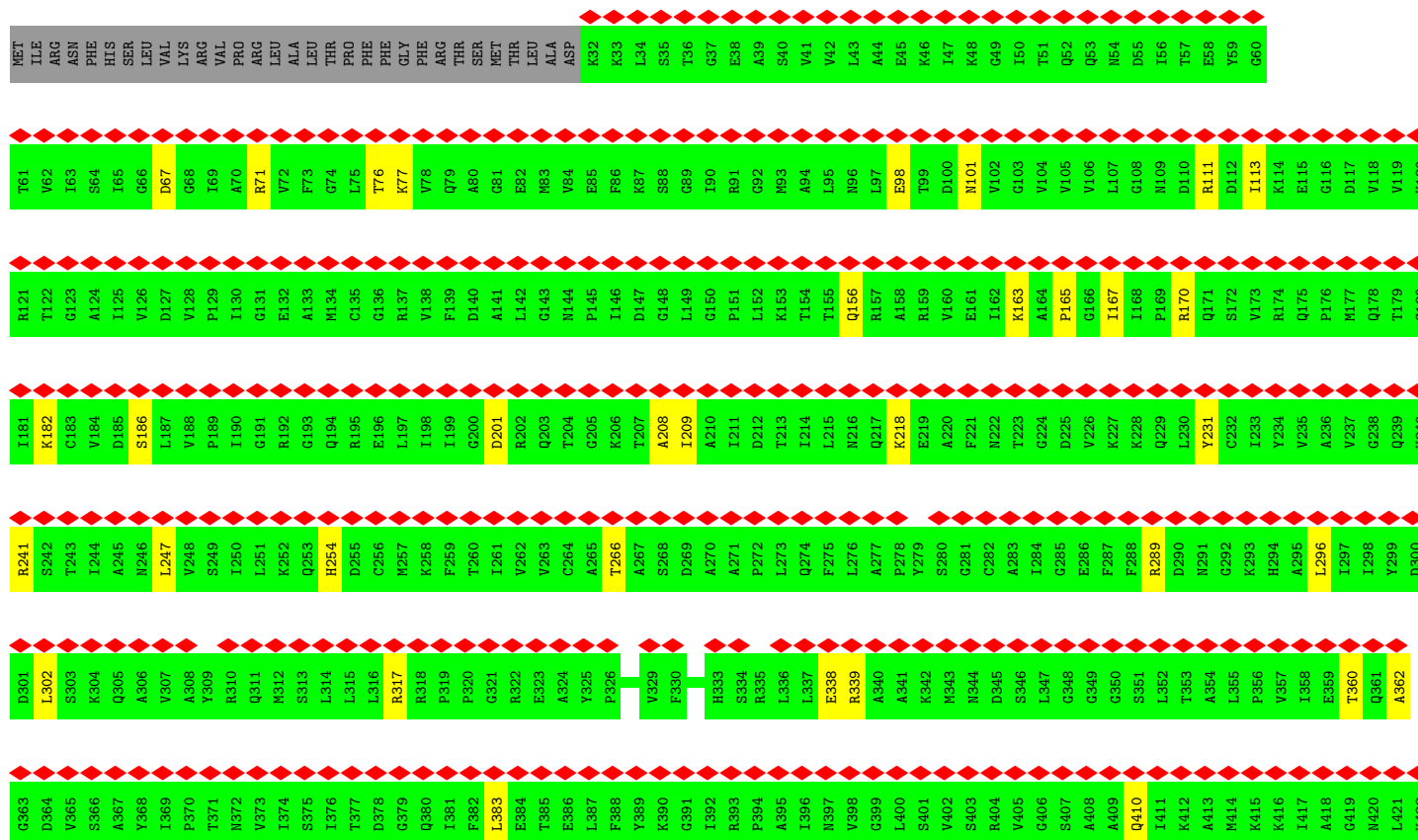
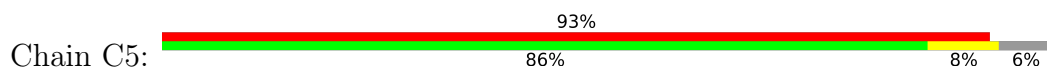
• Molecule 24: ATP synthase subunit alpha

Chain A4:

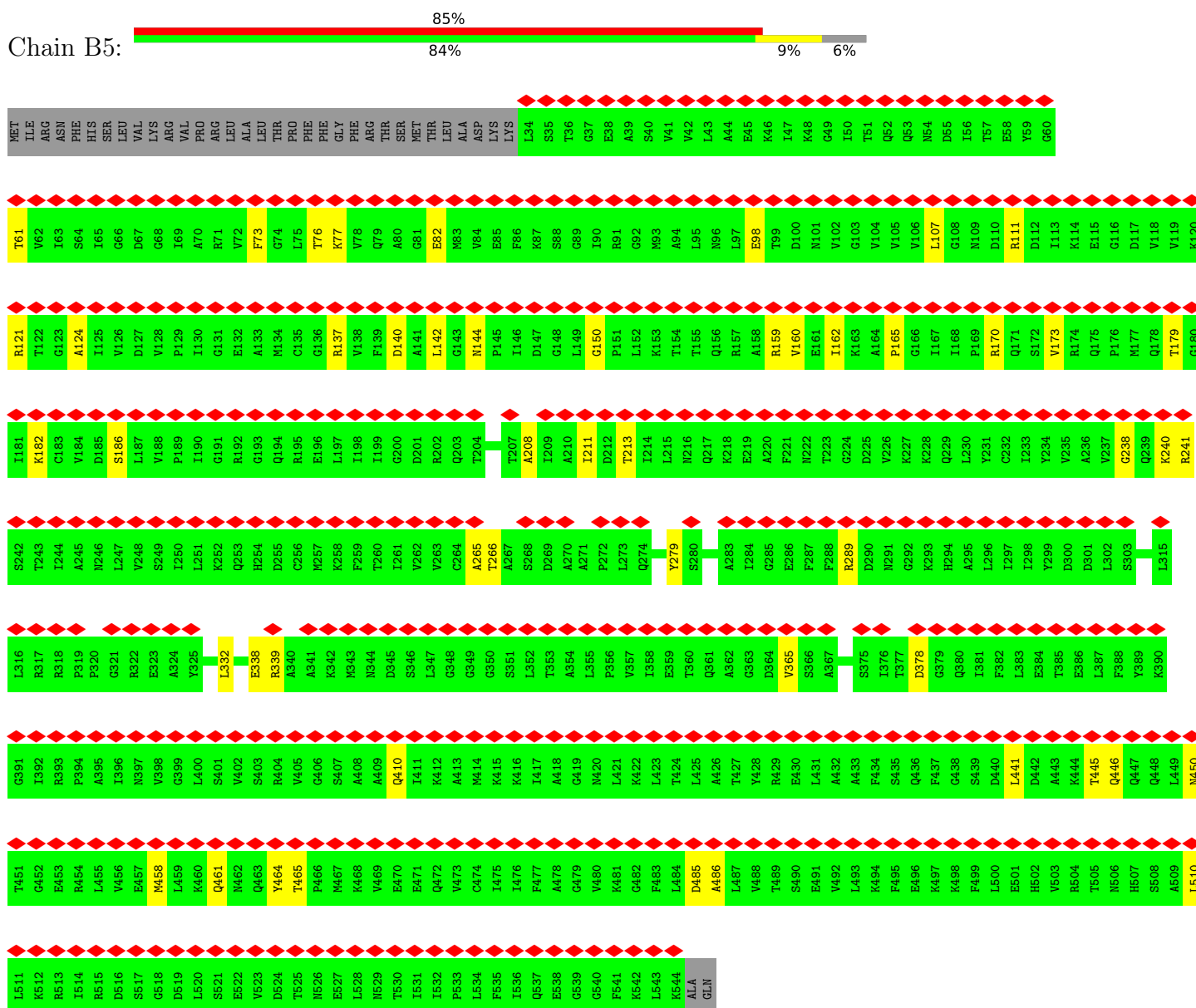




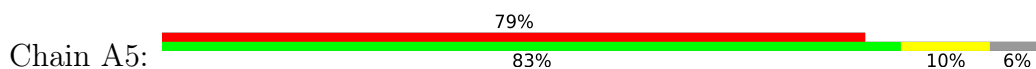
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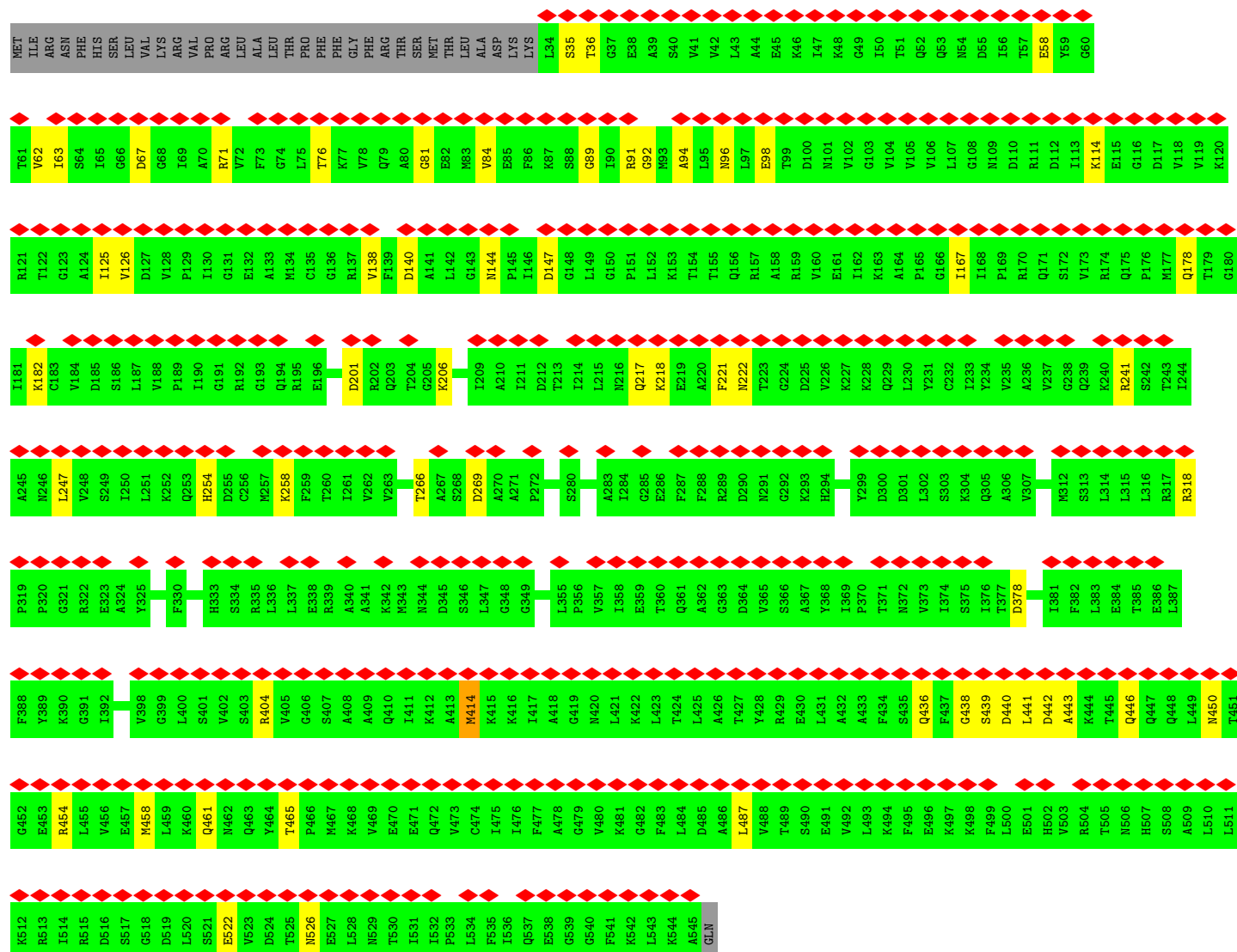


- Molecule 24: ATP synthase subunit alpha



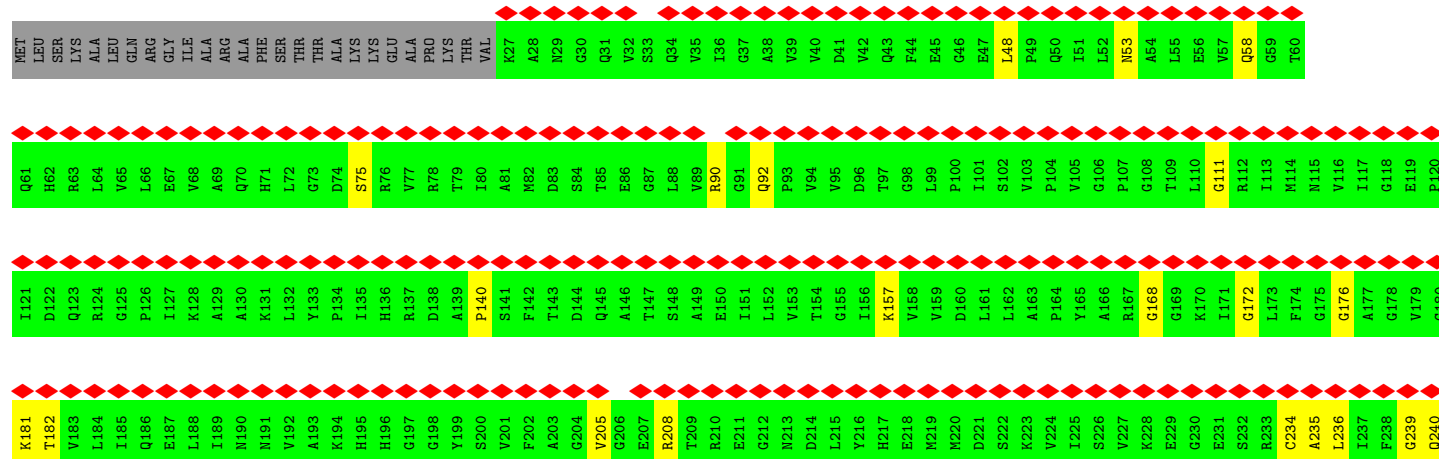
- Molecule 24: ATP synthase subunit alpha

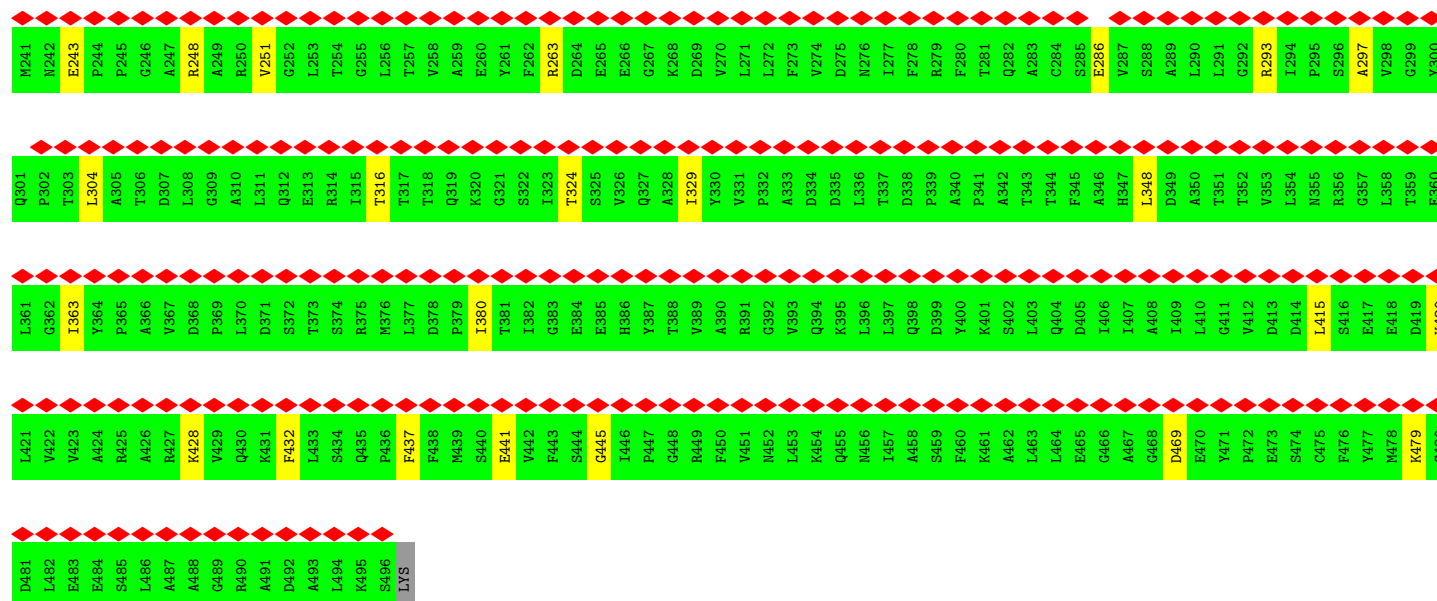




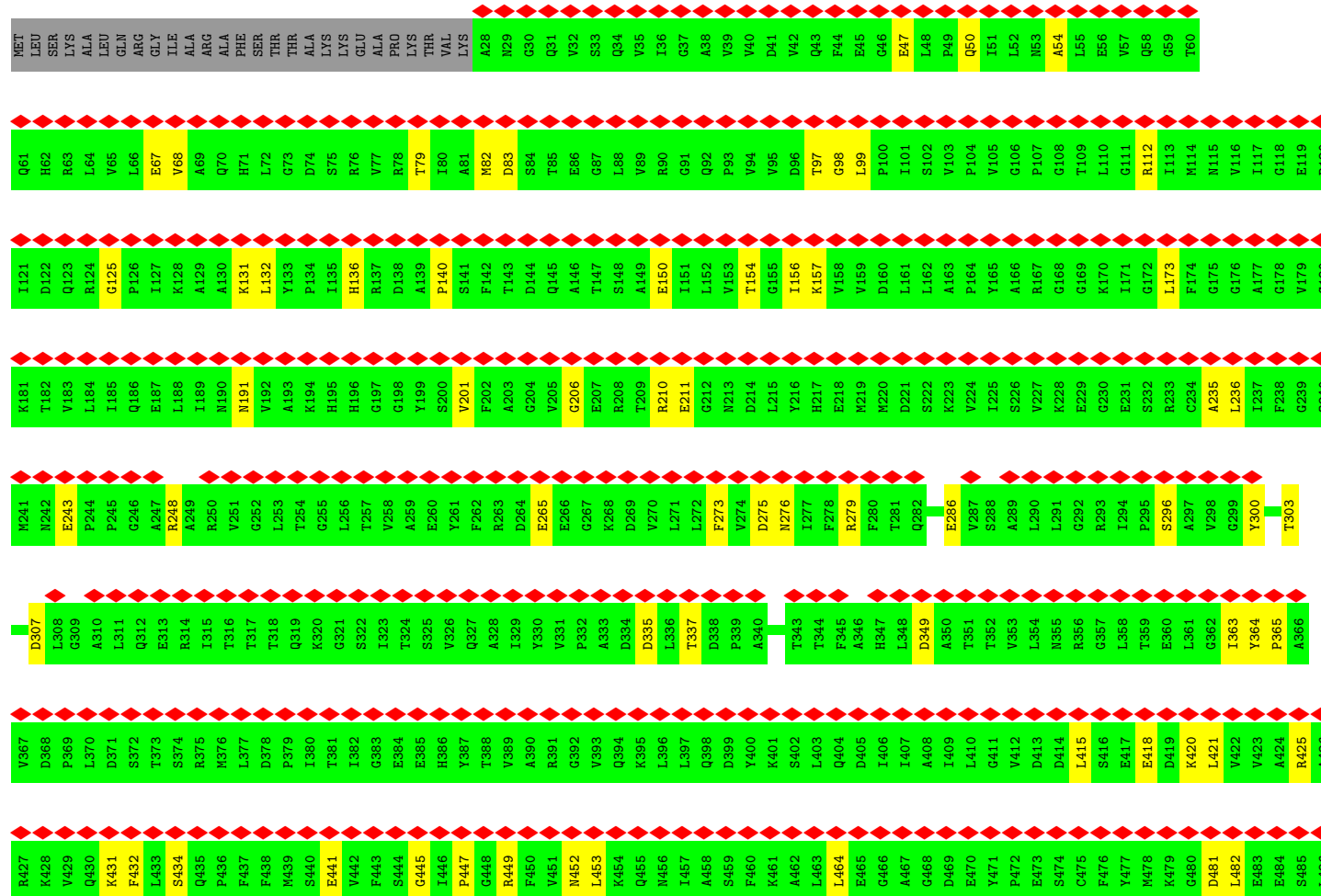
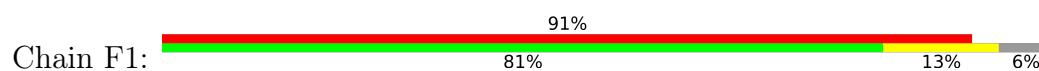
• Molecule 25: ATP synthase subunit beta

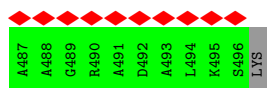
Chain D1: 94% 86% 9% 5%





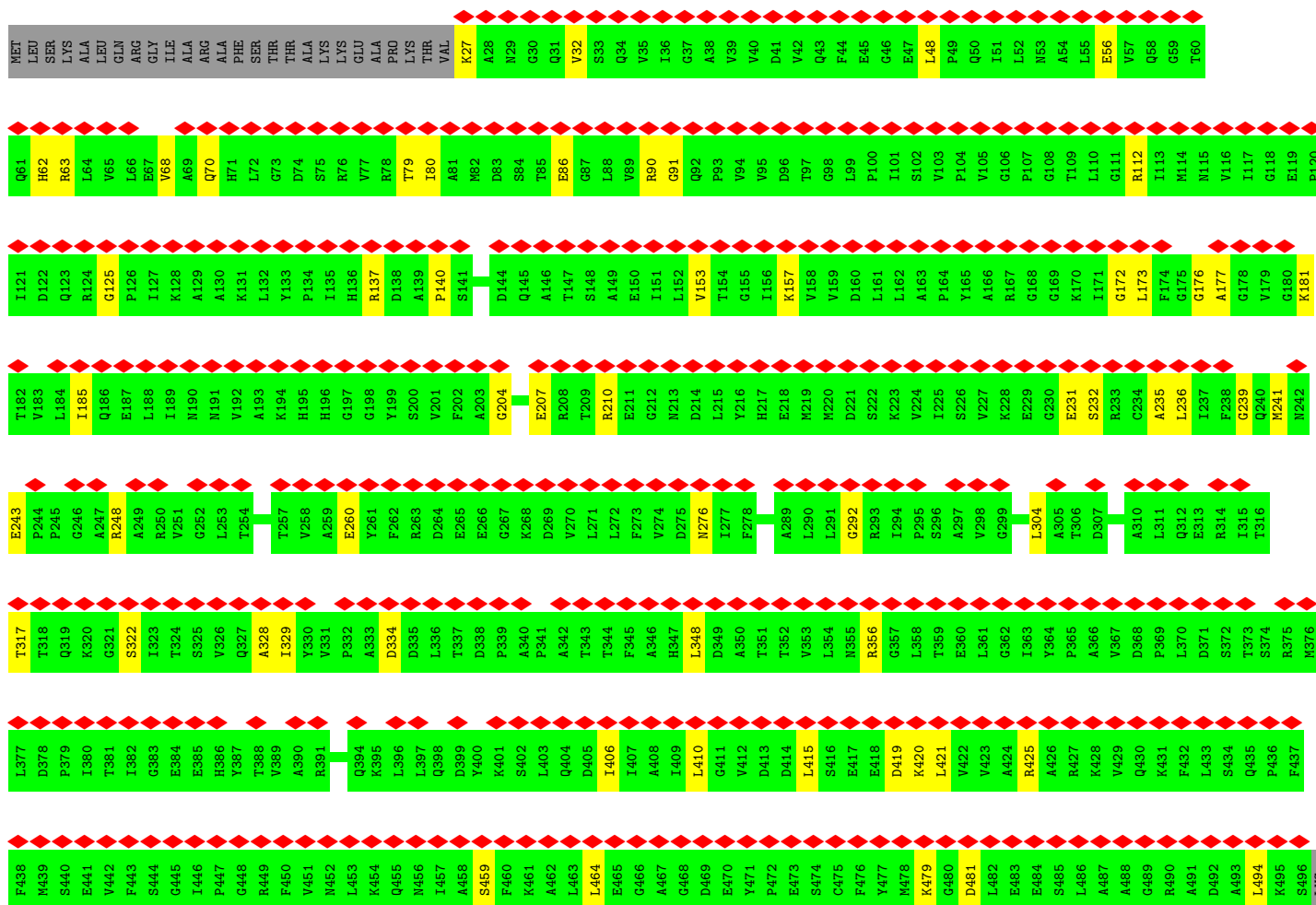
• Molecule 25: ATP synthase subunit beta



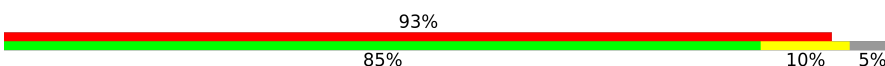


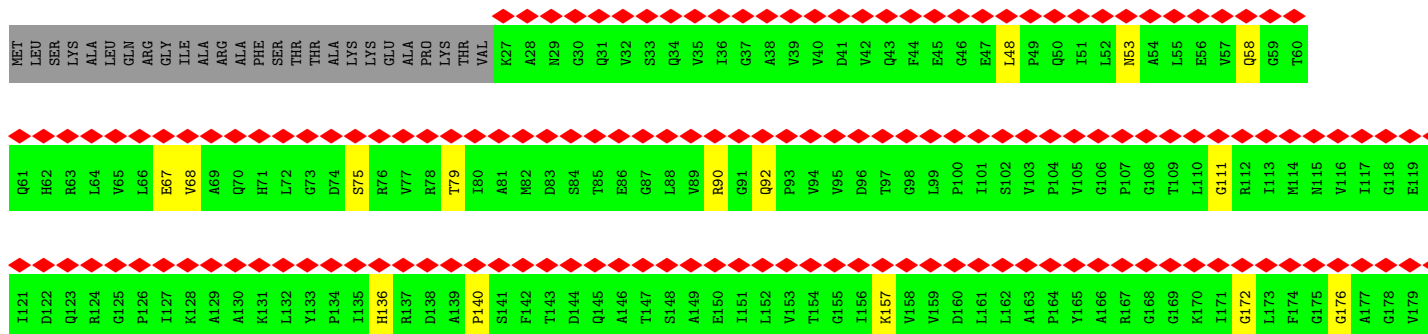
• Molecule 25: ATP synthase subunit beta

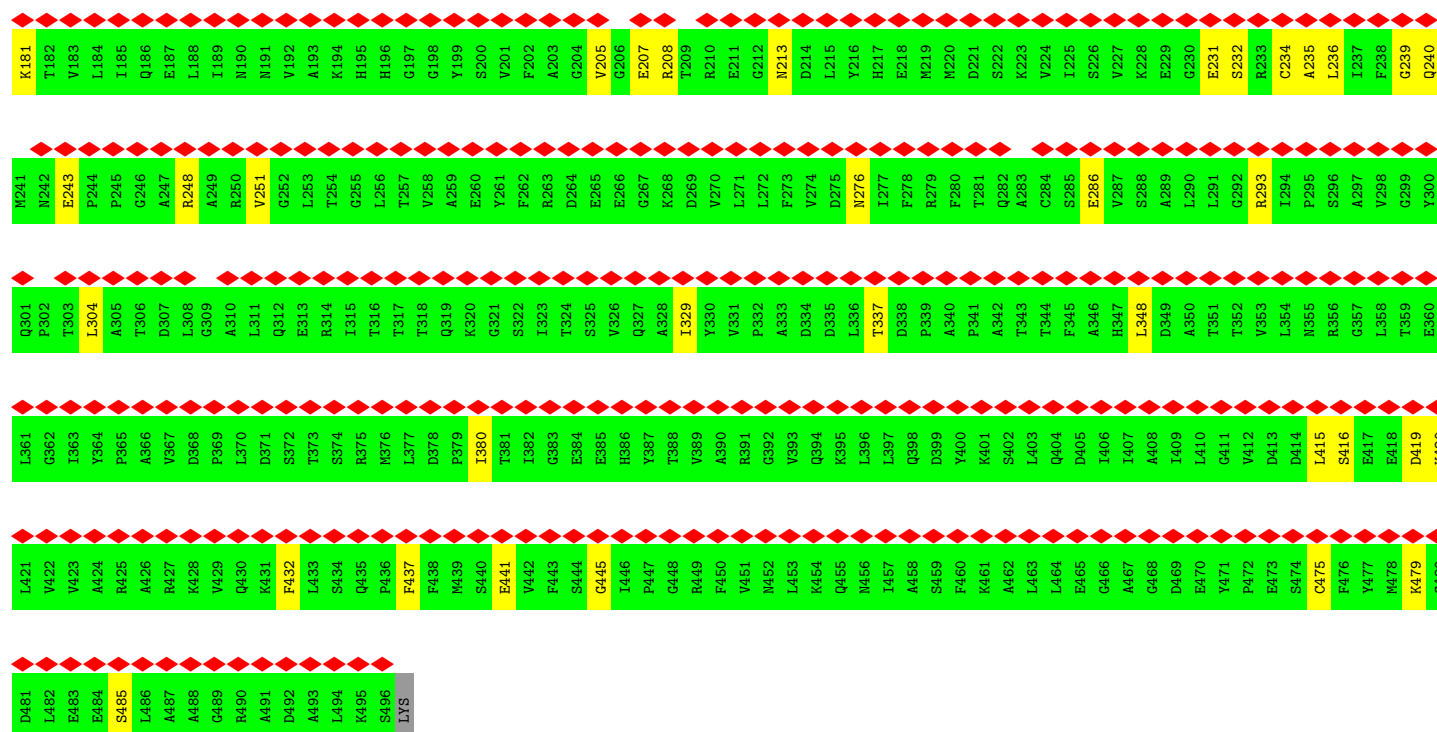
Chain E1: 



• Molecule 25: ATP synthase subunit beta

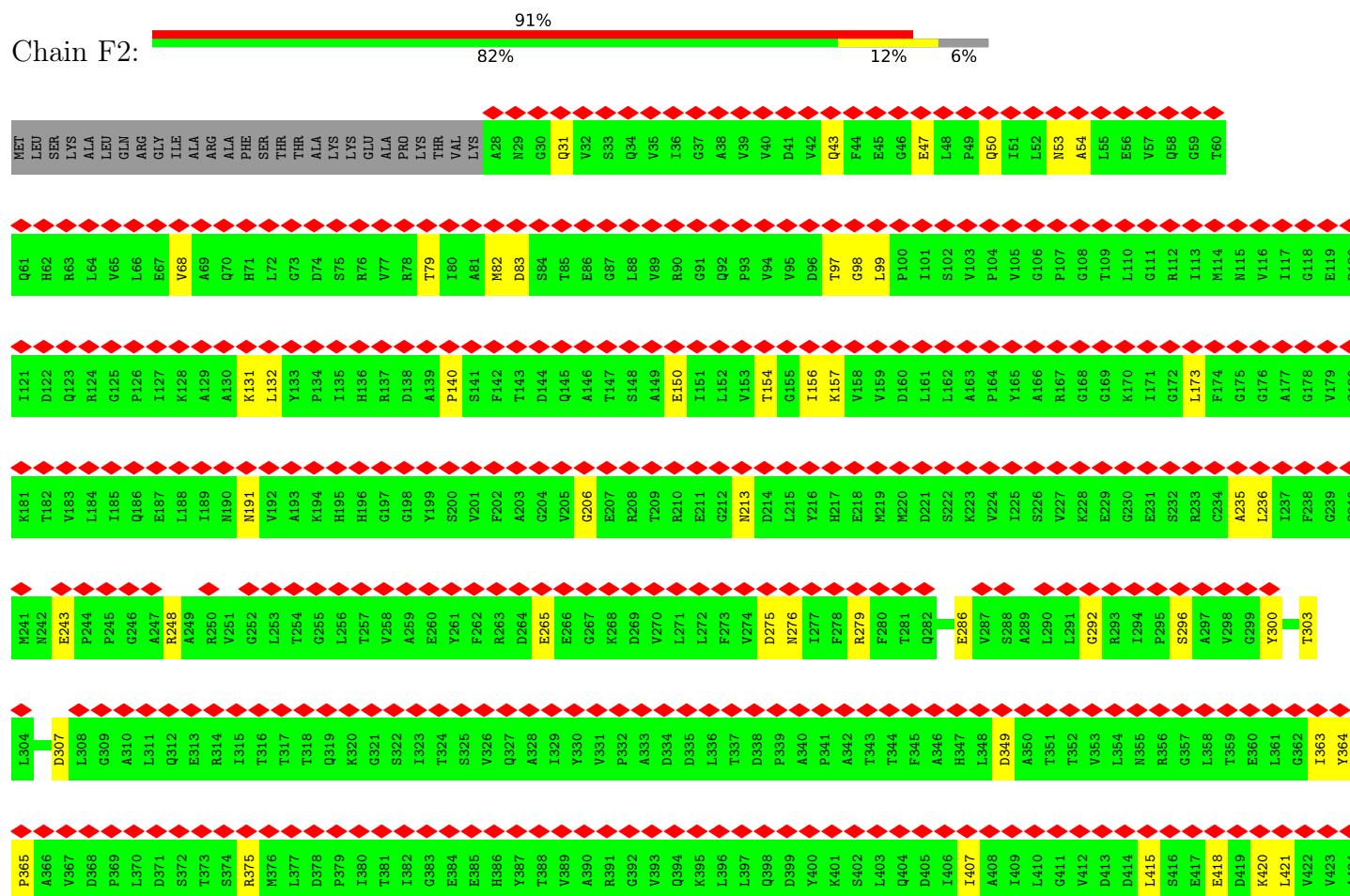
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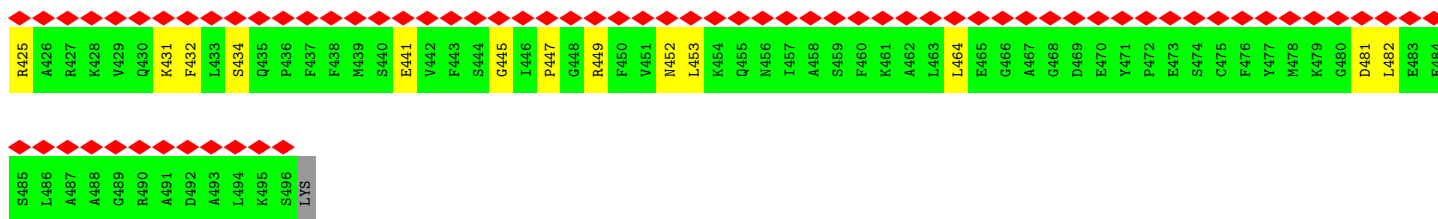




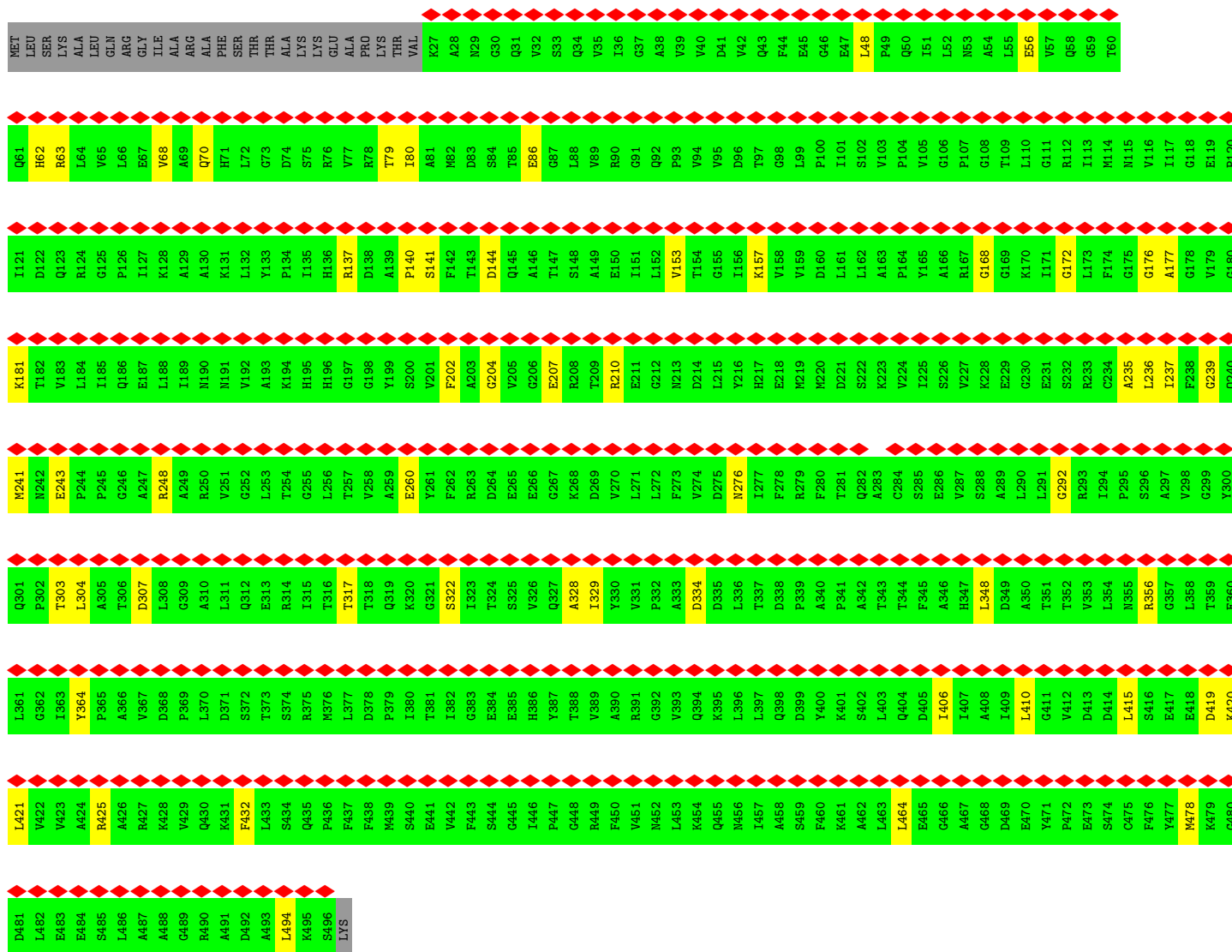
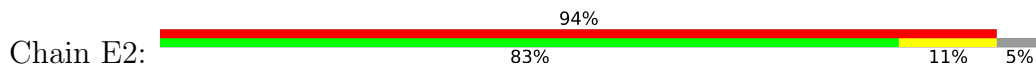
● Molecule 25: ATP synthase subunit beta

Chain F2:

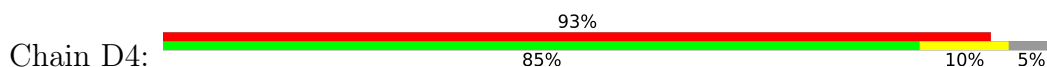


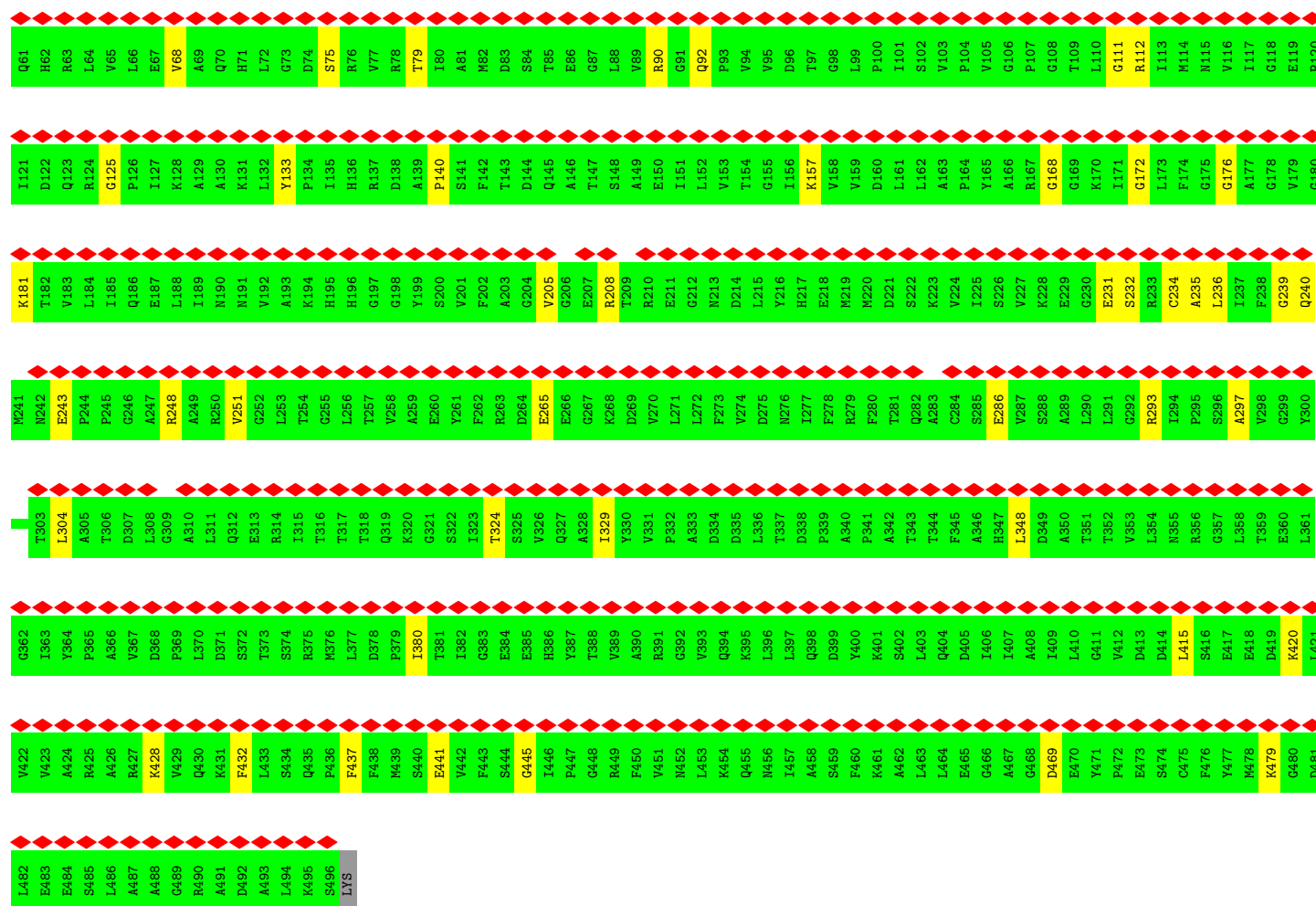


• Molecule 25: ATP synthase subunit beta

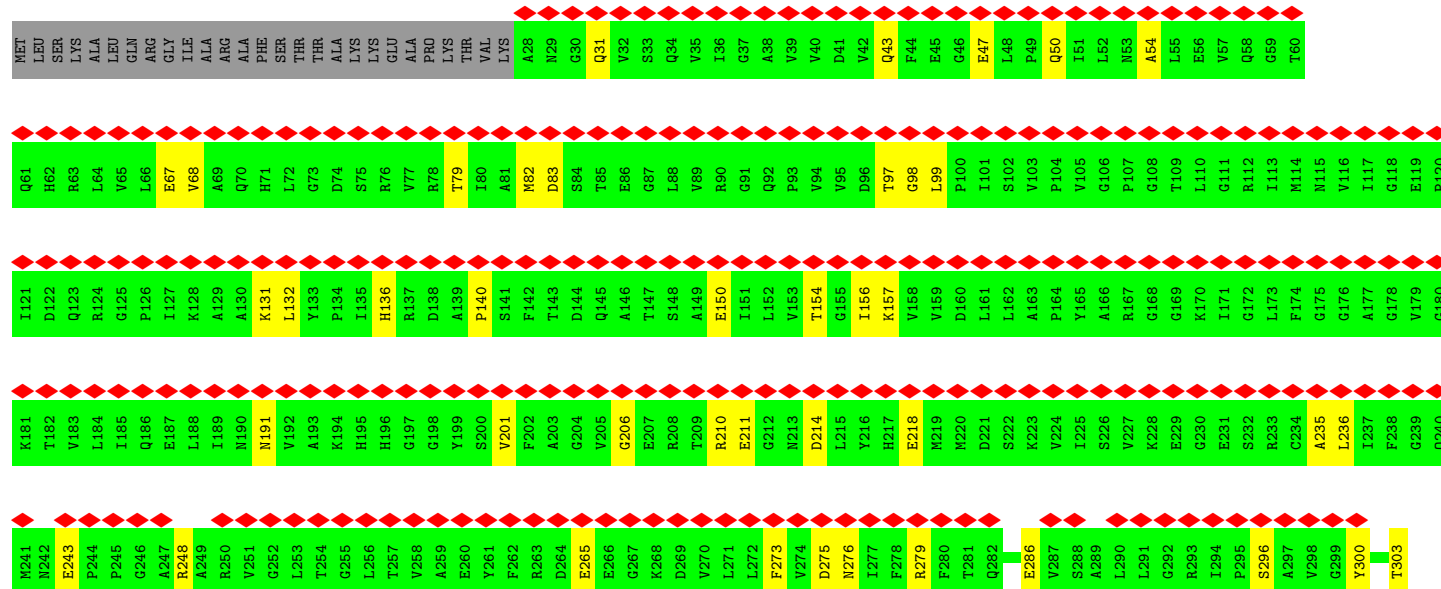
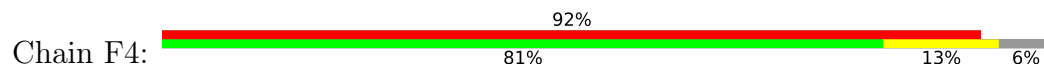


• Molecule 25: ATP synthase subunit beta



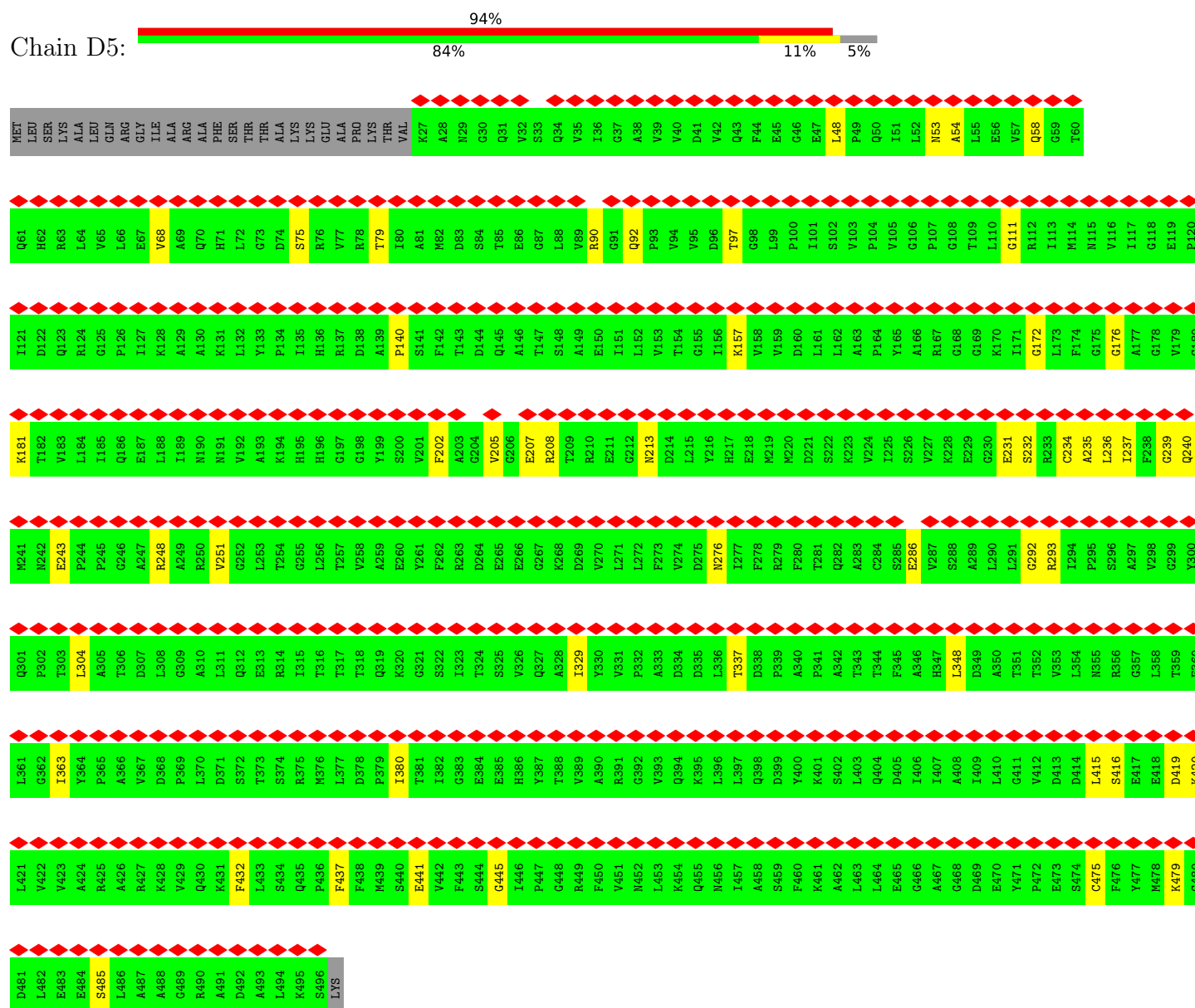


• Molecule 25: ATP synthase subunit beta



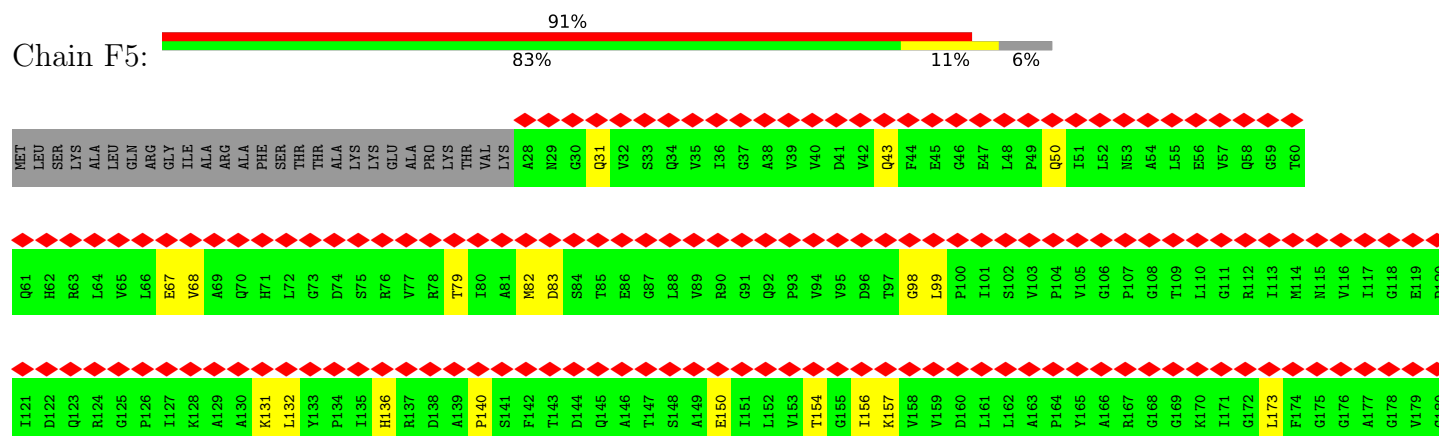
● Molecule 25: ATP synthase subunit beta

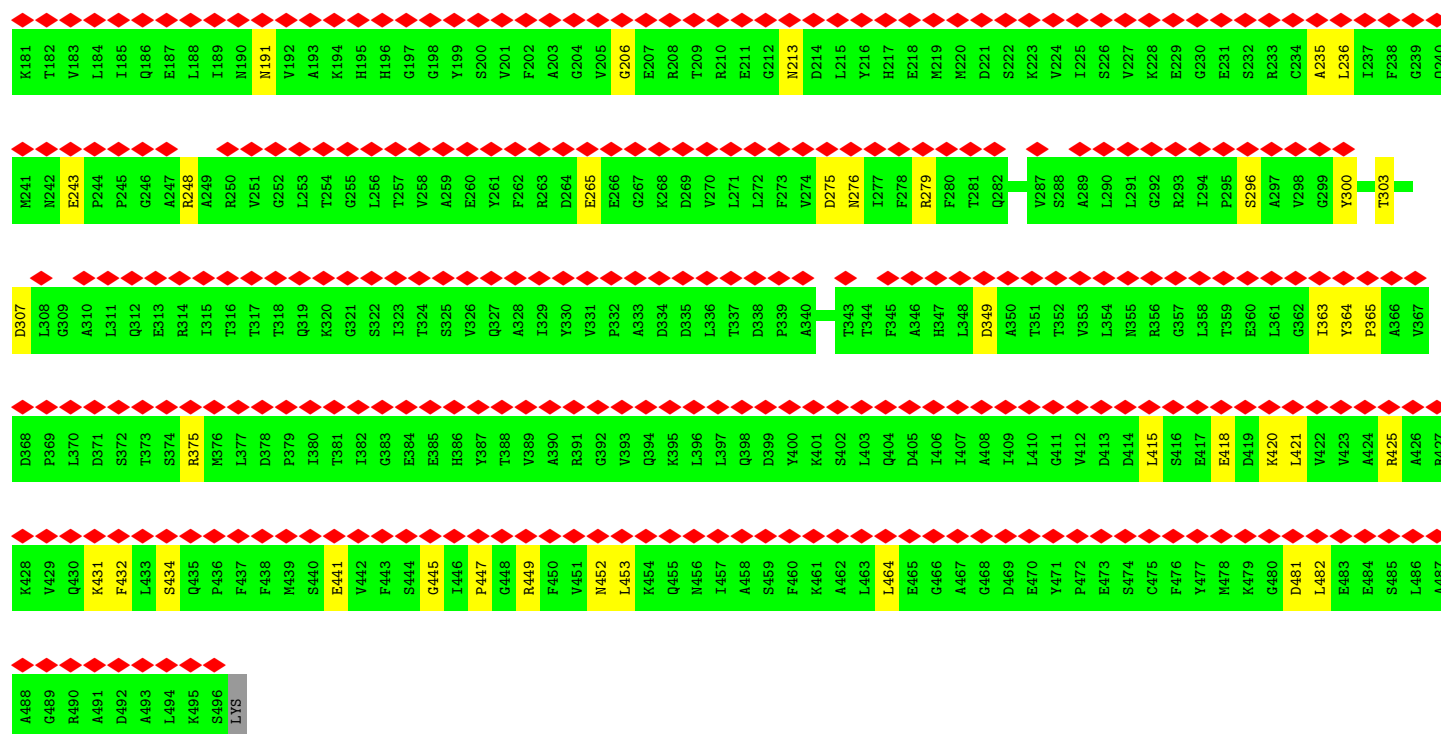
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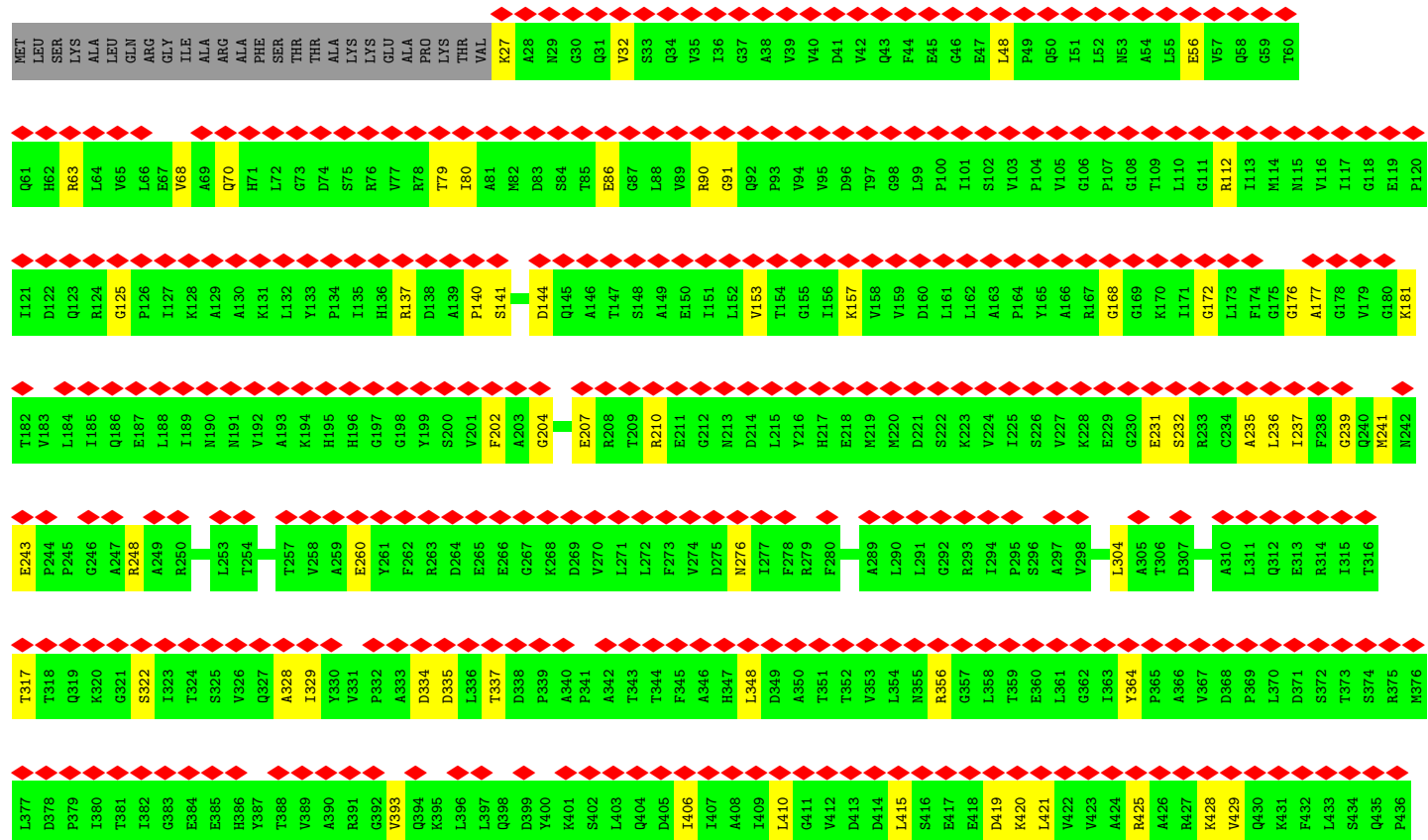
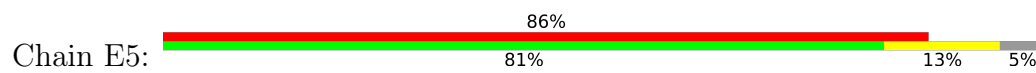
● Molecule 25: ATP synthase subunit beta

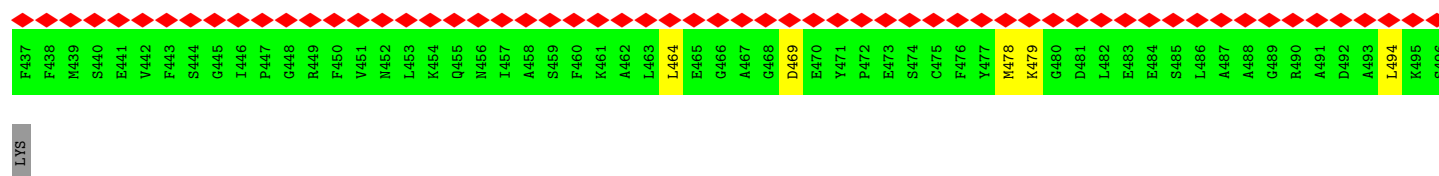
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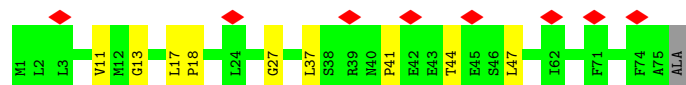
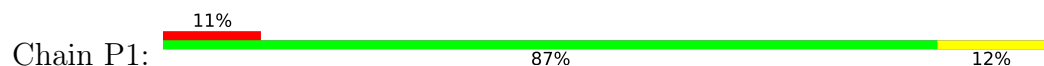


• Molecule 25: ATP synthase subunit beta

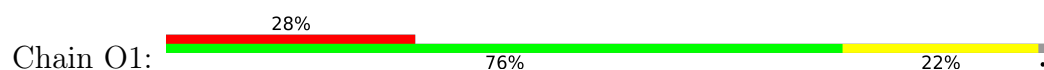




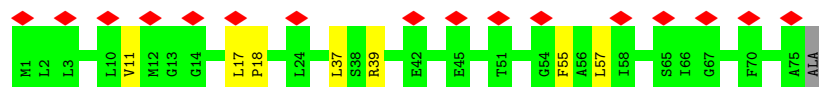
- Molecule 26: ATP synthase F0 subunit 9



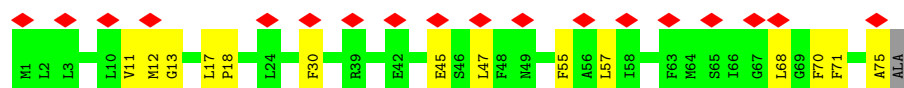
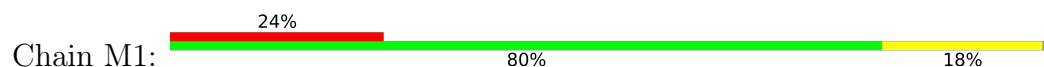
- Molecule 26: ATP synthase F0 subunit 9



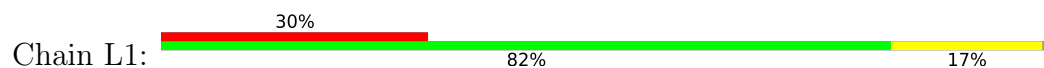
- Molecule 26: ATP synthase F0 subunit 9



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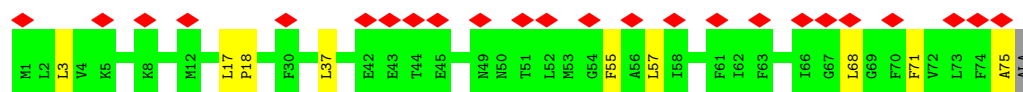


- Molecule 26: ATP synthase F0 subunit 9

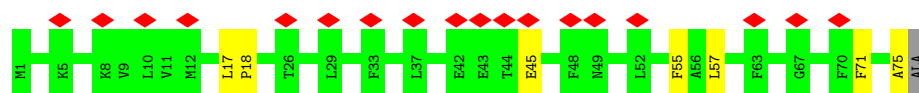
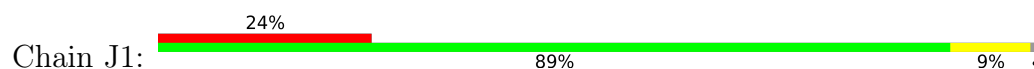


- Molecule 26: ATP synthase F0 subunit 9

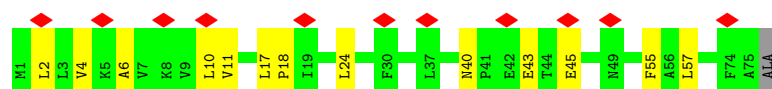
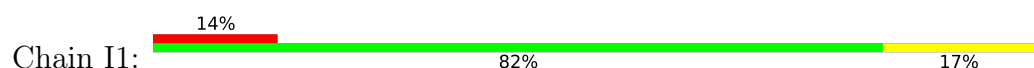




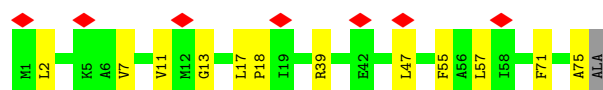
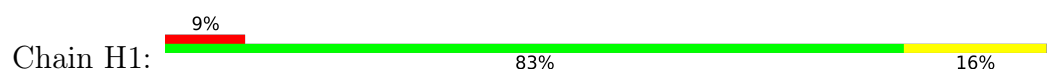
- Molecule 26: ATP synthase F0 subunit 9



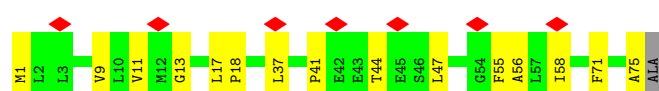
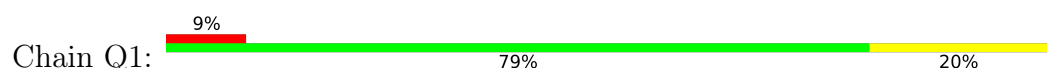
- Molecule 26: ATP synthase F0 subunit 9



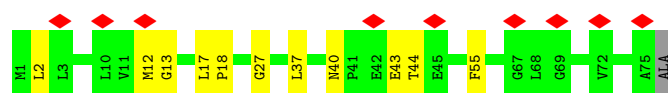
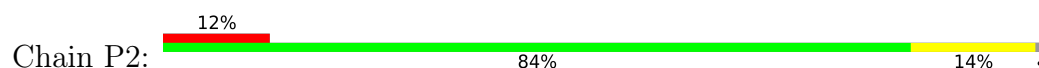
- Molecule 26: ATP synthase F0 subunit 9



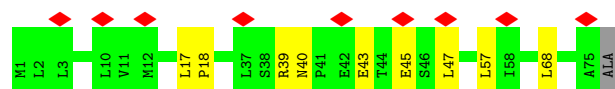
- Molecule 26: ATP synthase F0 subunit 9



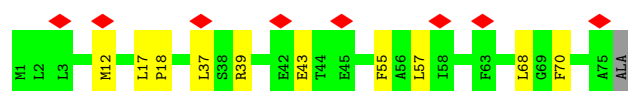
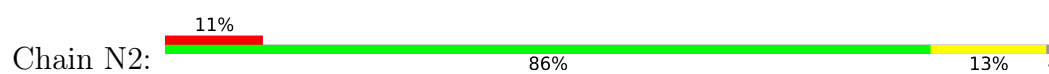
- Molecule 26: ATP synthase F0 subunit 9



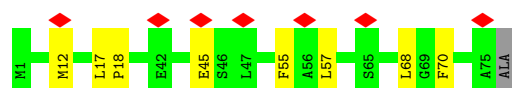
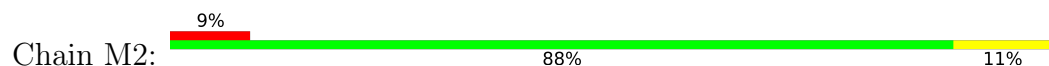
- Molecule 26: ATP synthase F0 subunit 9



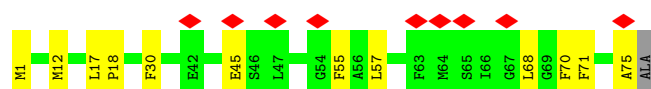
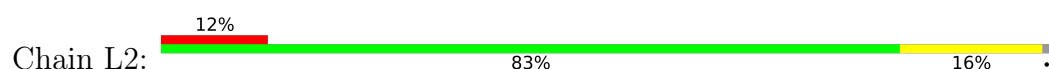
- Molecule 26: ATP synthase F0 subunit 9



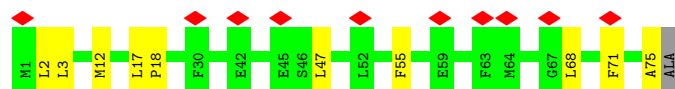
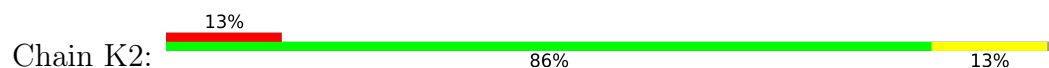
- Molecule 26: ATP synthase F0 subunit 9



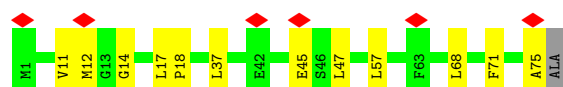
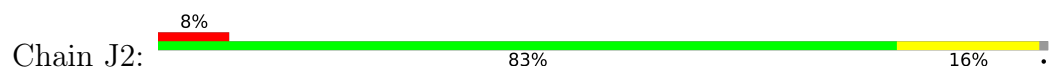
- Molecule 26: ATP synthase F0 subunit 9



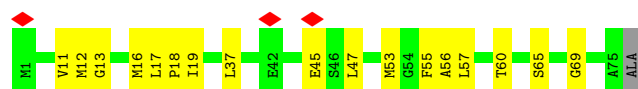
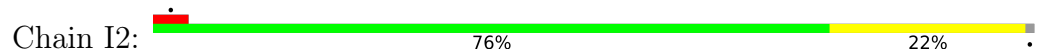
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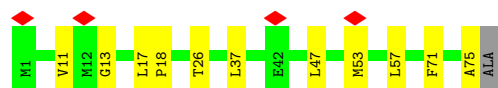
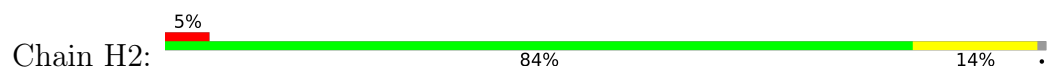
- Molecule 26: ATP synthase F0 subunit 9



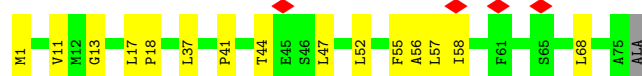
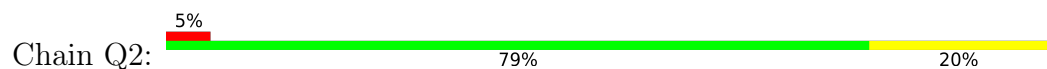
- Molecule 26: ATP synthase F0 subunit 9



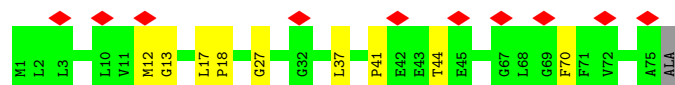
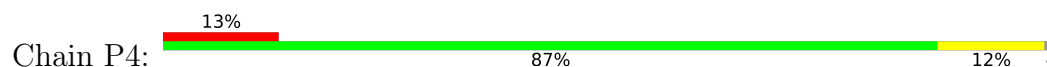
- Molecule 26: ATP synthase F0 subunit 9



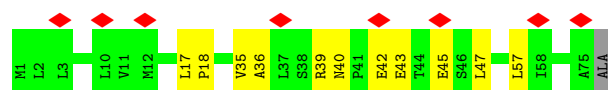
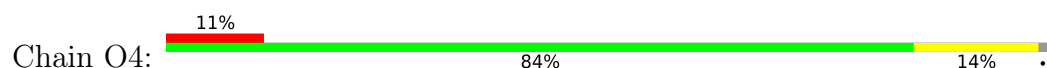
- Molecule 26: ATP synthase F0 subunit 9



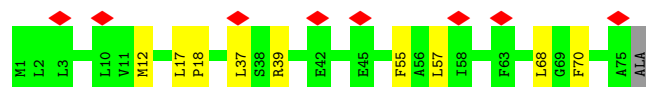
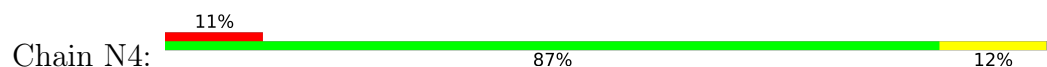
- Molecule 26: ATP synthase F0 subunit 9



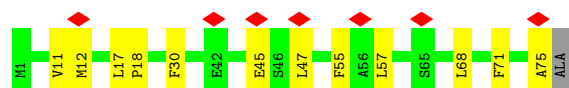
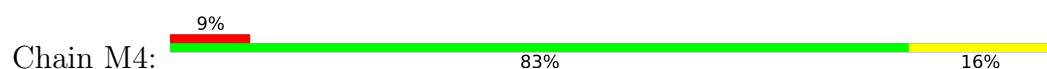
- Molecule 26: ATP synthase F0 subunit 9



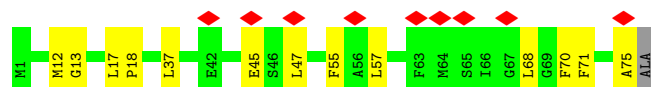
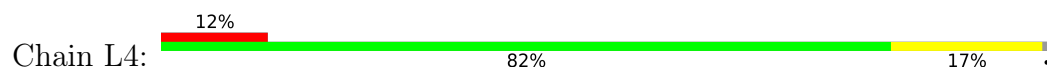
- Molecule 26: ATP synthase F0 subunit 9



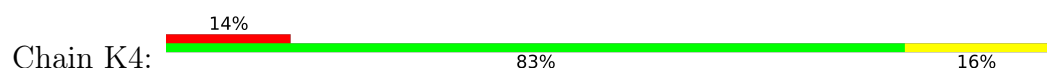
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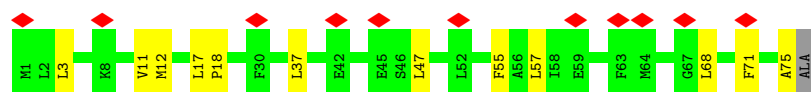


- Molecule 26: ATP synthase F0 subunit 9

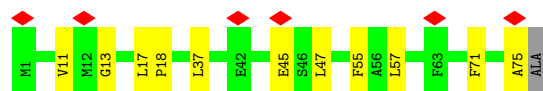
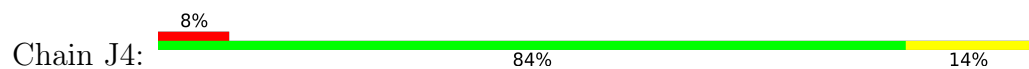


- Molecule 26: ATP synthase F0 subunit 9

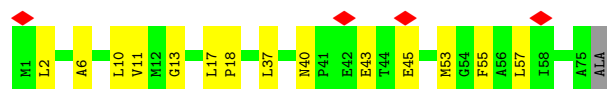
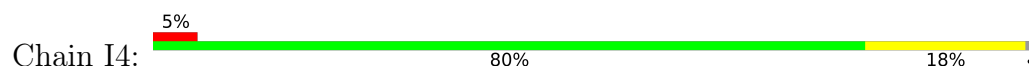




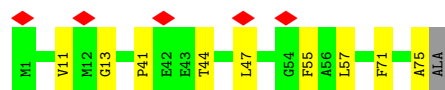
- Molecule 26: ATP synthase F0 subunit 9



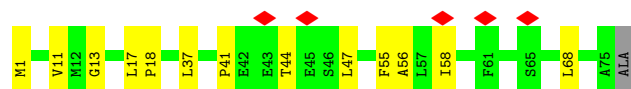
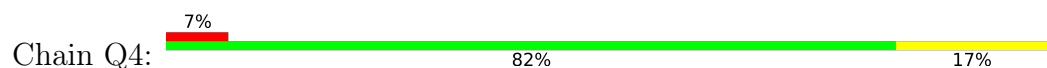
- Molecule 26: ATP synthase F0 subunit 9



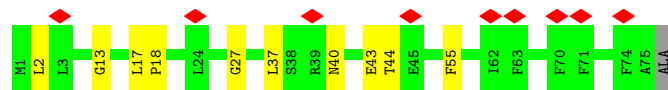
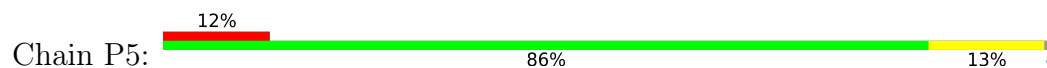
- Molecule 26: ATP synthase F0 subunit 9



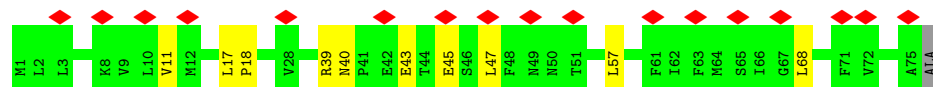
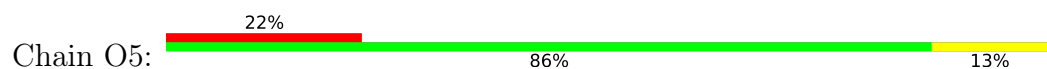
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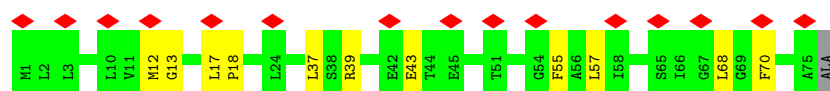
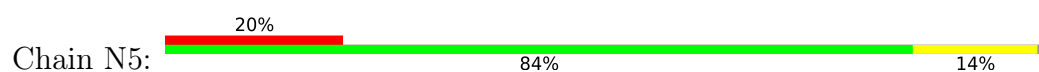
- Molecule 26: ATP synthase F0 subunit 9



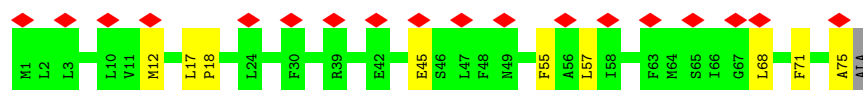
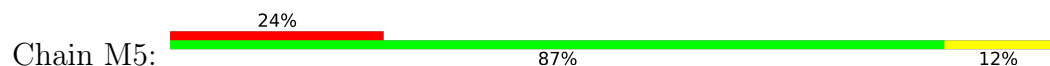
- Molecule 26: ATP synthase F0 subunit 9



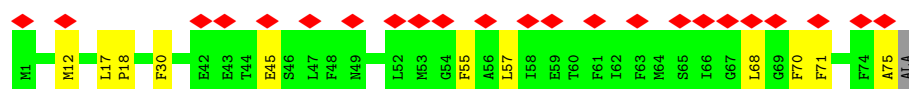
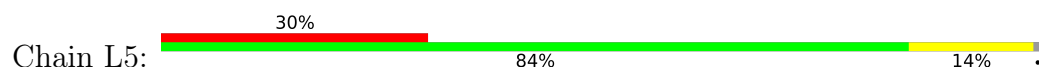
- Molecule 26: ATP synthase F0 subunit 9



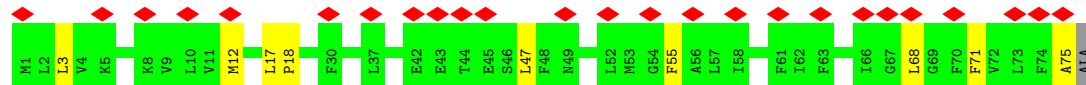
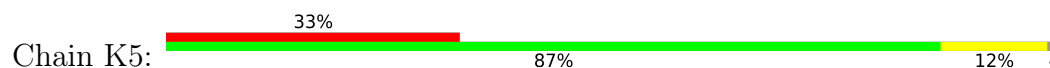
- Molecule 26: ATP synthase F0 subunit 9



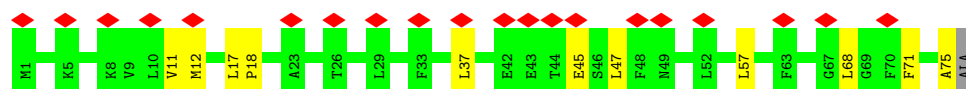
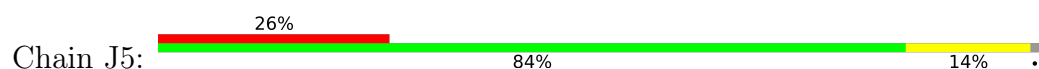
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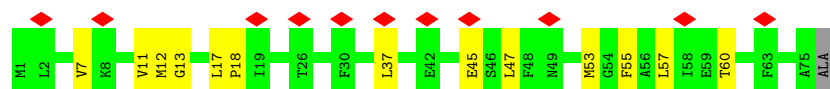
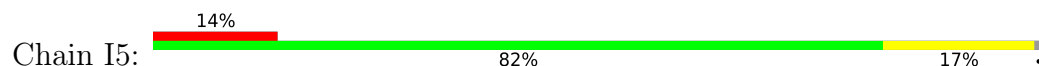
- Molecule 26: ATP synthase F0 subunit 9



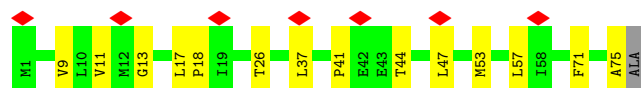
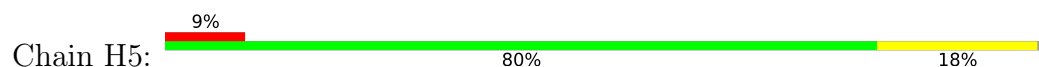
- Molecule 26: ATP synthase F0 subunit 9



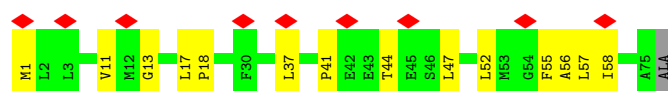
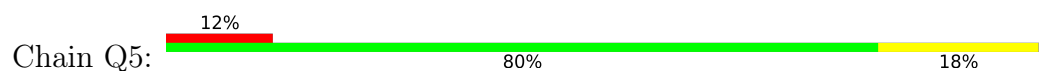
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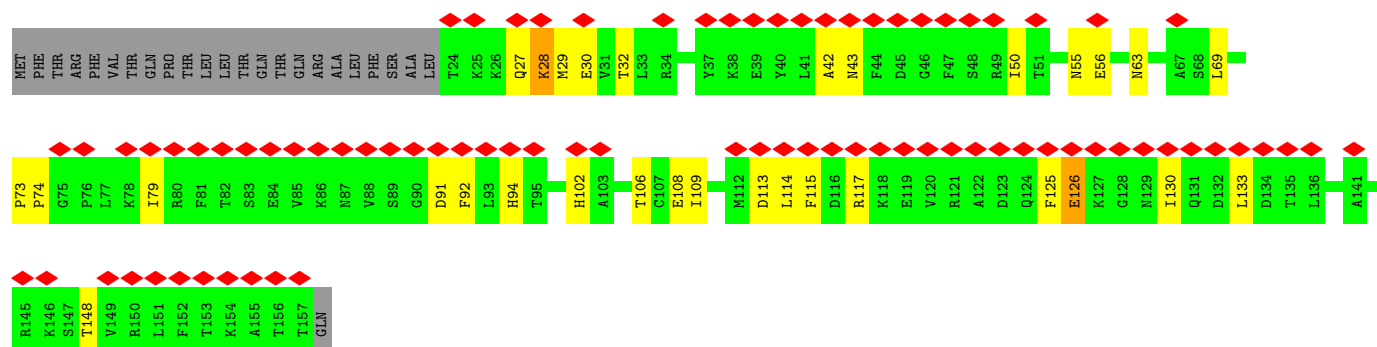
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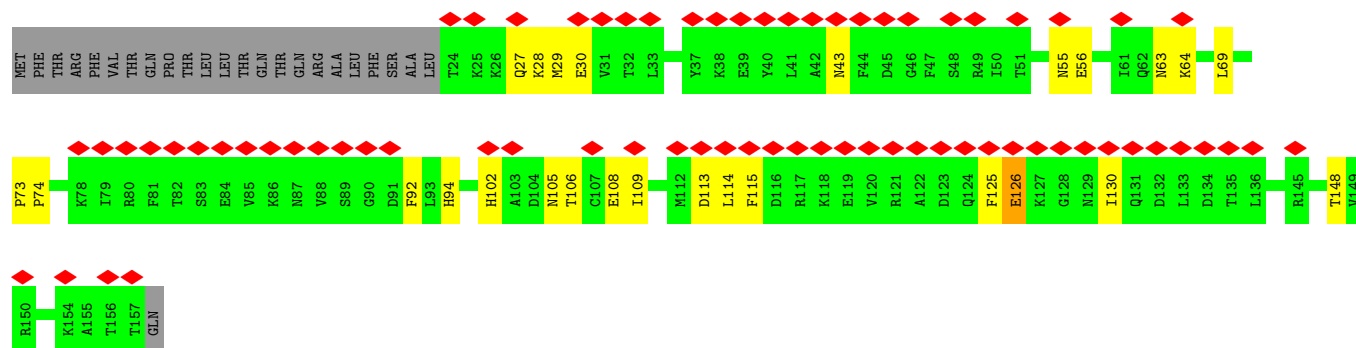
- Molecule 26: ATP synthase F0 subunit 9



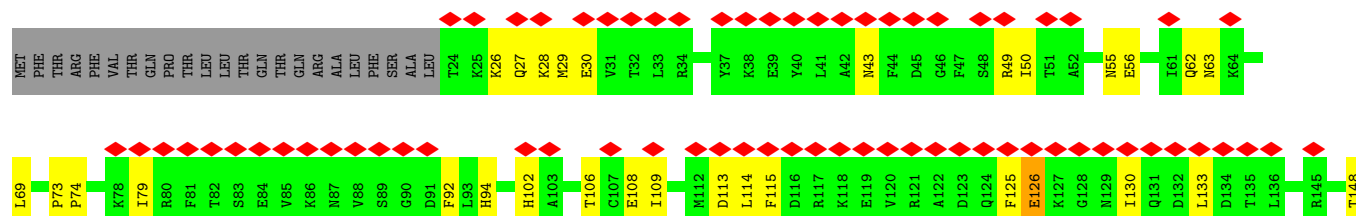
- Molecule 27: subunit delta

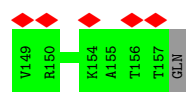


- Molecule 27: subunit delta

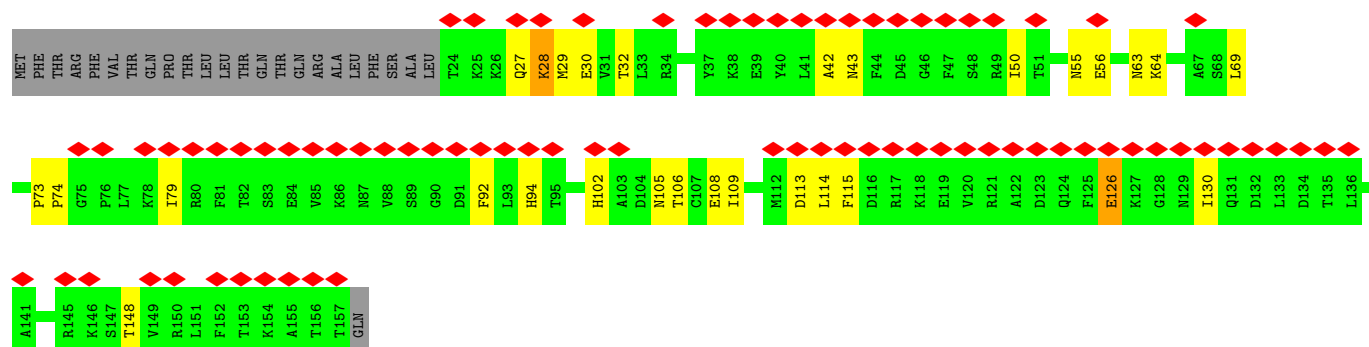


- Molecule 27: subunit delta

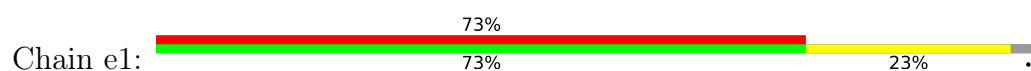




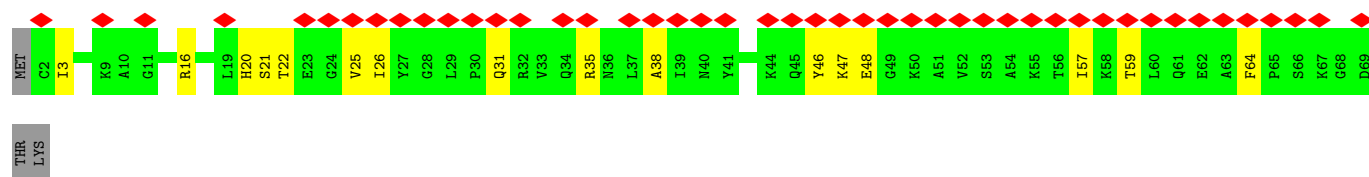
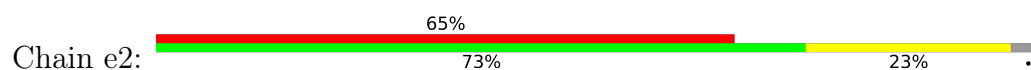
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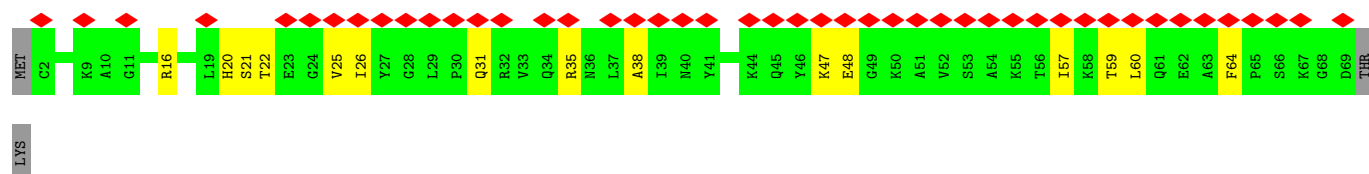
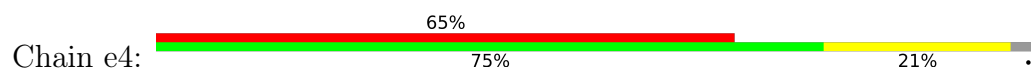
- Molecule 28: subunit epsilon



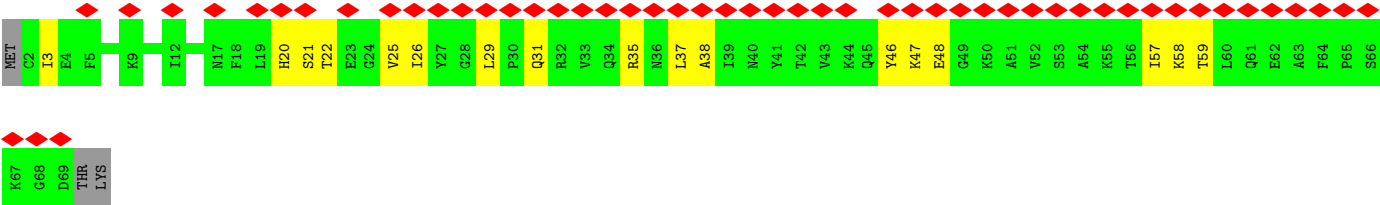
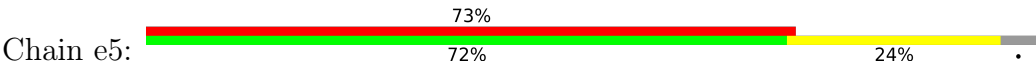
- Molecule 28: subunit epsilon



- Molecule 28: subunit epsilon



- Molecule 28: subunit epsilon



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	40691	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	0.070	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UQ8, CDL, PO4, MG, ADP, NAD, PC1, PEE, 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	0.16	0/3752	0.23	0/5109
1	A3	0.15	0/3752	0.23	0/5109
1	a	0.15	0/3752	0.23	0/5109
1	a3	0.16	0/3752	0.24	0/5109
2	B	0.13	0/2940	0.23	0/3969
2	B3	0.12	0/2940	0.22	0/3969
2	b	0.12	0/2940	0.23	0/3969
2	b3	0.13	0/2940	0.23	0/3969
3	D	0.12	0/1715	0.21	0/2321
3	D3	0.11	0/1715	0.21	0/2321
3	d	0.11	0/1715	0.21	0/2321
3	d3	0.12	0/1715	0.21	0/2321
4	F	0.18	0/1733	0.26	0/2327
4	F3	0.17	0/1733	0.27	0/2327
4	f	0.17	0/1733	0.26	0/2327
4	f3	0.18	0/1733	0.25	0/2327
5	I	0.16	0/1771	0.27	0/2394
5	I3	0.15	0/1771	0.27	0/2394
5	i	0.16	0/1771	0.28	0/2394
5	i3	0.16	0/1771	0.26	0/2394
6	K	0.11	0/1508	0.24	0/2024
6	K3	0.11	0/1508	0.24	0/2024
6	k	0.11	0/1508	0.23	0/2024
6	k3	0.11	0/1508	0.23	0/2024
7	C	0.15	0/866	0.26	0/1176
7	C3	0.14	0/866	0.25	0/1176
7	c	0.14	0/866	0.25	0/1176
7	c3	0.15	0/866	0.26	0/1176
8	G	0.12	0/2302	0.25	0/3115
8	G3	0.11	0/2302	0.25	0/3115
8	g	0.11	0/2302	0.25	0/3115
8	g3	0.12	0/2302	0.25	0/3115

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	H	0.14	0/2006	0.26	0/2704
9	H3	0.13	0/2006	0.26	0/2704
9	h	0.13	0/2006	0.25	0/2704
9	h3	0.13	0/2006	0.25	0/2704
10	J	0.16	0/2256	0.26	0/3069
10	J3	0.15	0/2256	0.25	0/3069
10	j	0.15	0/2256	0.25	0/3069
10	j3	0.16	0/2256	0.25	0/3069
11	L	0.17	0/2140	0.26	0/2903
11	L3	0.16	0/2140	0.27	0/2903
11	l	0.16	0/2140	0.27	0/2903
11	l3	0.17	0/2140	0.26	0/2903
12	M	0.16	0/1912	0.24	0/2598
12	M3	0.14	0/1912	0.24	0/2598
12	m	0.14	0/1912	0.24	0/2598
12	m3	0.15	0/1912	0.23	0/2598
13	N	0.16	0/1030	0.22	0/1393
13	N3	0.15	0/1030	0.23	0/1393
13	n	0.15	0/1030	0.23	0/1393
13	n3	0.16	0/1030	0.23	0/1393
14	O	0.13	0/821	0.22	0/1104
14	O3	0.13	0/821	0.22	0/1104
14	o	0.13	0/821	0.22	0/1104
14	o3	0.13	0/821	0.22	0/1104
15	P	0.10	0/1249	0.21	0/1695
15	P3	0.09	0/1249	0.21	0/1695
15	p	0.09	0/1249	0.21	0/1695
15	p3	0.10	0/1249	0.20	0/1695
16	Q	0.11	0/888	0.21	0/1200
16	Q3	0.09	0/888	0.21	0/1200
16	q	0.10	0/888	0.21	0/1200
16	q3	0.11	0/888	0.21	0/1200
17	R	0.15	0/1185	0.23	0/1594
17	R3	0.13	0/1185	0.23	0/1594
17	r	0.13	0/1225	0.24	0/1649
17	r3	0.15	0/1225	0.24	0/1649
18	S	0.14	0/1044	0.26	0/1414
18	S3	0.13	0/1044	0.25	0/1414
18	s	0.12	0/1037	0.25	0/1404
18	s3	0.13	0/1037	0.26	0/1404
19	E	0.09	0/3492	0.22	0/4720
19	E3	0.08	0/3492	0.21	0/4720
19	e	0.08	0/3492	0.21	0/4720

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	e3	0.09	0/3492	0.21	0/4720
20	i1	0.08	0/593	0.20	0/795
20	i2	0.07	0/563	0.19	0/753
20	i4	0.08	0/593	0.20	0/795
20	i5	0.08	0/563	0.20	0/753
21	t	0.10	0/3103	0.26	0/4200
21	t3	0.11	0/3103	0.25	0/4200
22	G1	0.07	0/1507	0.22	0/2027
22	G2	0.07	0/1507	0.21	0/2027
22	G4	0.07	0/1507	0.22	0/2027
22	G5	0.07	0/1507	0.21	0/2027
23	g1	0.07	0/2156	0.22	0/2900
23	g2	0.07	0/2156	0.21	0/2900
23	g4	0.07	0/2156	0.22	0/2900
23	g5	0.07	0/2156	0.22	0/2900
24	A1	0.07	0/3961	0.21	0/5346
24	A2	0.07	0/3961	0.21	0/5346
24	A4	0.07	0/3961	0.21	0/5346
24	A5	0.07	0/3961	0.21	0/5346
24	B1	0.07	0/3956	0.21	0/5339
24	B2	0.07	0/3956	0.21	0/5339
24	B4	0.07	0/3956	0.21	0/5339
24	B5	0.07	0/3956	0.21	0/5339
24	C1	0.07	0/3974	0.21	0/5361
24	C2	0.07	0/3974	0.21	0/5361
24	C4	0.07	0/3974	0.21	0/5361
24	C5	0.07	0/3974	0.21	0/5361
25	D1	0.07	0/3613	0.21	0/4900
25	D2	0.07	0/3613	0.21	0/4900
25	D4	0.07	0/3613	0.21	0/4900
25	D5	0.07	0/3613	0.21	0/4900
25	E1	0.07	0/3613	0.21	0/4900
25	E2	0.07	0/3613	0.21	0/4900
25	E4	0.07	0/3613	0.21	0/4900
25	E5	0.07	0/3613	0.21	0/4900
25	F1	0.07	0/3604	0.22	0/4889
25	F2	0.07	0/3604	0.21	0/4889
25	F4	0.07	0/3604	0.21	0/4889
25	F5	0.07	0/3604	0.21	0/4889
26	H1	0.09	0/572	0.20	0/771
26	H2	0.09	0/572	0.21	0/771
26	H4	0.09	0/572	0.20	0/771
26	H5	0.09	0/572	0.21	0/771

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	I1	0.09	0/572	0.21	0/771
26	I2	0.11	0/572	0.25	0/771
26	I4	0.09	0/572	0.21	0/771
26	I5	0.11	0/572	0.25	0/771
26	J1	0.08	0/572	0.19	0/771
26	J2	0.09	0/572	0.20	0/771
26	J4	0.08	0/572	0.20	0/771
26	J5	0.08	0/572	0.19	0/771
26	K1	0.07	0/572	0.19	0/771
26	K2	0.08	0/572	0.18	0/771
26	K4	0.08	0/572	0.19	0/771
26	K5	0.07	0/572	0.18	0/771
26	L1	0.07	0/572	0.18	0/771
26	L2	0.07	0/572	0.19	0/771
26	L4	0.07	0/572	0.18	0/771
26	L5	0.07	0/572	0.18	0/771
26	M1	0.07	0/572	0.18	0/771
26	M2	0.07	0/572	0.18	0/771
26	M4	0.07	0/572	0.18	0/771
26	M5	0.07	0/572	0.18	0/771
26	N1	0.07	0/572	0.18	0/771
26	N2	0.07	0/572	0.18	0/771
26	N4	0.07	0/572	0.18	0/771
26	N5	0.07	0/572	0.18	0/771
26	O1	0.07	0/572	0.19	0/771
26	O2	0.07	0/572	0.19	0/771
26	O4	0.07	0/572	0.19	0/771
26	O5	0.07	0/572	0.19	0/771
26	P1	0.08	0/572	0.19	0/771
26	P2	0.08	0/572	0.20	0/771
26	P4	0.07	0/572	0.20	0/771
26	P5	0.08	0/572	0.19	0/771
26	Q1	0.08	0/572	0.19	0/771
26	Q2	0.08	0/572	0.19	0/771
26	Q4	0.08	0/572	0.19	0/771
26	Q5	0.08	0/572	0.19	0/771
27	d1	0.09	0/1081	0.26	0/1459
27	d2	0.09	0/1081	0.26	0/1459
27	d4	0.09	0/1081	0.26	0/1459
27	d5	0.09	0/1081	0.27	0/1459
28	e1	0.08	0/547	0.24	0/735
28	e2	0.08	0/547	0.26	0/735
28	e4	0.09	0/547	0.25	0/735

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
28	e5	0.08	0/547	0.25	0/735
All	All	0.11	0/281952	0.23	0/381166

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
25	F4	0	1
25	F5	0	1
28	e2	0	1
28	e5	0	1
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	F1	364	TYR	Peptide
25	F2	364	TYR	Peptide
25	F4	364	TYR	Peptide
25	F5	364	TYR	Peptide
28	e2	46	TYR	Peptide
28	e5	46	TYR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3628	3529	3529	18	0
1	A3	3628	3529	3529	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	3628	3527	3529	31	0
1	a3	3628	3527	3529	26	0
2	B	2875	2849	2850	22	0
2	B3	2875	2849	2850	22	0
2	b	2875	2851	2851	20	0
2	b3	2875	2851	2851	17	0
3	D	1676	1598	1598	27	0
3	D3	1676	1598	1598	28	0
3	d	1676	1598	1598	25	0
3	d3	1676	1598	1598	22	0
4	F	1682	1692	1692	12	0
4	F3	1682	1692	1692	9	0
4	f	1682	1691	1691	13	0
4	f3	1682	1691	1690	10	0
5	I	1720	1740	1740	15	0
5	I3	1720	1740	1740	14	0
5	i	1720	1742	1741	16	0
5	i3	1720	1742	1741	13	0
6	K	1473	1430	1430	8	0
6	K3	1473	1430	1430	10	0
6	k	1473	1429	1429	10	0
6	k3	1473	1429	1429	11	0
7	C	841	830	830	15	0
7	C3	841	830	830	11	0
7	c	841	830	830	8	0
7	c3	841	830	830	9	0
8	G	2220	2118	2118	14	0
8	G3	2220	2118	2118	17	0
8	g	2220	2118	2119	12	0
8	g3	2220	2118	2118	11	0
9	H	1953	1883	1882	8	0
9	H3	1953	1883	1882	9	0
9	h	1953	1883	1882	20	0
9	h3	1953	1883	1882	20	0
10	J	2199	2147	2147	14	0
10	J3	2199	2147	2147	15	0
10	j	2199	2147	2147	16	0
10	j3	2199	2147	2147	15	0
11	L	2071	1999	2000	23	0
11	L3	2071	1999	2000	28	0
11	l	2071	1999	2000	25	0
11	l3	2071	1999	2000	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	M	1861	1835	1835	12	0
12	M3	1861	1835	1835	13	0
12	m	1861	1835	1835	10	0
12	m3	1861	1835	1835	11	0
13	N	998	962	962	5	0
13	N3	998	962	962	10	0
13	n	998	962	962	7	0
13	n3	998	962	962	4	0
14	O	805	794	794	0	0
14	O3	805	794	794	0	0
14	o	805	794	794	3	0
14	o3	805	794	794	2	0
15	P	1217	1196	1196	4	0
15	P3	1217	1196	1196	4	0
15	p	1217	1196	1196	6	0
15	p3	1217	1196	1196	6	0
16	Q	875	874	874	9	0
16	Q3	875	874	874	10	0
16	q	875	874	874	10	0
16	q3	875	874	874	8	0
17	R	1154	1134	1134	11	0
17	R3	1154	1134	1134	9	0
17	r	1193	1180	1180	12	0
17	r3	1193	1180	1180	13	0
18	S	1023	1016	1016	17	0
18	S3	1023	1016	1016	17	0
18	s	1016	1009	1009	21	0
18	s3	1016	1009	1009	23	0
19	E	3395	3286	3285	25	0
19	E3	3395	3286	3285	23	0
19	e	3395	3286	3285	20	0
19	e3	3395	3286	3285	25	0
20	i1	585	582	582	9	0
20	i2	556	556	556	4	0
20	i4	585	582	582	6	0
20	i5	556	556	556	3	0
21	t	3013	2876	2876	46	0
21	t3	3013	2876	2876	46	0
22	G1	1485	1515	1515	18	0
22	G2	1485	1515	1515	15	0
22	G4	1485	1515	1515	18	0
22	G5	1485	1515	1515	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	g1	2126	2206	2206	24	0
23	g2	2126	2206	2206	26	0
23	g4	2126	2206	2206	27	0
23	g5	2126	2206	2206	22	0
24	A1	3909	4037	4037	45	0
24	A2	3909	4037	4037	39	0
24	A4	3909	4037	4037	39	0
24	A5	3909	4037	4037	37	0
24	B1	3904	4030	4030	39	0
24	B2	3904	4030	4030	38	0
24	B4	3904	4030	4030	38	0
24	B5	3904	4030	4030	33	0
24	C1	3922	4058	4058	31	0
24	C2	3922	4058	4058	30	0
24	C4	3922	4058	4058	29	0
24	C5	3922	4058	4058	33	0
25	D1	3554	3581	3581	30	0
25	D2	3554	3581	3581	31	0
25	D4	3554	3581	3581	29	0
25	D5	3554	3581	3581	33	0
25	E1	3554	3581	3581	38	0
25	E2	3554	3581	3581	37	0
25	E4	3554	3581	3581	37	0
25	E5	3554	3581	3581	42	0
25	F1	3545	3568	3568	41	0
25	F2	3545	3568	3568	43	0
25	F4	3545	3568	3568	42	0
25	F5	3545	3568	3568	38	0
26	H1	561	587	587	16	0
26	H2	561	587	587	13	0
26	H4	561	587	587	11	0
26	H5	561	587	587	13	0
26	I1	561	587	587	14	0
26	I2	561	587	587	24	0
26	I4	561	587	587	14	0
26	I5	561	587	587	19	0
26	J1	561	587	587	6	0
26	J2	561	587	587	13	0
26	J4	561	587	587	10	0
26	J5	561	587	587	10	0
26	K1	561	587	587	8	0
26	K2	561	587	587	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	K4	561	587	587	11	0
26	K5	561	587	587	9	0
26	L1	561	587	587	14	0
26	L2	561	587	587	13	0
26	L4	561	587	587	14	0
26	L5	561	587	587	11	0
26	M1	561	587	587	14	0
26	M2	561	587	587	10	0
26	M4	561	587	587	13	0
26	M5	561	587	587	9	0
26	N1	561	587	587	9	0
26	N2	561	587	587	11	0
26	N4	561	587	587	10	0
26	N5	561	587	587	12	0
26	O1	561	587	587	13	0
26	O2	561	587	587	8	0
26	O4	561	587	587	9	0
26	O5	561	587	587	9	0
26	P1	561	587	587	8	0
26	P2	561	587	587	11	0
26	P4	561	587	587	8	0
26	P5	561	587	587	11	0
26	Q1	561	587	587	17	0
26	Q2	561	587	587	17	0
26	Q4	561	587	587	15	0
26	Q5	561	587	587	15	0
27	d1	1062	1082	1082	27	0
27	d2	1062	1082	1082	23	0
27	d4	1062	1082	1082	25	0
27	d5	1062	1082	1082	25	0
28	e1	537	559	559	13	0
28	e2	537	559	559	11	0
28	e4	537	559	559	12	0
28	e5	537	559	559	11	0
29	A	100	156	156	0	0
29	A3	100	156	156	1	0
29	B	400	624	624	8	0
29	B3	400	624	624	8	0
29	F	200	312	312	14	0
29	F3	100	156	156	2	0
29	I	200	312	312	3	0
29	I3	300	468	468	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	J	200	312	312	0	0
29	J3	200	312	312	0	0
29	K	200	312	312	1	0
29	K3	200	312	312	2	0
29	L	200	312	312	8	0
29	L3	100	156	156	1	0
29	P	100	156	156	0	0
29	P3	100	156	156	0	0
29	a	100	156	156	2	0
29	a3	200	312	312	14	0
29	b	100	156	156	1	0
29	b3	100	156	156	1	0
29	f	300	468	468	4	0
29	f3	300	468	468	2	0
29	g	100	156	156	1	0
29	g3	100	156	156	1	0
29	i	100	156	156	0	0
29	i3	200	312	312	2	0
29	j	200	312	312	0	0
29	j3	200	312	312	0	0
29	k	100	156	156	1	0
29	k3	100	156	156	1	0
29	l	200	312	312	7	0
29	l3	200	312	312	7	0
29	p	100	156	156	0	0
29	p3	100	156	156	0	0
29	r	100	156	156	1	0
30	D	54	88	88	0	0
30	D3	54	88	88	1	0
30	G	108	176	176	1	0
30	G3	108	176	176	1	0
30	d	54	88	88	0	0
30	d3	54	88	88	0	0
30	g	108	176	176	0	0
30	g3	108	176	176	0	0
31	F	5	0	0	0	0
31	F3	5	0	0	0	0
31	f	5	0	0	1	0
31	f3	5	0	0	0	0
32	I	53	74	74	8	0
32	I3	53	74	74	7	0
32	i	53	74	74	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	i3	53	74	74	5	0
33	A1	31	11	12	1	0
33	A2	31	11	12	0	0
33	A4	31	11	12	0	0
33	A5	31	11	12	0	0
33	B1	31	11	12	2	0
33	B2	31	11	12	2	0
33	B4	31	11	12	2	0
33	B5	31	11	12	2	0
33	C1	31	11	12	0	0
33	C2	31	11	12	1	0
33	C4	31	11	12	0	0
33	C5	31	11	12	1	0
33	G	31	11	12	1	0
33	G3	31	11	12	2	0
33	g	31	11	12	1	0
33	g3	31	11	12	1	0
34	A1	1	0	0	0	0
34	A2	1	0	0	0	0
34	A4	1	0	0	0	0
34	A5	1	0	0	0	0
34	B1	1	0	0	0	0
34	B2	1	0	0	0	0
34	B4	1	0	0	0	0
34	B5	1	0	0	0	0
34	C1	1	0	0	0	0
34	C2	1	0	0	0	0
34	C4	1	0	0	0	0
34	C5	1	0	0	0	0
34	D1	1	0	0	0	0
34	D2	1	0	0	0	0
34	D4	1	0	0	0	0
34	D5	1	0	0	0	0
34	E1	1	0	0	0	0
34	E2	1	0	0	0	0
34	E4	1	0	0	0	0
34	E5	1	0	0	0	0
34	G	1	0	0	0	0
34	G3	1	0	0	0	0
34	g	1	0	0	0	0
34	g3	1	0	0	0	0
35	A	48	75	73	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	J	51	82	82	1	0
35	L	48	75	73	1	0
35	L3	51	82	82	0	0
35	a3	48	75	73	1	0
35	j3	51	82	82	0	0
35	l3	48	75	73	0	0
35	m	51	82	82	0	0
36	E	44	26	25	1	0
36	E3	44	26	25	0	0
36	e	44	26	25	0	0
36	e3	44	26	25	2	0
37	B1	27	11	12	0	0
37	B2	27	11	12	0	0
37	B4	27	11	12	0	0
37	B5	27	11	12	0	0
37	D1	27	11	11	2	0
37	D2	27	11	11	0	0
37	D4	27	11	11	0	0
37	D5	27	11	11	0	0
All	All	284056	287810	287818	2332	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (2332) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:s3:36:VAL:O	21:t3:407:ARG:NH2	2.00	0.94
26:H2:47:LEU:HD23	26:Q2:37:LEU:HD23	1.52	0.91
18:s:36:VAL:O	21:t:407:ARG:NH2	2.08	0.87
1:a3:374:ILE:O	11:L3:128:TYR:OH	1.94	0.86
24:B2:289:ARG:NH1	24:B2:339:ARG:O	2.09	0.86
26:H5:47:LEU:HD23	26:Q5:37:LEU:HD23	1.55	0.86
11:l:128:TYR:OH	1:A:374:ILE:O	1.92	0.85
21:t3:226:SER:OG	21:t3:229:SER:OG	1.94	0.85
21:t:185:ASP:OD1	21:t:188:ARG:NH1	2.09	0.85
19:e3:58:ASP:OD2	19:e3:360:ARG:NH1	2.09	0.85
21:t3:417:ASP:OD2	21:t3:422:ARG:NH1	2.10	0.85
21:t:173:ARG:NH1	21:t:296:ASN:O	2.11	0.84
24:B4:289:ARG:NH1	24:B4:339:ARG:O	2.10	0.84
21:t:417:ASP:OD2	21:t:422:ARG:NH1	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:p3:88:VAL:O	15:p3:92:SER:OG	1.96	0.84
11:l3:128:TYR:OH	1:A3:374:ILE:O	1.94	0.84
24:B5:159:ARG:NH2	25:E5:86:GLU:OE1	2.11	0.84
1:a:374:ILE:O	11:L:128:TYR:OH	1.96	0.84
24:B1:159:ARG:NH2	25:E1:86:GLU:OE1	2.11	0.84
21:t3:185:ASP:OD1	21:t3:188:ARG:NH1	2.11	0.83
24:B4:159:ARG:NH2	25:E4:86:GLU:OE1	2.11	0.83
21:t:226:SER:OG	21:t:229:SER:OG	1.95	0.83
28:e1:31:GLN:OE1	28:e1:35:ARG:NH1	2.12	0.82
24:B2:159:ARG:NH2	25:E2:86:GLU:OE1	2.12	0.82
21:t3:173:ARG:NH1	21:t3:296:ASN:O	2.13	0.82
24:C4:289:ARG:NH1	24:C4:339:ARG:O	2.12	0.82
26:P4:37:LEU:HD11	26:P4:44:THR:HG22	1.61	0.82
28:e5:31:GLN:OE1	28:e5:35:ARG:NH1	2.12	0.81
24:B5:289:ARG:NH1	24:B5:339:ARG:O	2.12	0.81
2:B:140:SER:OG	4:F:159:TRP:O	1.98	0.81
23:g5:215:THR:OG1	26:O5:39:ARG:O	1.98	0.81
24:B2:240:LYS:NZ	25:F2:349:ASP:OD1	2.14	0.81
19:e:58:ASP:OD2	19:e:360:ARG:NH1	2.13	0.81
24:B1:289:ARG:NH1	24:B1:339:ARG:O	2.13	0.81
26:P1:37:LEU:HD11	26:P1:44:THR:HG22	1.61	0.80
19:E3:58:ASP:OD2	19:E3:360:ARG:NH1	2.15	0.80
24:B4:240:LYS:NZ	25:F4:349:ASP:OD1	2.13	0.80
19:E:58:ASP:OD2	19:E:360:ARG:NH1	2.15	0.80
4:f:76:ARG:NH1	29:f:303:CDL:OB4	2.14	0.80
24:C2:289:ARG:NH1	24:C2:339:ARG:O	2.15	0.80
24:A4:436:GLN:NE2	25:E4:419:ASP:OD2	2.15	0.80
4:f3:76:ARG:NH1	29:f3:303:CDL:OB4	2.14	0.79
28:e4:31:GLN:OE1	28:e4:35:ARG:NH1	2.14	0.79
2:B3:140:SER:OG	4:F3:159:TRP:O	1.99	0.79
24:A2:436:GLN:NE2	25:E2:419:ASP:OD2	2.16	0.79
25:D4:415:LEU:O	25:D4:420:LYS:NZ	2.16	0.79
28:e2:31:GLN:OE1	28:e2:35:ARG:NH1	2.15	0.79
21:t3:158:ARG:NH2	21:t3:394:LEU:O	2.16	0.79
27:d1:30:GLU:OE1	27:d1:43:ASN:ND2	2.16	0.79
15:p:88:VAL:O	15:p:92:SER:OG	2.01	0.78
24:C1:289:ARG:NH1	24:C1:339:ARG:O	2.17	0.78
25:F2:275:ASP:OD2	25:F2:279:ARG:NH2	2.17	0.78
25:F4:131:LYS:NZ	25:F4:265:GLU:OE2	2.17	0.78
25:E5:425:ARG:NH1	25:E5:464:LEU:O	2.17	0.78
25:D2:415:LEU:O	25:D2:420:LYS:NZ	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:c:61:SER:OG	7:c:63:GLU:OE1	2.02	0.78
9:h:229:LYS:NZ	18:s:24:TRP:O	2.17	0.78
23:g2:215:THR:OG1	26:O2:39:ARG:O	2.01	0.78
24:B5:170:ARG:NH2	24:B5:338:GLU:O	2.17	0.78
5:i3:43:GLU:OE2	9:h3:267:THR:OG1	1.99	0.77
29:I3:301:CDL:O1	17:R3:31:GLU:OE1	2.01	0.77
24:C2:461:GLN:NE2	24:C2:465:THR:O	2.17	0.77
24:C4:461:GLN:NE2	24:C4:465:THR:O	2.18	0.77
24:A2:218:LYS:NZ	24:A2:254:HIS:O	2.18	0.77
25:F2:131:LYS:NZ	25:F2:265:GLU:OE2	2.18	0.77
25:D1:415:LEU:O	25:D1:420:LYS:NZ	2.18	0.77
24:B5:240:LYS:NZ	25:F5:349:ASP:OD1	2.18	0.76
24:B5:241:ARG:NH1	25:F5:140:PRO:O	2.18	0.76
25:F4:275:ASP:OD2	25:F4:279:ARG:NH2	2.18	0.76
25:D5:415:LEU:O	25:D5:420:LYS:NZ	2.19	0.76
24:C5:289:ARG:NH1	24:C5:339:ARG:O	2.19	0.76
25:F5:425:ARG:NH2	25:F5:464:LEU:O	2.19	0.76
24:A5:218:LYS:NZ	24:A5:254:HIS:O	2.19	0.76
25:F2:425:ARG:NH2	25:F2:464:LEU:O	2.19	0.76
25:D5:157:LYS:NZ	25:D5:479:LYS:O	2.14	0.75
25:F5:275:ASP:OD2	25:F5:279:ARG:NH2	2.19	0.75
12:m:49:MET:O	12:m:217:GLN:NE2	2.19	0.75
25:F4:425:ARG:NH2	25:F4:464:LEU:O	2.19	0.75
8:g:41:ASN:N	16:q:152:ALA:O	2.19	0.75
20:i5:87:ARG:NH1	20:i4:99:GLU:OE1	2.20	0.75
24:B4:170:ARG:NH2	24:B4:338:GLU:O	2.19	0.75
20:i2:87:ARG:NH1	20:i1:99:GLU:OE1	2.20	0.75
29:I:301:CDL:O1	17:R:31:GLU:OE1	2.02	0.75
25:F1:275:ASP:OD2	25:F1:279:ARG:NH2	2.19	0.75
24:B2:170:ARG:NH2	24:B2:338:GLU:O	2.20	0.75
24:C5:461:GLN:NE2	24:C5:465:THR:O	2.19	0.75
8:g3:107:ASN:OD1	8:g3:142:ARG:NH1	2.20	0.75
10:J:213:ARG:NH2	10:J:216:THR:O	2.20	0.75
25:E1:425:ARG:NH1	25:E1:464:LEU:O	2.20	0.75
24:C2:241:ARG:NH1	25:D2:140:PRO:O	2.20	0.75
7:c3:61:SER:OG	7:c3:63:GLU:OE1	2.03	0.75
12:M3:49:MET:O	12:M3:217:GLN:NE2	2.19	0.74
8:g:107:ASN:OD1	8:g:142:ARG:NH1	2.20	0.74
8:G3:107:ASN:OD1	8:G3:142:ARG:NH1	2.20	0.74
9:h:250:ASP:OD2	17:r:20:ARG:NH1	2.21	0.74
9:H:250:ASP:OD2	18:S:49:ARG:NH2	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:t:335:TYR:O	21:t:373:ASN:ND2	2.20	0.74
24:B1:241:ARG:NH1	25:F1:140:PRO:O	2.21	0.74
3:D3:145:ASP:OD2	7:C3:76:LYS:NZ	2.19	0.74
24:A5:436:GLN:NE2	25:E5:419:ASP:OD2	2.20	0.74
2:b:169:ARG:NH2	29:b:401:CDL:OB3	2.20	0.74
8:G:107:ASN:OD1	8:G:142:ARG:NH1	2.20	0.74
2:b3:112:ARG:NH2	29:f3:303:CDL:OA4	2.21	0.74
4:f:50:ARG:NH1	21:t:215:CYS:O	2.21	0.74
24:B1:240:LYS:NZ	25:F1:349:ASP:OD1	2.21	0.74
24:B4:241:ARG:NH1	25:F4:140:PRO:O	2.21	0.74
27:d4:30:GLU:OE1	27:d4:43:ASN:ND2	2.21	0.74
24:B2:241:ARG:NH1	25:F2:140:PRO:O	2.20	0.74
26:J1:45:GLU:N	26:J1:45:GLU:OE1	2.21	0.73
10:j3:213:ARG:NH2	10:j3:216:THR:O	2.20	0.73
24:A5:114:LYS:NZ	25:E5:48:LEU:O	2.21	0.73
24:A4:182:LYS:NZ	24:A4:458:MET:O	2.16	0.73
24:A4:294:HIS:HD1	24:A4:351:SER:HG	1.34	0.73
11:l:193:ARG:NH1	17:r:108:ASP:OD2	2.21	0.73
12:m:14:ARG:NH1	13:n:113:GLU:OE2	2.20	0.73
25:D2:157:LYS:NZ	25:D2:479:LYS:O	2.15	0.73
21:t3:135:GLU:OE1	21:t3:136:ALA:N	2.22	0.73
26:Q5:37:LEU:HD11	26:Q5:44:THR:HG22	1.70	0.73
12:M3:14:ARG:NH1	13:N3:113:GLU:OE2	2.21	0.73
24:C1:218:LYS:NZ	24:C1:254:HIS:O	2.22	0.73
25:D4:157:LYS:NZ	25:D4:479:LYS:O	2.16	0.73
22:G1:145:GLU:OE1	22:G1:145:GLU:N	2.22	0.73
24:B1:170:ARG:NH2	24:B1:338:GLU:O	2.22	0.73
24:A2:182:LYS:NZ	24:A2:458:MET:O	2.21	0.73
24:C1:461:GLN:NE2	24:C1:465:THR:O	2.21	0.73
2:b3:343:SER:O	2:b3:347:ASN:ND2	2.22	0.73
9:h3:225:HIS:NE2	18:s3:27:LEU:O	2.21	0.73
26:L4:45:GLU:N	26:L4:45:GLU:OE1	2.21	0.72
26:J4:45:GLU:OE1	26:J4:45:GLU:N	2.21	0.72
27:d5:30:GLU:OE1	27:d5:43:ASN:ND2	2.21	0.72
22:G4:145:GLU:OE1	22:G4:145:GLU:N	2.22	0.72
26:L5:45:GLU:OE1	26:L5:45:GLU:N	2.23	0.72
12:m3:49:MET:O	12:m3:217:GLN:NE2	2.22	0.72
22:G5:145:GLU:N	22:G5:145:GLU:OE1	2.21	0.72
26:L1:45:GLU:OE1	26:L1:45:GLU:N	2.21	0.72
26:L2:45:GLU:OE1	26:L2:45:GLU:N	2.23	0.72
16:q3:63:LYS:NZ	16:q3:66:ASP:OD1	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A4:378:ASP:O	24:A4:404:ARG:NH1	2.22	0.72
12:M:49:MET:O	12:M:217:GLN:NE2	2.22	0.72
29:l:302:CDL:H812	26:I1:10:LEU:HD11	1.70	0.72
2:b3:169:ARG:NH2	29:b3:401:CDL:OB3	2.23	0.72
25:D2:207:GLU:OE2	25:D2:276:ASN:ND2	2.22	0.72
2:B:343:SER:O	2:B:347:ASN:ND2	2.22	0.71
22:G2:145:GLU:N	22:G2:145:GLU:OE1	2.22	0.71
11:l3:200:ARG:NH2	17:r3:88:ASN:OD1	2.23	0.71
24:C5:241:ARG:NH1	25:D5:140:PRO:O	2.21	0.71
8:g3:41:ASN:N	16:q3:152:ALA:O	2.24	0.71
26:I1:45:GLU:OE1	26:I1:45:GLU:N	2.23	0.71
2:B:329:GLU:OE1	24:A1:35:SER:OG	2.08	0.71
24:A2:454:ARG:NH2	24:A2:487:LEU:O	2.23	0.71
23:g5:218:GLU:OE1	26:N5:39:ARG:NE	2.22	0.71
11:l:66:GLU:OE2	11:l:69:ARG:NH1	2.23	0.71
3:D:145:ASP:OD2	7:C:76:LYS:NZ	2.24	0.71
2:B3:329:GLU:OE1	24:A4:35:SER:OG	2.07	0.71
23:g2:79:GLU:O	23:g2:83:GLN:NE2	2.23	0.71
11:L:33:SER:OG	11:L:35:ASP:OD1	2.05	0.71
8:g3:47:LYS:NZ	8:g3:151:ASP:OD2	2.16	0.71
10:J3:54:SER:O	11:L3:94:ARG:NH1	2.23	0.71
24:A4:218:LYS:NZ	24:A4:254:HIS:O	2.24	0.71
25:E4:415:LEU:O	25:E4:420:LYS:NZ	2.23	0.71
11:L3:33:SER:OG	11:L3:35:ASP:OD1	2.06	0.70
9:H:244:PRO:O	21:t:241:LYS:NZ	2.18	0.70
24:C2:517:SER:OG	24:C2:519:ASP:OD1	2.08	0.70
25:F4:54:ALA:O	25:F4:97:THR:OG1	2.04	0.70
10:J:54:SER:O	11:L:94:ARG:NH1	2.24	0.70
24:C2:156:GLN:OE1	24:C2:156:GLN:N	2.23	0.70
27:d2:126:GLU:OE1	27:d2:126:GLU:N	2.24	0.70
2:B3:343:SER:O	2:B3:347:ASN:ND2	2.23	0.70
24:A1:294:HIS:HD1	24:A1:351:SER:HG	1.38	0.70
7:c3:66:ARG:NH1	18:s3:69:ASP:OD1	2.24	0.70
24:C4:156:GLN:OE1	24:C4:156:GLN:N	2.23	0.70
24:B4:107:LEU:HD13	24:B4:142:LEU:HD21	1.73	0.70
2:b:343:SER:O	2:b:347:ASN:ND2	2.24	0.70
24:A2:378:ASP:O	24:A2:404:ARG:NH1	2.25	0.70
24:C5:156:GLN:OE1	24:C5:156:GLN:N	2.23	0.70
27:d5:126:GLU:OE1	27:d5:126:GLU:N	2.24	0.70
23:g1:79:GLU:O	23:g1:83:GLN:NE2	2.24	0.70
25:E1:415:LEU:O	25:E1:420:LYS:NZ	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d2:30:GLU:OE1	27:d2:43:ASN:ND2	2.25	0.70
27:d4:28:LYS:O	27:d4:63:ASN:ND2	2.24	0.70
24:A1:378:ASP:O	24:A1:404:ARG:NH1	2.25	0.70
26:I4:45:GLU:OE1	26:I4:45:GLU:N	2.23	0.70
23:g5:79:GLU:O	23:g5:83:GLN:NE2	2.24	0.70
23:g2:218:GLU:OE1	26:N2:39:ARG:NE	2.25	0.70
10:j3:54:SER:O	11:l3:94:ARG:NH1	2.24	0.70
19:e3:239:PHE:N	19:e3:247:ASP:OD2	2.24	0.70
12:M3:3:ASN:ND2	12:M3:40:GLU:OE2	2.25	0.70
21:t3:335:TYR:O	21:t3:373:ASN:ND2	2.25	0.70
24:B5:208:ALA:N	33:B5:1003:ATP:O2A	2.25	0.70
24:A5:454:ARG:NH2	24:A5:487:LEU:O	2.24	0.70
26:I1:40:ASN:ND2	26:I1:43:GLU:OE2	2.24	0.70
26:J2:57:LEU:HD23	26:I2:55:PHE:CD2	2.26	0.70
9:h3:229:LYS:NZ	18:s3:24:TRP:O	2.24	0.70
24:A5:378:ASP:O	24:A5:404:ARG:NH1	2.25	0.70
24:C2:218:LYS:NZ	24:C2:254:HIS:O	2.25	0.70
19:e3:426:GLY:O	19:e3:430:LYS:NZ	2.17	0.70
10:J:150:ASP:OD1	17:R:142:ARG:NH2	2.25	0.69
7:C3:66:ARG:NH1	18:S3:69:ASP:OD1	2.25	0.69
24:C5:218:LYS:NZ	24:C5:254:HIS:O	2.25	0.69
21:t:135:GLU:OE1	21:t:136:ALA:N	2.24	0.69
21:t:253:ILE:HD11	21:t:263:VAL:HG22	1.72	0.69
24:C1:156:GLN:OE1	24:C1:156:GLN:N	2.24	0.69
11:L3:44:VAL:HG21	26:K5:3:LEU:HB2	1.74	0.69
25:D4:176:GLY:O	25:D4:181:LYS:NZ	2.25	0.69
26:O4:40:ASN:ND2	26:O4:43:GLU:OE2	2.25	0.69
19:E3:85:GLN:OE1	19:E3:420:TYR:OH	2.09	0.69
23:g4:79:GLU:O	23:g4:83:GLN:NE2	2.24	0.69
9:h3:250:ASP:OD2	17:r3:20:ARG:NH1	2.26	0.69
25:E4:207:GLU:OE2	25:E4:276:ASN:ND2	2.25	0.69
7:C:66:ARG:NH1	18:S:69:ASP:OD1	2.24	0.69
23:g1:215:THR:OG1	26:O1:39:ARG:O	2.09	0.69
24:A1:436:GLN:NE2	25:E1:419:ASP:OD2	2.26	0.69
2:b:112:ARG:NH2	29:f:303:CDL:OA4	2.26	0.69
24:B1:208:ALA:N	33:B1:1003:ATP:O2A	2.24	0.69
25:E1:207:GLU:OE2	25:E1:276:ASN:ND2	2.25	0.69
6:k3:146:ASN:OD1	6:k3:150:GLN:NE2	2.25	0.69
27:d4:126:GLU:N	27:d4:126:GLU:OE1	2.25	0.69
10:j:54:SER:O	11:l:94:ARG:NH1	2.25	0.69
25:F1:131:LYS:NZ	25:F1:265:GLU:OE2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:H2:57:LEU:HD23	26:Q2:55:PHE:CE2	2.28	0.69
24:B4:378:ASP:OD2	25:E4:210:ARG:NE	2.26	0.69
26:H5:57:LEU:HD23	26:Q5:55:PHE:CE2	2.28	0.69
8:G:47:LYS:NZ	8:G:151:ASP:OD2	2.18	0.69
24:C4:218:LYS:NZ	24:C4:254:HIS:O	2.25	0.69
25:F4:363:ILE:HG22	25:F4:365:PRO:HD2	1.74	0.69
25:E4:176:GLY:O	25:E4:181:LYS:NZ	2.26	0.69
26:J5:45:GLU:OE1	26:J5:45:GLU:N	2.26	0.69
10:j:213:ARG:NH2	10:j:216:THR:O	2.26	0.69
29:I3:303:CDL:H812	26:I4:10:LEU:HD11	1.73	0.69
27:d1:126:GLU:N	27:d1:126:GLU:OE1	2.25	0.68
25:F5:131:LYS:NZ	25:F5:265:GLU:OE2	2.22	0.68
24:B1:107:LEU:HD13	24:B1:142:LEU:HD21	1.73	0.68
11:l:193:ARG:NH2	17:r:106:THR:O	2.27	0.68
24:B2:208:ALA:N	33:B2:1003:ATP:O2A	2.25	0.68
26:O2:40:ASN:ND2	26:O2:43:GLU:OE2	2.26	0.68
26:J2:45:GLU:OE1	26:J2:45:GLU:N	2.27	0.68
24:B5:165:PRO:O	24:B5:170:ARG:NH1	2.25	0.68
8:g:153:LYS:NZ	33:g:301:ATP:O1A	2.25	0.68
29:B:402:CDL:OB7	4:F:104:LYS:NZ	2.25	0.68
25:F2:363:ILE:HG22	25:F2:365:PRO:HD2	1.76	0.68
10:J3:213:ARG:NH2	10:J3:216:THR:O	2.26	0.68
1:A:211:ASP:OD2	3:D:198:ARG:NH2	2.26	0.68
24:A1:218:LYS:NZ	24:A1:254:HIS:O	2.26	0.68
2:B3:188:GLU:OE2	21:t3:311:ALA:N	2.27	0.68
10:j3:194:ARG:NH1	12:m3:191:ASP:OD1	2.27	0.68
24:C5:517:SER:OG	24:C5:519:ASP:OD1	2.10	0.68
9:h:225:HIS:NE2	18:s:27:LEU:O	2.26	0.68
25:E2:425:ARG:NH1	25:E2:464:LEU:O	2.27	0.68
25:D2:176:GLY:O	25:D2:181:LYS:NZ	2.25	0.68
2:b3:329:GLU:OE1	24:A5:35:SER:OG	2.12	0.68
24:C1:241:ARG:NH1	25:D1:140:PRO:O	2.27	0.68
27:d1:28:LYS:O	27:d1:63:ASN:ND2	2.27	0.68
24:B2:165:PRO:O	24:B2:170:ARG:NH1	2.27	0.68
26:Q2:37:LEU:HD11	26:Q2:44:THR:HG22	1.74	0.68
25:F1:54:ALA:O	25:F1:97:THR:OG1	2.07	0.68
25:F1:363:ILE:HG22	25:F1:365:PRO:HD2	1.74	0.68
4:F3:2:SER:N	4:F3:5:GLU:OE1	2.27	0.68
24:C4:241:ARG:NH1	25:D4:140:PRO:O	2.27	0.68
26:Q1:37:LEU:HD11	26:Q1:44:THR:HG22	1.74	0.67
23:g4:215:THR:OG1	26:O4:39:ARG:O	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j3:147:GLU:N	10:j3:147:GLU:OE1	2.27	0.67
24:C5:186:SER:O	24:C5:410:GLN:NE2	2.26	0.67
6:k:125:SER:HA	26:P2:2:LEU:HD12	1.77	0.67
19:e:85:GLN:OE1	19:e:420:TYR:OH	2.12	0.67
4:f3:50:ARG:NH1	21:t3:215:CYS:O	2.28	0.67
9:h3:218:ARG:NH2	9:h3:221:GLU:OE2	2.27	0.67
25:D5:207:GLU:OE2	25:D5:276:ASN:ND2	2.27	0.67
6:k3:41:ASP:OD2	8:g3:242:ARG:NH1	2.27	0.67
25:E5:177:ALA:O	25:E5:356:ARG:NH2	2.26	0.67
7:c:66:ARG:NH1	18:s:69:ASP:OD1	2.26	0.67
2:B3:169:ARG:NH2	29:B3:402:CDL:OB3	2.27	0.67
25:F5:363:ILE:HG22	25:F5:365:PRO:HD2	1.76	0.67
4:f:13:TRP:O	21:t:442:ARG:NH1	2.27	0.67
9:H:217:GLU:OE1	9:H:217:GLU:N	2.28	0.67
25:E4:425:ARG:NH1	25:E4:464:LEU:O	2.28	0.67
24:B1:186:SER:O	24:B1:410:GLN:NE2	2.28	0.67
25:E2:176:GLY:O	25:E2:181:LYS:NZ	2.27	0.67
26:P2:37:LEU:HD11	26:P2:44:THR:HG22	1.77	0.67
24:B4:461:GLN:NE2	24:B4:465:THR:O	2.28	0.67
2:B:282:GLU:OE1	2:B:282:GLU:N	2.28	0.67
3:D:99:ASN:ND2	18:S:143:ASP:O	2.28	0.67
25:F1:425:ARG:NH2	25:F1:464:LEU:O	2.28	0.67
2:b:282:GLU:OE1	2:b:282:GLU:N	2.27	0.67
4:f3:13:TRP:O	21:t3:442:ARG:NH1	2.28	0.67
2:B3:282:GLU:N	2:B3:282:GLU:OE1	2.28	0.67
24:B5:461:GLN:NE2	24:B5:465:THR:O	2.28	0.67
10:j:147:GLU:OE1	10:j:147:GLU:N	2.28	0.66
24:B1:165:PRO:O	24:B1:170:ARG:NH1	2.27	0.66
24:B2:461:GLN:NE2	24:B2:465:THR:O	2.28	0.66
24:B4:165:PRO:O	24:B4:170:ARG:NH1	2.28	0.66
26:M4:68:LEU:HD11	26:L4:12:MET:HE3	1.77	0.66
25:F1:243:GLU:O	25:F1:248:ARG:NH1	2.28	0.66
25:F1:415:LEU:O	25:F1:420:LYS:NZ	2.28	0.66
10:J3:194:ARG:NH1	12:M3:191:ASP:OD1	2.29	0.66
25:F4:206:GLY:O	25:F4:279:ARG:NE	2.29	0.66
8:G:242:ARG:O	19:E:186:LYS:NZ	2.24	0.66
25:F5:452:ASN:OD1	25:F5:453:LEU:N	2.29	0.66
10:j:194:ARG:NH1	12:m:191:ASP:OD1	2.27	0.66
25:F1:452:ASN:OD1	25:F1:453:LEU:N	2.29	0.66
21:t3:253:ILE:HD11	21:t3:263:VAL:HG22	1.77	0.66
25:F4:452:ASN:OD1	25:F4:453:LEU:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:t:95:ARG:O	21:t:98:ASN:ND2	2.28	0.66
25:F5:415:LEU:O	25:F5:420:LYS:NZ	2.28	0.66
1:a:323:GLN:OE1	1:a:326:ARG:NE	2.23	0.66
24:B1:378:ASP:OD2	25:E1:210:ARG:NE	2.29	0.66
25:E1:176:GLY:O	25:E1:181:LYS:NZ	2.27	0.66
26:I2:45:GLU:N	26:I2:45:GLU:OE1	2.29	0.66
26:H2:53:MET:CE	26:Q2:52:LEU:HD21	2.26	0.66
11:L3:193:ARG:NH1	17:R3:108:ASP:OD2	2.28	0.66
24:B1:461:GLN:NE2	24:B1:465:THR:O	2.29	0.66
2:b3:282:GLU:N	2:b3:282:GLU:OE1	2.28	0.66
19:E:85:GLN:OE1	19:E:420:TYR:OH	2.14	0.66
22:G1:40:GLU:OE1	22:G1:133:LYS:NZ	2.29	0.66
24:A1:89:GLY:O	24:A1:91:ARG:NH2	2.28	0.66
3:D:122:SER:O	3:D:125:LEU:N	2.29	0.65
25:D1:157:LYS:NZ	25:D1:479:LYS:O	2.17	0.65
25:F2:452:ASN:OD1	25:F2:453:LEU:N	2.29	0.65
24:B5:61:THR:O	24:B5:73:PHE:N	2.29	0.65
26:N2:68:LEU:HD11	26:M2:12:MET:HE3	1.76	0.65
9:H3:217:GLU:OE1	9:H3:217:GLU:N	2.27	0.65
26:P5:37:LEU:HD11	26:P5:44:THR:HG22	1.78	0.65
11:l:33:SER:OG	11:l:35:ASP:OD1	2.08	0.65
19:E:305:GLU:OE1	19:E:305:GLU:N	2.30	0.65
11:L3:24:LYS:O	11:L3:28:ASN:ND2	2.30	0.65
24:A4:522:GLU:O	24:A4:526:ASN:ND2	2.30	0.65
26:I5:45:GLU:OE1	26:I5:45:GLU:N	2.29	0.65
25:E5:176:GLY:O	25:E5:181:LYS:NZ	2.29	0.65
19:e3:305:GLU:N	19:e3:305:GLU:OE1	2.30	0.65
1:a:209:ASP:OD1	2:b:173:ARG:NH1	2.29	0.65
11:L:44:VAL:HG21	26:K2:3:LEU:HB2	1.78	0.65
24:A1:461:GLN:NE2	24:A1:465:THR:O	2.29	0.65
25:E1:137:ARG:NH1	25:E1:260:GLU:OE1	2.28	0.65
3:D3:122:SER:O	3:D3:125:LEU:N	2.29	0.65
25:E4:137:ARG:NH1	25:E4:260:GLU:OE1	2.29	0.65
6:k:41:ASP:OD2	8:g:242:ARG:NH1	2.30	0.65
1:a3:209:ASP:OD1	2:b3:173:ARG:NH1	2.30	0.65
26:H1:57:LEU:HD23	26:Q1:55:PHE:CE2	2.31	0.65
25:D2:475:CYS:SG	25:D2:485:SER:OG	2.54	0.65
25:F4:415:LEU:O	25:F4:420:LYS:NZ	2.29	0.65
19:E:303:ARG:NH2	19:E:308:ASP:OD2	2.29	0.65
21:t:158:ARG:NH2	21:t:394:LEU:O	2.30	0.65
10:J3:150:ASP:OD1	17:R3:142:ARG:NH2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:E3:303:ARG:NH1	19:E3:315:GLY:O	2.28	0.65
24:A5:461:GLN:NE2	24:A5:465:THR:O	2.29	0.65
19:e:305:GLU:OE1	19:e:305:GLU:N	2.30	0.64
24:B2:61:THR:O	24:B2:73:PHE:N	2.30	0.64
24:A2:461:GLN:NE2	24:A2:465:THR:O	2.30	0.64
3:d3:99:ASN:ND2	18:s3:143:ASP:O	2.30	0.64
24:A5:182:LYS:NZ	24:A5:458:MET:O	2.26	0.64
24:A1:182:LYS:NZ	24:A1:458:MET:O	2.20	0.64
25:F2:415:LEU:O	25:F2:420:LYS:NZ	2.30	0.64
9:h3:258:PHE:O	11:l3:118:ARG:NH1	2.31	0.64
19:e3:119:GLN:OE1	19:e3:129:ARG:NH1	2.29	0.64
24:B4:208:ALA:N	33:B4:1003:ATP:O2A	2.28	0.64
24:A4:461:GLN:NE2	24:A4:465:THR:O	2.29	0.64
11:l3:193:ARG:NH2	17:r3:106:THR:O	2.31	0.64
3:D3:34:GLN:NE2	3:D3:68:ASN:O	2.30	0.64
4:F3:87:LYS:NZ	29:I3:302:CDL:O1	2.30	0.64
25:F5:243:GLU:O	25:F5:248:ARG:NH1	2.30	0.64
24:A2:522:GLU:O	24:A2:526:ASN:ND2	2.31	0.64
24:B5:378:ASP:OD2	25:E5:210:ARG:NE	2.29	0.64
24:A5:241:ARG:NH1	25:E5:140:PRO:O	2.30	0.64
4:F:87:LYS:NZ	29:L:302:CDL:O1	2.30	0.64
24:C1:163:LYS:NZ	25:F1:83:ASP:OD2	2.30	0.64
26:O1:40:ASN:ND2	26:O1:43:GLU:OE2	2.30	0.64
25:F2:206:GLY:O	25:F2:279:ARG:NE	2.31	0.64
24:C5:182:LYS:NZ	24:C5:458:MET:O	2.28	0.64
24:A5:89:GLY:O	24:A5:91:ARG:NH2	2.29	0.64
19:e:119:GLN:OE1	19:e:129:ARG:NH1	2.29	0.64
10:J:194:ARG:NH1	12:M:191:ASP:OD1	2.30	0.64
1:a3:211:ASP:OD2	3:d3:198:ARG:NH2	2.30	0.64
24:A5:67:ASP:OD1	25:E5:70:GLN:NE2	2.30	0.64
27:d4:92:PHE:CD2	27:d4:114:LEU:HD21	2.33	0.64
15:p3:111:LYS:O	17:r3:75:ASN:ND2	2.27	0.64
26:O4:57:LEU:HD23	26:N4:55:PHE:CD2	2.33	0.64
26:H4:71:PHE:O	26:H4:75:ALA:N	2.30	0.64
26:H1:71:PHE:O	26:H1:75:ALA:N	2.31	0.63
24:A2:241:ARG:NH1	25:E2:140:PRO:O	2.30	0.63
11:L:123:ARG:NE	29:L:302:CDL:OA4	2.30	0.63
27:d5:28:LYS:O	27:d5:105:ASN:ND2	2.31	0.63
23:g1:106:CYS:SG	23:g1:110:ASN:ND2	2.72	0.63
24:A2:114:LYS:NZ	25:E2:48:LEU:O	2.25	0.63
26:I4:57:LEU:HD23	26:H4:55:PHE:CE2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:G5:56:SER:HB2	22:G5:61:LEU:HD21	1.81	0.63
25:D5:176:GLY:O	25:D5:181:LYS:NZ	2.32	0.63
26:O5:40:ASN:ND2	26:O5:43:GLU:OE2	2.31	0.63
11:L:200:ARG:NH2	17:R:88:ASN:OD1	2.31	0.63
21:t3:116:ARG:NH1	21:t3:172:ASP:OD1	2.32	0.63
26:L4:57:LEU:HD23	26:K4:55:PHE:CD2	2.33	0.63
6:K:41:ASP:OD2	8:G:242:ARG:NH1	2.32	0.63
3:d3:130:ASN:OD1	18:s3:89:ARG:NH2	2.31	0.63
5:i3:136:ASN:ND2	11:l3:191:TYR:O	2.31	0.63
21:t3:95:ARG:O	21:t3:98:ASN:ND2	2.31	0.63
23:g4:106:CYS:SG	23:g4:110:ASN:ND2	2.72	0.63
25:E5:137:ARG:NH1	25:E5:260:GLU:OE1	2.32	0.63
26:J5:57:LEU:HD23	26:I5:55:PHE:CD2	2.34	0.63
19:E3:305:GLU:OE1	19:E3:305:GLU:N	2.30	0.63
4:F:2:SER:N	4:F:5:GLU:OE1	2.32	0.63
25:D1:176:GLY:O	25:D1:181:LYS:NZ	2.31	0.63
11:l3:33:SER:OG	11:l3:35:ASP:OD1	2.09	0.63
22:G4:56:SER:HB2	22:G4:61:LEU:HD21	1.81	0.63
26:N5:68:LEU:HD11	26:M5:12:MET:HE3	1.80	0.63
24:C1:186:SER:O	24:C1:410:GLN:NE2	2.31	0.63
24:B1:61:THR:O	24:B1:73:PHE:N	2.32	0.63
24:A4:89:GLY:O	24:A4:91:ARG:NH2	2.32	0.63
24:C5:201:ASP:OD1	24:C5:360:THR:OG1	2.16	0.63
24:B2:378:ASP:OD2	25:E2:210:ARG:NE	2.31	0.62
5:I3:156:GLU:O	5:I3:160:ARG:NH1	2.32	0.62
24:B4:140:ASP:OD1	24:B4:144:ASN:N	2.32	0.62
25:F4:243:GLU:O	25:F4:248:ARG:NH1	2.32	0.62
2:B:169:ARG:NH2	29:B:402:CDL:OB3	2.32	0.62
19:E:169:GLU:OE1	19:E:169:GLU:N	2.33	0.62
24:B4:61:THR:O	24:B4:73:PHE:N	2.31	0.62
25:D5:243:GLU:O	25:D5:248:ARG:NH1	2.31	0.62
24:A5:63:ILE:N	24:A5:71:ARG:O	2.32	0.62
16:q:116:TYR:OH	16:q:140:GLU:OE2	2.17	0.62
22:G2:56:SER:HB2	22:G2:61:LEU:HD21	1.81	0.62
26:M2:68:LEU:HD11	26:L2:12:MET:HE3	1.81	0.62
3:D3:30:ALA:O	3:D3:70:GLN:NE2	2.33	0.62
21:t3:122:GLY:N	21:t3:159:ASN:OD1	2.33	0.62
2:b:329:GLU:OE1	24:A2:35:SER:OG	2.17	0.62
29:B:403:CDL:OB3	29:B:403:CDL:O1	2.14	0.62
26:M1:68:LEU:HD11	26:L1:12:MET:HE3	1.80	0.62
11:l3:186:GLU:OE2	13:N3:169:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:P4:41:PRO:O	26:P4:44:THR:HG23	2.00	0.62
26:H4:47:LEU:HD23	26:Q4:37:LEU:HD23	1.82	0.62
26:Q4:37:LEU:HD11	26:Q4:44:THR:HG22	1.81	0.62
16:Q:63:LYS:NZ	16:Q:66:ASP:OD1	2.33	0.62
8:g3:257:GLU:OE1	8:g3:257:GLU:N	2.33	0.62
24:B4:186:SER:O	24:B4:410:GLN:NE2	2.33	0.62
26:J4:57:LEU:HD23	26:I4:55:PHE:CD2	2.33	0.62
26:I4:40:ASN:ND2	26:I4:43:GLU:OE2	2.33	0.62
24:B5:186:SER:O	24:B5:410:GLN:NE2	2.32	0.62
26:M5:57:LEU:HD23	26:L5:55:PHE:CD2	2.35	0.62
26:H1:47:LEU:HD23	26:Q1:37:LEU:HD23	1.82	0.62
26:M2:57:LEU:HD23	26:L2:55:PHE:CD2	2.35	0.62
19:E3:169:GLU:OE1	19:E3:169:GLU:N	2.33	0.62
28:e5:20:HIS:NE2	28:e5:59:THR:O	2.30	0.62
8:g:257:GLU:OE1	8:g:257:GLU:N	2.33	0.62
25:D1:90:ARG:NH1	24:A1:98:GLU:O	2.33	0.61
25:F1:206:GLY:O	25:F1:279:ARG:NE	2.33	0.61
26:P1:41:PRO:O	26:P1:44:THR:HG23	1.99	0.61
22:G1:56:SER:HB2	22:G1:61:LEU:HD21	1.81	0.61
24:A2:89:GLY:O	24:A2:91:ARG:NH2	2.32	0.61
26:L2:57:LEU:HD23	26:K2:55:PHE:CD2	2.34	0.61
2:B3:106:GLU:HA	18:S3:32:MET:HE1	1.81	0.61
21:t3:137:CYS:O	21:t3:283:ASN:ND2	2.34	0.61
26:H4:57:LEU:HD23	26:Q4:55:PHE:CE2	2.35	0.61
5:i:43:GLU:OE2	9:h:267:THR:OG1	2.04	0.61
6:K:96:MET:HA	6:K:96:MET:HE3	1.82	0.61
25:F2:296:SER:N	25:F2:300:TYR:O	2.32	0.61
32:i:302:UQ8:H20B	29:r:201:CDL:H771	1.82	0.61
26:O1:57:LEU:HD23	26:N1:55:PHE:CD2	2.36	0.61
32:I3:304:UQ8:H25A	32:I3:304:UQ8:C29	2.30	0.61
23:g4:79:GLU:OE2	23:g4:217:HIS:ND1	2.31	0.61
5:i:190:GLN:OE1	5:i:190:GLN:N	2.33	0.61
24:A1:522:GLU:O	24:A1:526:ASN:ND2	2.33	0.61
27:d2:92:PHE:CD2	27:d2:114:LEU:HD21	2.35	0.61
23:g4:160:ASN:ND2	28:e4:38:ALA:O	2.33	0.61
25:D5:90:ARG:NH1	24:A5:98:GLU:O	2.34	0.61
6:K:12:ASN:OD1	33:G:301:ATP:N6	2.33	0.61
1:a3:323:GLN:OE1	1:a3:326:ARG:NE	2.23	0.61
19:e3:85:GLN:OE1	19:e3:420:TYR:OH	2.19	0.61
24:C5:71:ARG:NH1	24:C5:98:GLU:OE2	2.33	0.61
26:H5:71:PHE:O	26:H5:75:ALA:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:178:ILE:HG23	29:I3:302:CDL:H473	1.83	0.61
25:D5:475:CYS:SG	25:D5:485:SER:OG	2.58	0.61
26:M1:57:LEU:HD23	26:L1:55:PHE:CD2	2.36	0.61
19:E3:303:ARG:NH2	19:E3:308:ASP:OD2	2.32	0.61
24:A4:63:ILE:N	24:A4:71:ARG:O	2.33	0.61
28:e1:22:THR:O	28:e1:26:ILE:HG23	2.00	0.61
23:g5:206:GLN:OE1	23:g5:206:GLN:N	2.33	0.61
25:F5:296:SER:N	25:F5:300:TYR:O	2.34	0.61
15:p:111:LYS:O	17:r:75:ASN:ND2	2.31	0.60
24:C2:201:ASP:OD1	24:C2:360:THR:OG1	2.19	0.60
9:h3:234:LYS:NZ	18:s3:61:ASP:OD2	2.34	0.60
1:A3:209:ASP:OD1	2:B3:173:ARG:NH1	2.34	0.60
21:t3:100:LEU:HD12	21:t3:100:LEU:O	2.01	0.60
24:A4:241:ARG:NH1	25:E4:140:PRO:O	2.32	0.60
19:e:108:GLU:OE2	19:e:110:LEU:HD12	2.00	0.60
19:e:303:ARG:NH1	19:e:315:GLY:O	2.33	0.60
1:A:184:PHE:HB2	32:I:303:UQ8:H15B	1.83	0.60
24:B1:140:ASP:OD1	24:B1:144:ASN:N	2.33	0.60
9:H3:250:ASP:OD2	18:S3:49:ARG:NH2	2.34	0.60
26:K4:71:PHE:O	26:K4:75:ALA:N	2.34	0.60
26:I4:57:LEU:HD23	26:H4:55:PHE:CD2	2.36	0.60
26:K1:71:PHE:O	26:K1:75:ALA:N	2.34	0.60
26:M2:45:GLU:OE1	26:M2:45:GLU:N	2.34	0.60
24:C5:111:ARG:NH1	25:D5:53:ASN:OD1	2.33	0.60
25:D5:111:GLY:N	25:D5:234:CYS:O	2.34	0.60
21:t:116:ARG:NH1	21:t:172:ASP:OD1	2.34	0.60
6:K3:96:MET:HA	6:K3:96:MET:HE3	1.82	0.60
12:M:14:ARG:NH1	13:N:113:GLU:OE2	2.34	0.60
21:t:100:LEU:HD12	21:t:100:LEU:O	2.02	0.60
27:d1:92:PHE:CD2	27:d1:114:LEU:HD21	2.36	0.60
25:F2:98:GLY:C	25:F2:99:LEU:HD12	2.27	0.60
26:H2:71:PHE:O	26:H2:75:ALA:N	2.34	0.60
25:F5:206:GLY:O	25:F5:279:ARG:NE	2.35	0.60
9:h:237:PRO:O	17:r:20:ARG:NH2	2.35	0.60
24:C2:186:SER:O	24:C2:410:GLN:NE2	2.34	0.60
25:D2:48:LEU:HD21	25:D2:75:SER:HA	1.84	0.60
26:L2:71:PHE:O	26:L2:75:ALA:N	2.35	0.60
25:D4:48:LEU:HD21	25:D4:75:SER:HA	1.84	0.60
25:F4:98:GLY:C	25:F4:99:LEU:HD12	2.27	0.60
24:A1:63:ILE:N	24:A1:71:ARG:O	2.32	0.60
21:t3:336:SER:OG	21:t3:339:VAL:O	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A5:222:ASN:OD1	24:A5:258:LYS:NZ	2.34	0.60
3:D:108:TYR:OH	18:S:135:ASN:OD1	2.07	0.60
24:B2:82:GLU:OE2	24:B2:124:ALA:N	2.35	0.60
25:F1:363:ILE:HG23	25:F1:434:SER:HB3	1.83	0.60
19:e:395:ALA:O	19:e:406:HIS:ND1	2.34	0.60
25:E1:243:GLU:O	25:E1:248:ARG:NH1	2.35	0.60
23:g2:206:GLN:OE1	23:g2:206:GLN:N	2.33	0.60
26:J2:71:PHE:O	26:J2:75:ALA:N	2.35	0.60
29:a3:502:CDL:H441	26:I5:60:THR:HG23	1.84	0.60
6:K3:12:ASN:OD1	33:G3:301:ATP:N6	2.35	0.60
23:g5:149:LEU:HD12	23:g5:149:LEU:O	2.01	0.60
19:e3:108:GLU:OE2	19:e3:110:LEU:HD12	2.01	0.59
19:E3:119:GLN:OE1	19:E3:129:ARG:NH1	2.33	0.59
19:E3:165:ASN:ND2	19:E3:205:CYS:SG	2.75	0.59
24:A4:317:ARG:NH1	25:E4:292:GLY:O	2.35	0.59
25:F5:447:PRO:O	25:F5:449:ARG:NH1	2.35	0.59
24:A5:522:GLU:O	24:A5:526:ASN:ND2	2.33	0.59
25:E5:243:GLU:O	25:E5:248:ARG:NH1	2.34	0.59
26:L1:57:LEU:HD23	26:K1:55:PHE:CD2	2.37	0.59
23:g2:149:LEU:O	23:g2:149:LEU:HD12	2.02	0.59
24:B2:140:ASP:OD1	24:B2:144:ASN:N	2.33	0.59
5:i3:190:GLN:N	5:i3:190:GLN:OE1	2.35	0.59
29:B3:403:CDL:OB3	29:B3:403:CDL:O1	2.16	0.59
3:D3:99:ASN:ND2	18:S3:143:ASP:O	2.35	0.59
3:D3:122:SER:OG	18:S3:123:ASP:OD1	2.14	0.59
25:F4:363:ILE:HG23	25:F4:434:SER:HB3	1.83	0.59
25:E4:204:GLY:O	25:E4:239:GLY:N	2.35	0.59
22:G5:51:LEU:HD22	22:G5:114:LEU:HD22	1.83	0.59
2:B:211:HIS:NE2	3:D:129:GLU:OE1	2.34	0.59
23:g1:206:GLN:OE1	23:g1:206:GLN:N	2.36	0.59
9:h3:253:GLU:OE2	21:t3:422:ARG:NH2	2.35	0.59
23:g4:206:GLN:OE1	23:g4:206:GLN:N	2.35	0.59
26:M4:57:LEU:HD23	26:L4:55:PHE:CD2	2.36	0.59
10:j:228:GLN:OE1	10:j:232:ASN:ND2	2.35	0.59
25:E1:204:GLY:O	25:E1:239:GLY:N	2.36	0.59
26:K2:71:PHE:O	26:K2:75:ALA:N	2.35	0.59
25:E5:204:GLY:O	25:E5:239:GLY:N	2.34	0.59
26:O2:57:LEU:HD23	26:N2:55:PHE:CE2	2.38	0.59
26:K4:57:LEU:HD23	26:J4:55:PHE:CD2	2.37	0.59
24:C5:487:LEU:HD21	24:C5:536:ILE:HG23	1.85	0.59
26:K5:71:PHE:O	26:K5:75:ALA:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:k:146:ASN:OD1	6:k:150:GLN:NE2	2.35	0.59
3:D:29:GLN:O	3:D:33:ASN:ND2	2.36	0.59
25:F1:98:GLY:C	25:F1:99:LEU:HD12	2.28	0.59
27:d5:113:ASP:OD1	27:d5:114:LEU:N	2.35	0.59
19:E:119:GLN:OE1	19:E:129:ARG:NH1	2.34	0.59
23:g1:149:LEU:HD12	23:g1:149:LEU:O	2.03	0.59
2:B3:112:ARG:NH1	4:F3:74:ASN:O	2.36	0.59
3:D3:41:ILE:HD13	3:D3:60:LEU:HD12	1.84	0.59
28:e4:20:HIS:NE2	28:e4:59:THR:O	2.34	0.59
25:F5:98:GLY:C	25:F5:99:LEU:HD12	2.27	0.59
26:P5:55:PHE:CZ	26:Q5:57:LEU:HD22	2.37	0.59
27:d5:92:PHE:CD2	27:d5:114:LEU:HD21	2.38	0.59
11:l:186:GLU:OE2	13:N:169:ARG:NH2	2.34	0.59
19:e:239:PHE:N	19:e:247:ASP:OD2	2.36	0.59
23:g1:73:GLN:OE1	23:g1:73:GLN:N	2.34	0.59
24:A1:317:ARG:NH1	25:E1:292:GLY:O	2.36	0.59
22:G2:51:LEU:HD22	22:G2:114:LEU:HD22	1.85	0.59
26:O2:57:LEU:HD23	26:N2:55:PHE:CD2	2.38	0.59
11:l3:123:ARG:NE	29:l3:301:CDL:OA4	2.36	0.59
19:e3:303:ARG:NH2	19:e3:308:ASP:OD2	2.36	0.59
27:d4:113:ASP:OD1	27:d4:114:LEU:N	2.36	0.59
28:e4:22:THR:O	28:e4:26:ILE:HG23	2.02	0.59
23:g5:73:GLN:N	23:g5:73:GLN:OE1	2.35	0.59
19:e:346:THR:OG1	19:e:396:HIS:NE2	2.28	0.58
15:P:111:LYS:O	17:R:75:ASN:ND2	2.32	0.58
26:P2:55:PHE:CZ	26:Q2:57:LEU:HD22	2.38	0.58
24:C4:163:LYS:NZ	25:F4:83:ASP:OD2	2.35	0.58
26:L5:71:PHE:O	26:L5:75:ALA:N	2.36	0.58
32:I:303:UQ8:H25A	32:I:303:UQ8:C29	2.32	0.58
19:E:51:CYS:O	19:E:55:PHE:N	2.35	0.58
24:C2:487:LEU:HD21	24:C2:536:ILE:HG23	1.84	0.58
3:D:34:GLN:NE2	3:D:68:ASN:O	2.36	0.58
24:A1:241:ARG:NH1	25:E1:140:PRO:O	2.34	0.58
26:L5:57:LEU:HD23	26:K5:55:PHE:CD2	2.38	0.58
10:j:102:GLN:OE1	10:j:102:GLN:N	2.33	0.58
25:F2:363:ILE:HG23	25:F2:434:SER:HB3	1.85	0.58
25:E2:137:ARG:NH1	25:E2:260:GLU:OE1	2.36	0.58
25:E2:204:GLY:O	25:E2:239:GLY:N	2.33	0.58
27:d2:55:ASN:OD1	27:d2:56:GLU:N	2.37	0.58
23:g4:149:LEU:HD12	23:g4:149:LEU:O	2.04	0.58
25:F4:296:SER:N	25:F4:300:TYR:O	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B5:238:GLY:N	24:B5:265:ALA:O	2.35	0.58
11:l:124:VAL:HG13	29:l:301:CDL:H312	1.84	0.58
23:g2:73:GLN:N	23:g2:73:GLN:OE1	2.36	0.58
2:b3:211:HIS:NE2	3:d3:129:GLU:OE1	2.35	0.58
2:B3:78:HIS:NE2	29:I3:301:CDL:OA4	2.36	0.58
25:D4:111:GLY:N	25:D4:234:CYS:O	2.35	0.58
25:F1:296:SER:N	25:F1:300:TYR:O	2.32	0.58
24:A2:63:ILE:N	24:A2:71:ARG:O	2.35	0.58
3:d:41:ILE:HD13	3:d:60:LEU:HD12	1.85	0.58
2:B:106:GLU:HA	18:S:32:MET:HE1	1.85	0.58
5:I:49:ILE:HD12	29:L:302:CDL:OB3	2.03	0.58
21:t:158:ARG:NH1	21:t:398:ASP:OD2	2.37	0.58
25:D2:243:GLU:O	25:D2:248:ARG:NH1	2.35	0.58
27:d2:28:LYS:O	27:d2:63:ASN:ND2	2.36	0.58
27:d2:113:ASP:OD1	27:d2:114:LEU:N	2.36	0.58
1:a3:14:TYR:N	1:a3:17:PHE:O	2.37	0.58
5:I3:49:ILE:HD12	29:I3:302:CDL:OB3	2.03	0.58
5:i:136:ASN:ND2	11:l:191:TYR:O	2.34	0.58
18:S:134:GLU:OE2	18:S:137:ARG:NH2	2.36	0.58
6:k3:125:SER:HA	26:P5:2:LEU:HD12	1.85	0.58
26:O5:57:LEU:HD23	26:N5:55:PHE:CE2	2.39	0.58
3:d:99:ASN:ND2	18:s:143:ASP:O	2.36	0.58
19:e:303:ARG:NH2	19:e:308:ASP:OD2	2.35	0.58
23:g2:125:ARG:O	23:g2:126:SER:OG	2.14	0.58
11:l:200:ARG:NH2	17:r:88:ASN:OD1	2.37	0.58
3:D:122:SER:OG	18:S:123:ASP:OD1	2.11	0.58
27:d1:113:ASP:OD1	27:d1:114:LEU:N	2.36	0.58
4:f3:67:LYS:NZ	29:B3:403:CDL:OA7	2.37	0.58
16:Q3:116:TYR:OH	16:Q3:140:GLU:OE2	2.21	0.58
23:g5:125:ARG:O	23:g5:126:SER:OG	2.19	0.58
24:B5:107:LEU:HD13	24:B5:142:LEU:HD21	1.86	0.58
26:M5:45:GLU:OE1	26:M5:45:GLU:N	2.34	0.58
10:J:147:GLU:OE1	10:J:147:GLU:N	2.37	0.57
24:A4:454:ARG:NH2	24:A4:487:LEU:O	2.37	0.57
27:d4:102:HIS:NE2	27:d4:108:GLU:OE2	2.34	0.57
10:j3:28:ASP:OD1	10:j3:31:THR:N	2.36	0.57
8:G3:242:ARG:O	19:E3:186:LYS:NZ	2.26	0.57
8:G3:257:GLU:OE1	8:G3:257:GLU:N	2.37	0.57
15:P3:111:LYS:O	17:R3:75:ASN:ND2	2.35	0.57
24:C5:170:ARG:NH2	24:C5:338:GLU:O	2.37	0.57
24:A5:140:ASP:OD1	24:A5:144:ASN:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ILE:HG23	29:L:302:CDL:H473	1.84	0.57
25:D1:111:GLY:N	25:D1:234:CYS:O	2.33	0.57
10:j3:102:GLN:OE1	10:j3:102:GLN:N	2.34	0.57
11:l3:16:GLU:N	11:l3:16:GLU:OE1	2.37	0.57
19:e:426:GLY:O	19:e:430:LYS:NZ	2.23	0.57
24:C1:517:SER:OG	24:C1:519:ASP:OD1	2.22	0.57
8:G3:122:ALA:O	8:G3:129:LYS:NZ	2.29	0.57
24:B1:77:LYS:O	24:B1:121:ARG:NH1	2.37	0.57
23:g2:160:ASN:ND2	28:e2:38:ALA:O	2.36	0.57
11:l3:113:ARG:NH2	29:l3:301:CDL:OB4	2.34	0.57
26:H5:53:MET:CE	26:Q5:52:LEU:HD21	2.35	0.57
18:s:118:LYS:O	18:s:122:HIS:ND1	2.37	0.57
8:G:257:GLU:OE1	8:G:257:GLU:N	2.37	0.57
26:M1:45:GLU:OE1	26:M1:45:GLU:N	2.36	0.57
24:C2:111:ARG:NH1	25:D2:53:ASN:OD1	2.37	0.57
24:A2:67:ASP:OD1	25:E2:70:GLN:NE2	2.38	0.57
24:A2:140:ASP:OD1	24:A2:144:ASN:N	2.37	0.57
19:e3:395:ALA:O	19:e3:406:HIS:ND1	2.37	0.57
23:g5:93:SER:OG	23:g5:179:ASP:OD1	2.22	0.57
25:F5:363:ILE:HG23	25:F5:434:SER:HB3	1.85	0.57
24:B1:82:GLU:OE2	24:B1:124:ALA:N	2.38	0.57
5:i3:61:MET:HE1	12:m3:97:ASN:HB2	1.87	0.57
11:l3:124:VAL:HG13	29:l3:301:CDL:H312	1.86	0.57
23:g5:106:CYS:SG	23:g5:110:ASN:ND2	2.77	0.57
25:E5:141:SER:OG	25:E5:144:ASP:OD1	2.10	0.57
26:M5:68:LEU:HD11	26:L5:12:MET:HE3	1.87	0.57
27:d5:55:ASN:OD1	27:d5:56:GLU:N	2.38	0.57
29:F:302:CDL:C40	26:I2:57:LEU:HD11	2.34	0.57
13:N:124:GLY:C	13:N:125:LEU:HD22	2.30	0.57
24:A1:67:ASP:OD1	25:E1:70:GLN:NE2	2.37	0.57
23:g4:73:GLN:OE1	23:g4:73:GLN:N	2.35	0.57
24:B5:140:ASP:OD1	24:B5:144:ASN:N	2.35	0.57
3:D:58:THR:HG22	24:A1:538:GLU:OE1	2.04	0.57
26:P1:37:LEU:HD23	26:Q1:47:LEU:HD23	1.87	0.57
28:e1:20:HIS:NE2	28:e1:59:THR:O	2.36	0.57
11:l3:193:ARG:NH1	17:r3:108:ASP:OD2	2.38	0.57
10:J3:147:GLU:OE1	10:J3:147:GLU:N	2.38	0.57
23:g4:26:LEU:HD21	23:g4:281:ARG:HA	1.85	0.57
15:P:126:ASP:OD2	17:R:148:TYR:OH	2.22	0.57
23:g1:218:GLU:OE1	26:N1:39:ARG:NE	2.38	0.57
12:m3:14:ARG:NH1	13:n3:113:GLU:OE2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C4:487:LEU:HD21	24:C4:536:ILE:HG23	1.85	0.57
24:B4:82:GLU:OE2	24:B4:124:ALA:N	2.37	0.57
24:C5:67:ASP:OD1	25:D5:293:ARG:NH2	2.38	0.57
24:B5:82:GLU:OE2	24:B5:124:ALA:N	2.37	0.57
15:P:88:VAL:O	15:P:92:SER:OG	2.17	0.56
24:C5:163:LYS:NZ	25:F5:83:ASP:OD2	2.29	0.56
25:E5:157:LYS:NZ	25:E5:479:LYS:O	2.28	0.56
29:F:302:CDL:H441	26:I2:60:THR:HG23	1.86	0.56
13:n3:124:GLY:C	13:n3:125:LEU:HD22	2.30	0.56
11:l:16:GLU:OE1	11:l:16:GLU:N	2.37	0.56
16:q:63:LYS:NZ	16:q:66:ASP:OD1	2.26	0.56
19:E:303:ARG:NH1	19:E:315:GLY:O	2.38	0.56
25:F1:447:PRO:O	25:F1:449:ARG:NH1	2.38	0.56
25:E1:157:LYS:NZ	25:E1:479:LYS:O	2.27	0.56
26:O1:57:LEU:HD23	26:N1:55:PHE:CE2	2.40	0.56
25:F2:447:PRO:O	25:F2:449:ARG:NH1	2.37	0.56
19:E3:56:ASP:O	19:E3:60:HIS:N	2.37	0.56
23:g4:292:ILE:HD11	25:D4:297:ALA:HA	1.87	0.56
24:C4:201:ASP:OD1	24:C4:360:THR:OG1	2.23	0.56
25:F4:447:PRO:O	25:F4:449:ARG:NH1	2.38	0.56
26:P4:37:LEU:HD23	26:Q4:47:LEU:HD23	1.86	0.56
27:d4:114:LEU:HD23	27:d4:115:PHE:N	2.20	0.56
1:a:226:THR:HG21	5:i:88:PHE:HD2	1.69	0.56
18:s3:134:GLU:OE2	18:s3:137:ARG:NH2	2.39	0.56
26:O4:57:LEU:HD23	26:N4:55:PHE:CE2	2.41	0.56
23:g1:26:LEU:HD21	23:g1:281:ARG:HA	1.87	0.56
25:F2:243:GLU:O	25:F2:248:ARG:NH1	2.38	0.56
28:e2:20:HIS:NE2	28:e2:59:THR:O	2.35	0.56
24:A4:140:ASP:OD1	24:A4:144:ASN:N	2.39	0.56
1:A:177:TRP:CE3	32:I:303:UQ8:H25B	2.40	0.56
24:B2:107:LEU:HD13	24:B2:142:LEU:HD21	1.87	0.56
24:B2:186:SER:O	24:B2:410:GLN:NE2	2.39	0.56
29:a3:502:CDL:C40	26:I5:57:LEU:HD11	2.35	0.56
3:D3:29:GLN:O	3:D3:33:ASN:ND2	2.38	0.56
13:n:124:GLY:C	13:n:125:LEU:HD22	2.31	0.56
1:A:412:LEU:O	1:A:416:THR:OG1	2.19	0.56
3:D:183:GLU:OE1	12:M:103:ARG:NE	2.35	0.56
24:C1:487:LEU:HD21	24:C1:536:ILE:HG23	1.87	0.56
10:j3:150:ASP:OD1	17:r3:142:ARG:NH2	2.38	0.56
11:L3:200:ARG:NH2	17:R3:88:ASN:OD1	2.39	0.56
19:E3:395:ALA:O	19:E3:406:HIS:ND1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:t3:158:ARG:NH1	21:t3:398:ASP:OD2	2.39	0.56
24:C1:111:ARG:NH1	25:D1:53:ASN:OD1	2.35	0.56
25:D2:111:GLY:N	25:D2:234:CYS:O	2.35	0.56
2:b3:363:ASP:N	2:b3:363:ASP:OD1	2.39	0.56
10:j3:228:GLN:OE1	10:j3:232:ASN:ND2	2.39	0.56
29:I3:302:CDL:OA4	11:L3:123:ARG:NE	2.37	0.56
24:C4:111:ARG:NH1	25:D4:53:ASN:OD1	2.36	0.56
30:G:303:PC1:H133	30:G:303:PC1:O13	2.06	0.56
25:D1:239:GLY:HA3	25:D1:251:VAL:HG11	1.88	0.56
23:g2:106:CYS:SG	23:g2:110:ASN:ND2	2.79	0.56
24:C2:170:ARG:NH2	24:C2:338:GLU:O	2.38	0.56
4:f3:39:PRO:O	21:t3:350:LYS:NZ	2.39	0.56
26:O5:45:GLU:OE1	26:O5:45:GLU:N	2.38	0.56
24:C1:170:ARG:NH2	24:C1:338:GLU:O	2.39	0.56
24:C1:201:ASP:OD1	24:C1:360:THR:OG1	2.21	0.56
24:A1:454:ARG:NH2	24:A1:487:LEU:O	2.39	0.56
8:g3:43:ARG:NH1	16:q3:121:GLU:OE1	2.39	0.56
6:K3:41:ASP:OD2	8:G3:242:ARG:NH1	2.39	0.56
11:l:44:VAL:HG21	26:K1:3:LEU:HB2	1.88	0.55
15:p3:2:SER:OG	15:p3:27:GLN:OE1	2.24	0.55
13:N3:124:GLY:C	13:N3:125:LEU:HD22	2.31	0.55
18:S3:111:GLN:N	18:S3:111:GLN:OE1	2.37	0.55
26:H4:57:LEU:HD23	26:Q4:55:PHE:CZ	2.40	0.55
26:O5:57:LEU:HD23	26:N5:55:PHE:CD2	2.41	0.55
9:h3:259:GLU:OE1	9:h3:259:GLU:N	2.39	0.55
24:B4:222:ASN:OD1	24:B4:258:LYS:NZ	2.37	0.55
15:p3:24:GLU:OE1	15:p3:24:GLU:N	2.38	0.55
3:D:41:ILE:HD13	3:D:60:LEU:HD12	1.87	0.55
25:D2:231:GLU:O	25:D2:232:SER:OG	2.24	0.55
24:A2:442:ASP:OD1	24:A2:443:ALA:N	2.40	0.55
8:g3:223:GLU:OE2	16:q3:130:LYS:NZ	2.39	0.55
19:e3:51:CYS:O	19:e3:55:PHE:N	2.40	0.55
24:B5:77:LYS:O	24:B5:121:ARG:NH1	2.40	0.55
5:i:156:GLU:O	5:i:160:ARG:NH1	2.40	0.55
9:h:240:ASP:OD1	21:t:457:LEU:HD21	2.07	0.55
27:d1:114:LEU:HD23	27:d1:115:PHE:N	2.21	0.55
29:a3:502:CDL:H401	26:I5:57:LEU:HD11	1.89	0.55
24:C4:490:SER:O	24:C4:494:LYS:NZ	2.40	0.55
25:E4:334:ASP:OD2	25:E4:356:ARG:NH1	2.40	0.55
11:l:69:ARG:HG2	11:l:70:PRO:HD3	1.88	0.55
1:A:209:ASP:OD1	2:B:173:ARG:NH1	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:t:122:GLY:N	21:t:159:ASN:OD1	2.39	0.55
25:D2:248:ARG:NH2	25:D2:286:GLU:OE1	2.39	0.55
27:d2:114:LEU:HD23	27:d2:115:PHE:N	2.21	0.55
1:A3:184:PHE:HB2	32:I3:304:UQ8:H15B	1.89	0.55
6:K3:37:ALA:N	29:K3:201:CDL:OA4	2.32	0.55
23:g4:218:GLU:OE1	26:N4:39:ARG:NE	2.40	0.55
24:A4:440:ASP:OD1	24:A4:441:LEU:N	2.39	0.55
26:J4:71:PHE:O	26:J4:75:ALA:N	2.39	0.55
24:B1:238:GLY:N	24:B1:265:ALA:O	2.37	0.55
25:E1:459:SER:OG	25:E1:481:ASP:OD1	2.24	0.55
27:d1:102:HIS:NE2	27:d1:108:GLU:OE2	2.37	0.55
10:J3:102:GLN:OE1	10:J3:102:GLN:N	2.35	0.55
26:N4:57:LEU:HD23	26:M4:55:PHE:CE2	2.41	0.55
23:g5:79:GLU:OE2	23:g5:217:HIS:ND1	2.38	0.55
26:I5:47:LEU:HD23	26:H5:37:LEU:HD23	1.89	0.55
23:g1:79:GLU:OE2	23:g1:217:HIS:ND1	2.36	0.55
26:K1:57:LEU:HD23	26:J1:55:PHE:CD2	2.42	0.55
23:g2:79:GLU:OE2	23:g2:217:HIS:ND1	2.37	0.55
24:C2:182:LYS:NZ	24:C2:458:MET:O	2.31	0.55
11:L3:193:ARG:NH2	17:R3:106:THR:O	2.40	0.55
24:C4:170:ARG:NH2	24:C4:338:GLU:O	2.40	0.55
24:B4:111:ARG:O	25:F4:50:GLN:NE2	2.37	0.55
26:M4:45:GLU:OE1	26:M4:45:GLU:N	2.37	0.55
23:g5:93:SER:O	23:g5:179:ASP:N	2.40	0.55
1:a:295:GLY:O	6:k:54:ARG:NH2	2.38	0.55
2:b:305:ASP:OD2	22:G2:206:ARG:NE	2.38	0.55
19:E:237:GLU:OE1	19:E:264:ASN:ND2	2.40	0.55
24:B1:111:ARG:O	25:F1:50:GLN:NE2	2.39	0.55
26:Q1:37:LEU:CD1	26:Q1:44:THR:HG22	2.37	0.55
21:t3:138:ASP:OD1	21:t3:139:LEU:N	2.40	0.55
10:j:28:ASP:OD1	10:j:31:THR:N	2.40	0.55
11:l:180:VAL:HG21	17:R:110:ALA:HB2	1.88	0.55
29:l:302:CDL:C81	26:I1:10:LEU:HD11	2.36	0.55
19:E:239:PHE:N	19:E:247:ASP:OD2	2.38	0.55
26:I2:47:LEU:HD23	26:H2:37:LEU:HD23	1.89	0.55
25:D4:90:ARG:NH1	24:A4:98:GLU:O	2.40	0.55
11:l:58:GLU:OE1	11:L3:74:LEU:HD21	2.07	0.54
29:F:302:CDL:H401	26:I2:57:LEU:HD11	1.88	0.54
9:H:93:ARG:NH1	16:Q:111:GLU:OE2	2.40	0.54
24:A1:266:THR:N	24:A1:269:ASP:OD2	2.39	0.54
25:E1:334:ASP:OD2	25:E1:356:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:E3:51:CYS:O	19:E3:55:PHE:N	2.38	0.54
25:F4:68:VAL:HA	25:F4:79:THR:HG22	1.88	0.54
9:h:259:GLU:OE1	9:h:259:GLU:N	2.40	0.54
24:A1:442:ASP:OD1	24:A1:443:ALA:N	2.39	0.54
26:N1:57:LEU:HD23	26:M1:55:PHE:CD2	2.42	0.54
27:d5:114:LEU:HD23	27:d5:115:PHE:N	2.22	0.54
6:k:106:ARG:NH2	6:k:155:SER:O	2.40	0.54
11:l:113:ARG:NH2	29:l:301:CDL:OB4	2.36	0.54
24:A1:178:GLN:O	24:A1:217:GLN:NE2	2.39	0.54
3:d3:87:ILE:O	3:d3:88:SER:OG	2.24	0.54
25:E5:207:GLU:OE2	25:E5:276:ASN:ND2	2.40	0.54
11:l:69:ARG:CG	11:l:70:PRO:HD3	2.37	0.54
25:F1:154:THR:O	25:F1:191:ASN:ND2	2.37	0.54
25:F2:68:VAL:HA	25:F2:79:THR:HG22	1.90	0.54
3:d3:183:GLU:OE1	12:m3:103:ARG:NE	2.40	0.54
1:A3:229:ASP:OD1	5:I3:70:ARG:NH2	2.40	0.54
26:N4:57:LEU:HD23	26:M4:55:PHE:CD2	2.42	0.54
24:C5:208:ALA:N	33:C5:601:ATP:O1A	2.38	0.54
9:h:218:ARG:NH2	9:h:221:GLU:OE2	2.41	0.54
23:g1:292:ILE:HD11	25:D1:297:ALA:HA	1.89	0.54
24:A4:442:ASP:OD1	24:A4:443:ALA:N	2.39	0.54
27:d4:55:ASN:OD1	27:d4:56:GLU:N	2.41	0.54
25:D1:48:LEU:HD21	25:D1:75:SER:HA	1.90	0.54
25:E1:177:ALA:O	25:E1:356:ARG:NH2	2.41	0.54
26:J1:57:LEU:HD23	26:I1:55:PHE:CD2	2.43	0.54
25:F5:481:ASP:OD1	25:F5:482:LEU:N	2.40	0.54
5:I:141:ARG:NE	12:M:66:ASP:O	2.33	0.54
21:t:99:HIS:ND1	21:t:99:HIS:O	2.41	0.54
24:C1:302:LEU:O	24:C1:302:LEU:HD13	2.08	0.54
28:e1:25:VAL:HG12	28:e1:25:VAL:O	2.07	0.54
26:P2:37:LEU:HD23	26:Q2:47:LEU:HD23	1.90	0.54
1:a3:184:PHE:HB2	32:i3:303:UQ8:H15B	1.90	0.54
29:I3:303:CDL:C81	26:I4:10:LEU:HD11	2.37	0.54
24:A4:84:VAL:O	24:A4:92:GLY:N	2.41	0.54
28:e4:25:VAL:O	28:e4:25:VAL:HG12	2.08	0.54
24:B5:111:ARG:O	25:F5:50:GLN:NE2	2.39	0.54
24:A1:440:ASP:OD1	24:A1:441:LEU:N	2.39	0.54
26:I1:57:LEU:HD23	26:H1:55:PHE:CD2	2.43	0.54
23:g2:26:LEU:HD21	23:g2:281:ARG:HA	1.89	0.54
26:O2:45:GLU:OE1	26:O2:45:GLU:N	2.39	0.54
26:K2:68:LEU:O	26:K2:68:LEU:HD23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d3:41:ILE:HD13	3:d3:60:LEU:HD12	1.89	0.54
2:B3:211:HIS:NE2	3:D3:129:GLU:OE1	2.37	0.54
3:D3:58:THR:HG22	24:A4:538:GLU:OE1	2.08	0.54
28:e5:22:THR:O	28:e5:26:ILE:HG23	2.07	0.54
12:m:13:LEU:HD21	12:m:18:LEU:HG	1.90	0.54
19:e:56:ASP:O	19:e:60:HIS:N	2.39	0.54
13:n3:169:ARG:NH2	11:L3:186:GLU:OE2	2.40	0.54
15:p3:89:PHE:O	15:p3:94:ASN:ND2	2.41	0.54
24:B4:279:TYR:OH	24:B4:332:LEU:O	2.25	0.54
23:g5:26:LEU:HD21	23:g5:281:ARG:HA	1.88	0.54
2:b:211:HIS:NE2	3:d:129:GLU:OE1	2.40	0.54
25:F1:481:ASP:OD1	25:F1:482:LEU:N	2.41	0.54
24:A1:84:VAL:O	24:A1:92:GLY:N	2.41	0.54
25:E2:207:GLU:OE2	25:E2:276:ASN:ND2	2.41	0.54
29:B3:402:CDL:OB7	4:F3:104:LYS:NZ	2.40	0.54
11:L3:69:ARG:CG	11:L3:70:PRO:HD3	2.38	0.54
27:d5:73:PRO:O	27:d5:94:HIS:NE2	2.41	0.54
1:a:226:THR:HG21	5:i:88:PHE:CD2	2.42	0.53
23:g2:93:SER:O	23:g2:179:ASP:N	2.37	0.53
1:A3:211:ASP:OD2	3:D3:198:ARG:NH2	2.40	0.53
15:P3:126:ASP:OD2	17:R3:148:TYR:OH	2.24	0.53
18:S:111:GLN:OE1	18:S:111:GLN:N	2.36	0.53
25:F1:68:VAL:HA	25:F1:79:THR:HG22	1.89	0.53
24:A1:206:LYS:NZ	33:A1:601:ATP:O2B	2.36	0.53
27:d1:55:ASN:OD1	27:d1:56:GLU:N	2.42	0.53
29:i3:301:CDL:H771	32:i3:303:UQ8:H20B	1.89	0.53
25:D4:239:GLY:HA3	25:D4:251:VAL:HG11	1.90	0.53
24:B4:77:LYS:O	24:B4:121:ARG:NH1	2.41	0.53
24:A4:266:THR:N	24:A4:269:ASP:OD2	2.40	0.53
23:g5:160:ASN:ND2	28:e5:38:ALA:O	2.40	0.53
5:I:66:VAL:HG21	7:C:45:VAL:HG21	1.89	0.53
10:J:102:GLN:OE1	10:J:102:GLN:N	2.35	0.53
19:E:395:ALA:O	19:E:406:HIS:ND1	2.42	0.53
24:A1:140:ASP:OD1	24:A1:144:ASN:N	2.39	0.53
25:E2:243:GLU:O	25:E2:248:ARG:NH1	2.42	0.53
25:E2:334:ASP:OD2	25:E2:356:ARG:NH1	2.41	0.53
24:A4:289:ARG:NH1	24:A4:339:ARG:O	2.41	0.53
23:g5:230:TYR:OH	28:e5:3:ILE:O	2.25	0.53
6:k:76:GLY:O	6:k:80:ASN:ND2	2.42	0.53
10:J:213:ARG:NH1	10:J:220:ASP:OD1	2.39	0.53
1:A3:412:LEU:O	1:A3:416:THR:OG1	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C4:113:ILE:HD12	24:C4:113:ILE:O	2.09	0.53
25:D4:248:ARG:NH2	25:D4:286:GLU:OE1	2.42	0.53
24:A4:186:SER:O	24:A4:410:GLN:NE2	2.41	0.53
24:C5:113:ILE:HD12	24:C5:113:ILE:O	2.09	0.53
25:F5:68:VAL:HA	25:F5:79:THR:HG22	1.90	0.53
26:H1:57:LEU:HD23	26:Q1:55:PHE:CZ	2.43	0.53
24:C2:113:ILE:O	24:C2:113:ILE:HD12	2.09	0.53
9:H3:93:ARG:NH1	16:Q3:111:GLU:OE2	2.42	0.53
26:K5:68:LEU:O	26:K5:68:LEU:HD23	2.08	0.53
9:h:234:LYS:NZ	18:s:61:ASP:OD2	2.40	0.53
26:P2:40:ASN:ND2	26:P2:43:GLU:OE1	2.41	0.53
1:A3:430:LYS:NZ	16:Q3:100:GLU:OE1	2.30	0.53
24:C4:302:LEU:O	24:C4:302:LEU:HD13	2.08	0.53
25:F4:154:THR:O	25:F4:191:ASN:ND2	2.40	0.53
5:i:61:MET:HE1	12:m:97:ASN:HB2	1.91	0.53
23:g1:160:ASN:ND2	28:e1:38:ALA:O	2.38	0.53
28:e2:22:THR:O	28:e2:26:ILE:HG23	2.09	0.53
22:G4:217:ILE:O	22:G4:218:SER:OG	2.25	0.53
26:L4:71:PHE:O	26:L4:75:ALA:N	2.42	0.53
23:g5:172:SER:OG	23:g5:204:ARG:NH1	2.42	0.53
25:F5:150:GLU:N	25:F5:150:GLU:OE1	2.42	0.53
25:E1:231:GLU:O	25:E1:232:SER:OG	2.24	0.53
24:A2:440:ASP:OD1	24:A2:441:LEU:N	2.42	0.53
4:f:39:PRO:O	21:t:350:LYS:NZ	2.42	0.53
15:p:24:GLU:N	15:p:24:GLU:OE1	2.38	0.53
29:I:301:CDL:H431	29:I:301:CDL:H471	1.90	0.53
18:s3:118:LYS:O	18:s3:122:HIS:ND1	2.42	0.53
29:I3:301:CDL:H431	29:I3:301:CDL:H471	1.91	0.53
16:Q3:63:LYS:NZ	16:Q3:66:ASP:OD1	2.41	0.53
24:C5:302:LEU:O	24:C5:302:LEU:HD13	2.09	0.53
25:F5:363:ILE:HD11	25:F5:431:LYS:HD3	1.91	0.53
24:A5:442:ASP:OD1	24:A5:443:ALA:N	2.40	0.53
1:A3:110:GLN:NE2	1:A3:143:ASN:OD1	2.41	0.53
5:I3:84:MET:SD	9:H3:77:ARG:NH2	2.81	0.53
7:C:69:THR:O	7:C:73:VAL:HG23	2.09	0.52
19:E:56:ASP:O	19:E:60:HIS:N	2.42	0.52
26:N1:57:LEU:HD23	26:M1:55:PHE:CE2	2.44	0.52
3:D3:108:TYR:OH	18:S3:135:ASN:OD1	2.10	0.52
1:a:184:PHE:HB2	32:i:302:UQ8:H15B	1.91	0.52
9:h:253:GLU:OE2	21:t:422:ARG:NH2	2.41	0.52
18:s:112:ASP:OD1	18:s:113:VAL:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:28:ASP:OD1	10:J:31:THR:N	2.41	0.52
21:t:138:ASP:OD1	21:t:139:LEU:N	2.42	0.52
25:E1:32:VAL:O	25:E1:91:GLY:N	2.36	0.52
26:I1:57:LEU:HD23	26:H1:55:PHE:CE2	2.43	0.52
25:D2:239:GLY:HA3	25:D2:251:VAL:HG11	1.90	0.52
25:F2:150:GLU:N	25:F2:150:GLU:OE1	2.42	0.52
24:A2:414:MET:HA	24:A2:414:MET:HE3	1.92	0.52
24:A4:279:TYR:OH	24:A4:332:LEU:O	2.26	0.52
25:D5:239:GLY:HA3	25:D5:251:VAL:HG11	1.91	0.52
25:F5:157:LYS:NZ	25:F5:432:PHE:O	2.42	0.52
24:A5:440:ASP:OD1	24:A5:441:LEU:N	2.42	0.52
6:K:146:ASN:OD1	6:K:150:GLN:NE2	2.42	0.52
19:E:281:ASN:O	19:E:285:GLY:N	2.40	0.52
24:B2:446:GLN:O	24:B2:450:ASN:ND2	2.42	0.52
26:N2:43:GLU:OE2	27:d2:64:LYS:NZ	2.39	0.52
30:G3:303:PC1:H133	30:G3:303:PC1:O13	2.08	0.52
26:P5:37:LEU:HD23	26:Q5:47:LEU:HD23	1.91	0.52
24:C1:490:SER:O	24:C1:494:LYS:NZ	2.42	0.52
22:G5:182:VAL:HG23	22:G5:182:VAL:O	2.10	0.52
1:a:430:LYS:NZ	16:q:100:GLU:OE1	2.29	0.52
13:n:169:ARG:NH2	11:L:186:GLU:OE2	2.39	0.52
25:F2:481:ASP:OD1	25:F2:482:LEU:N	2.40	0.52
25:E2:168:GLY:O	25:E2:317:THR:OG1	2.26	0.52
5:i3:141:ARG:NE	12:m3:66:ASP:O	2.34	0.52
1:A3:177:TRP:CE3	32:I3:304:UQ8:H25B	2.44	0.52
2:B3:363:ASP:OD1	2:B3:363:ASP:N	2.41	0.52
8:g:43:ARG:NH1	16:q:121:GLU:OE1	2.42	0.52
1:A:110:GLN:NE2	1:A:143:ASN:OD1	2.41	0.52
5:i3:66:VAL:HG21	7:c3:45:VAL:HG21	1.91	0.52
6:k3:76:GLY:O	6:k3:80:ASN:ND2	2.43	0.52
7:C3:69:THR:O	7:C3:73:VAL:HG23	2.10	0.52
27:d4:125:PHE:CE1	28:e4:25:VAL:HG13	2.45	0.52
1:a:398:SER:OG	29:F:302:CDL:H432	2.09	0.52
6:k:37:ALA:N	29:k:201:CDL:OA4	2.35	0.52
18:s:35:ARG:NH1	21:t:126:ASP:OD2	2.42	0.52
5:I:156:GLU:O	5:I:160:ARG:NH1	2.39	0.52
24:C1:113:ILE:HD12	24:C1:113:ILE:O	2.09	0.52
25:F1:150:GLU:OE1	25:F1:150:GLU:N	2.43	0.52
25:F1:303:THR:OG1	25:F1:307:ASP:OD2	2.24	0.52
1:a3:412:LEU:O	1:a3:416:THR:OG1	2.22	0.52
25:E5:334:ASP:OD2	25:E5:356:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:150:ASP:OD1	17:r:142:ARG:NH2	2.42	0.52
22:G1:182:VAL:O	22:G1:182:VAL:HG23	2.10	0.52
27:d2:102:HIS:NE2	27:d2:108:GLU:OE2	2.40	0.52
19:e3:169:GLU:OE1	19:e3:169:GLU:N	2.43	0.52
25:F5:154:THR:O	25:F5:191:ASN:ND2	2.41	0.52
26:N5:43:GLU:OE2	27:d5:64:LYS:NZ	2.39	0.52
4:f:37:THR:OG1	29:F:303:CDL:OB4	2.26	0.52
5:i:49:ILE:HD12	29:l:301:CDL:OB3	2.10	0.52
11:l:123:ARG:NE	29:l:301:CDL:OA4	2.40	0.52
5:I:136:ASN:ND2	11:L:191:TYR:O	2.36	0.52
8:G:197:GLU:OE1	8:G:197:GLU:N	2.39	0.52
25:F1:363:ILE:HD11	25:F1:431:LYS:HD3	1.91	0.52
19:e3:281:ASN:O	19:e3:285:GLY:N	2.40	0.52
24:C4:186:SER:O	24:C4:410:GLN:NE2	2.42	0.52
25:D5:48:LEU:HD21	25:D5:75:SER:HA	1.91	0.52
25:E5:415:LEU:O	25:E5:420:LYS:NZ	2.43	0.52
3:D:87:ILE:O	3:D:88:SER:OG	2.24	0.52
22:G1:51:LEU:HD22	22:G1:114:LEU:HD22	1.91	0.52
24:C1:71:ARG:NH1	24:C1:98:GLU:OE2	2.42	0.52
25:D1:243:GLU:O	25:D1:248:ARG:NH1	2.40	0.52
27:d1:30:GLU:HG3	27:d1:106:THR:HG23	1.91	0.52
27:d1:73:PRO:O	27:d1:94:HIS:NE2	2.42	0.52
28:e4:16:ARG:NH1	28:e4:64:PHE:O	2.43	0.52
24:A5:414:MET:HA	24:A5:414:MET:HE3	1.91	0.52
2:b:363:ASP:OD1	2:b:363:ASP:N	2.40	0.51
3:d:180:GLU:OE2	3:d:192:LYS:NZ	2.42	0.51
23:g1:80:SER:OG	26:O1:42:GLU:OE1	2.28	0.51
25:F2:31:GLN:O	25:F2:43:GLN:N	2.39	0.51
4:f3:27:ARG:NH1	21:t3:423:ASN:OD1	2.38	0.51
1:A3:295:GLY:O	6:K3:54:ARG:NH2	2.39	0.51
25:F4:150:GLU:OE1	25:F4:150:GLU:N	2.43	0.51
3:d:72:VAL:HG13	3:d:72:VAL:O	2.10	0.51
19:E:189:ASP:OD1	19:E:229:THR:OG1	2.27	0.51
26:Q1:41:PRO:O	26:Q1:44:THR:HG23	2.10	0.51
27:d2:73:PRO:O	27:d2:94:HIS:NE2	2.43	0.51
15:P3:88:VAL:O	15:P3:92:SER:OG	2.21	0.51
24:A4:414:MET:HA	24:A4:414:MET:HE3	1.93	0.51
3:D:54:ARG:O	3:D:58:THR:HG23	2.09	0.51
24:B2:238:GLY:N	24:B2:265:ALA:O	2.40	0.51
28:e2:16:ARG:NH1	28:e2:64:PHE:O	2.43	0.51
3:d3:72:VAL:HG13	3:d3:72:VAL:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m3:198:ASP:OD2	12:m3:202:ARG:NH1	2.41	0.51
6:K3:154:ASP:OD1	6:K3:155:SER:N	2.42	0.51
18:S3:134:GLU:OE2	18:S3:137:ARG:NH2	2.43	0.51
25:E4:32:VAL:O	25:E4:91:GLY:N	2.39	0.51
3:d:145:ASP:OD2	7:c:76:LYS:NZ	2.32	0.51
5:I:195:PRO:O	12:M:176:ARG:NH2	2.41	0.51
19:E:90:LYS:NZ	19:E:172:ARG:O	2.42	0.51
25:E2:317:THR:HG23	25:E2:322:SER:HA	1.92	0.51
18:s3:112:ASP:OD1	18:s3:113:VAL:N	2.41	0.51
8:G3:197:GLU:OE1	8:G3:197:GLU:N	2.39	0.51
25:F4:481:ASP:OD1	25:F4:482:LEU:N	2.41	0.51
24:C1:182:LYS:NZ	24:C1:458:MET:O	2.34	0.51
26:M1:71:PHE:O	26:M1:75:ALA:N	2.43	0.51
24:C2:302:LEU:O	24:C2:302:LEU:HD13	2.09	0.51
25:E4:328:ALA:C	25:E4:329:ILE:HD12	2.36	0.51
26:Q4:41:PRO:O	26:Q4:44:THR:HG23	2.11	0.51
26:I5:17:LEU:HB3	26:I5:18:PRO:HD3	1.93	0.51
2:B:333:LEU:HD13	24:A1:36:THR:HB	1.92	0.51
6:K:154:ASP:OD1	6:K:155:SER:N	2.41	0.51
13:N:107:ILE:HG23	13:N:110:HIS:HB3	1.92	0.51
21:t:336:SER:OG	21:t:339:VAL:O	2.29	0.51
25:F1:67:GLU:OE2	25:F1:136:HIS:NE2	2.42	0.51
24:C2:490:SER:O	24:C2:494:LYS:NZ	2.43	0.51
1:a3:430:LYS:NZ	16:q3:100:GLU:OE1	2.26	0.51
19:e3:346:THR:OG1	19:e3:396:HIS:NE2	2.28	0.51
2:B3:333:LEU:HD13	24:A4:36:THR:HB	1.91	0.51
10:J3:213:ARG:NH1	10:J3:220:ASP:OD1	2.41	0.51
12:M3:2:ASP:OD1	13:N3:61:THR:N	2.43	0.51
4:f:27:ARG:NH1	21:t:423:ASN:OD1	2.44	0.51
19:e:165:ASN:ND2	19:e:205:CYS:SG	2.78	0.51
22:G2:105:THR:HG22	22:G2:106:ASN:H	1.76	0.51
26:P2:13:GLY:HA3	26:Q2:11:VAL:HG13	1.93	0.51
25:F5:31:GLN:O	25:F5:43:GLN:N	2.38	0.51
18:s:45:PRO:O	21:t:354:ARG:NH1	2.44	0.51
25:D1:182:THR:N	37:D1:501:ADP:O1B	2.44	0.51
14:o3:104:LEU:HD12	15:p3:143:ARG:HG3	1.93	0.51
26:Q4:37:LEU:CD1	26:Q4:44:THR:HG22	2.40	0.51
1:A:158:GLU:OE1	11:L:176:ARG:NH1	2.42	0.51
25:E1:328:ALA:C	25:E1:329:ILE:HD12	2.36	0.51
27:d1:148:THR:HG21	28:e1:21:SER:HB3	1.93	0.51
24:B2:179:THR:HB	24:B2:213:THR:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:E2:202:PHE:O	25:E2:237:ILE:N	2.40	0.51
32:i3:303:UQ8:H28	11:l3:110:LEU:HD11	1.91	0.51
19:e3:303:ARG:NH1	19:e3:315:GLY:O	2.42	0.51
11:L3:69:ARG:HG2	11:L3:70:PRO:HD3	1.93	0.51
26:O4:45:GLU:OE1	26:O4:45:GLU:N	2.41	0.51
19:e:169:GLU:OE1	19:e:169:GLU:N	2.43	0.51
25:E2:328:ALA:C	25:E2:329:ILE:HD12	2.36	0.51
2:b3:305:ASP:OD2	22:G5:206:ARG:NE	2.42	0.51
17:r3:110:ALA:HB2	11:L3:180:VAL:HG21	1.92	0.51
25:D4:243:GLU:O	25:D4:248:ARG:NH1	2.42	0.51
24:A4:178:GLN:O	24:A4:217:GLN:NE2	2.44	0.51
27:d4:73:PRO:O	27:d4:94:HIS:NE2	2.44	0.51
2:B:363:ASP:OD1	2:B:363:ASP:N	2.41	0.50
22:G1:217:ILE:O	22:G1:218:SER:OG	2.25	0.50
25:F2:303:THR:OG1	25:F2:307:ASP:OD2	2.24	0.50
10:j3:213:ARG:NH1	10:j3:220:ASP:OD1	2.41	0.50
24:C4:98:GLU:OE1	24:C4:101:ASN:ND2	2.44	0.50
25:E4:459:SER:OG	25:E4:481:ASP:OD1	2.29	0.50
24:C5:490:SER:O	24:C5:494:LYS:NZ	2.44	0.50
25:F5:418:GLU:OE1	25:F5:418:GLU:N	2.44	0.50
1:a:14:TYR:N	1:a:17:PHE:O	2.44	0.50
16:Q:82:THR:OG1	18:S:103:SER:O	2.26	0.50
24:A2:222:ASN:OD1	24:A2:258:LYS:NZ	2.38	0.50
28:e2:25:VAL:O	28:e2:25:VAL:HG12	2.12	0.50
1:A3:158:GLU:OE1	11:L3:176:ARG:NH1	2.40	0.50
2:B3:305:ASP:OD2	22:G4:206:ARG:NE	2.45	0.50
22:G4:182:VAL:O	22:G4:182:VAL:HG23	2.10	0.50
26:P4:12:MET:HE3	26:Q4:68:LEU:HD11	1.93	0.50
26:I4:11:VAL:HG13	26:H4:13:GLY:CA	2.41	0.50
25:F5:235:ALA:C	25:F5:236:LEU:HD12	2.36	0.50
32:i:302:UQ8:H28	11:l:110:LEU:HD11	1.91	0.50
3:D:30:ALA:O	3:D:70:GLN:NE2	2.41	0.50
7:c3:82:ASP:OD1	7:c3:83:PHE:N	2.45	0.50
3:D3:54:ARG:O	3:D3:58:THR:HG23	2.12	0.50
25:E5:328:ALA:C	25:E5:329:ILE:HD12	2.37	0.50
25:F2:235:ALA:C	25:F2:236:LEU:HD12	2.36	0.50
24:A2:266:THR:N	24:A2:269:ASP:OD2	2.39	0.50
32:I3:304:UQ8:H25A	32:I3:304:UQ8:C28	2.42	0.50
22:G4:105:THR:HG22	22:G4:106:ASN:H	1.76	0.50
25:F4:418:GLU:OE1	25:F4:418:GLU:N	2.42	0.50
25:E4:56:GLU:OE2	25:E4:63:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A5:241:ARG:CG	24:A5:266:THR:HG21	2.41	0.50
22:G1:105:THR:HG22	22:G1:106:ASN:H	1.76	0.50
25:D1:248:ARG:NH2	25:D1:286:GLU:OE1	2.45	0.50
25:F1:235:ALA:C	25:F1:236:LEU:HD12	2.37	0.50
1:a3:226:THR:HG21	5:i3:88:PHE:HD2	1.77	0.50
7:c3:76:LYS:O	18:s3:79:GLN:NE2	2.44	0.50
5:l3:142:THR:N	11:l3:164:CYS:O	2.42	0.50
25:F4:248:ARG:NH2	25:F4:286:GLU:OE1	2.45	0.50
25:E4:243:GLU:O	25:E4:248:ARG:NH1	2.44	0.50
27:d5:130:ILE:H	27:d5:130:ILE:HD12	1.76	0.50
10:j:72:ASN:ND2	10:j:95:ASN:OD1	2.41	0.50
21:t:241:LYS:O	21:t:245:GLY:N	2.40	0.50
25:F1:418:GLU:OE1	25:F1:418:GLU:N	2.42	0.50
22:G2:182:VAL:HG23	22:G2:182:VAL:O	2.10	0.50
25:E2:415:LEU:O	25:E2:420:LYS:NZ	2.40	0.50
17:r3:98:GLN:OE1	17:r3:101:ARG:NH1	2.43	0.50
24:B5:446:GLN:O	24:B5:450:ASN:ND2	2.45	0.50
26:P5:13:GLY:HA3	26:Q5:11:VAL:HG13	1.93	0.50
24:C1:98:GLU:OE1	24:C1:101:ASN:ND2	2.43	0.50
26:l1:11:VAL:HG13	26:H1:13:GLY:CA	2.42	0.50
25:D2:208:ARG:O	25:D2:240:GLN:NE2	2.45	0.50
2:b3:229:GLU:OE2	2:b3:232:ARG:NH2	2.41	0.50
18:s3:35:ARG:NH1	21:t3:126:ASP:OD2	2.44	0.50
21:t3:327:ARG:NH2	21:t3:401:HIS:O	2.44	0.50
25:D4:235:ALA:C	25:D4:236:LEU:HD12	2.37	0.50
27:d4:30:GLU:HG3	27:d4:106:THR:HG23	1.94	0.50
3:d:130:ASN:OD1	18:s:89:ARG:NH2	2.44	0.50
12:m:198:ASP:OD2	12:m:202:ARG:NH1	2.40	0.50
24:B2:111:ARG:NH1	25:F2:53:ASN:OD1	2.43	0.50
18:s3:37:MET:SD	21:t3:407:ARG:NH2	2.85	0.50
24:C4:165:PRO:O	24:C4:170:ARG:NH1	2.45	0.50
22:G5:105:THR:HG22	22:G5:106:ASN:H	1.76	0.50
25:D5:416:SER:OG	25:D5:419:ASP:OD1	2.30	0.50
25:E5:317:THR:HG23	25:E5:322:SER:HA	1.94	0.50
27:d5:102:HIS:NE2	27:d5:108:GLU:OE2	2.44	0.50
24:C2:163:LYS:HZ3	25:F2:83:ASP:CG	2.18	0.50
24:C2:165:PRO:O	24:C2:170:ARG:NH1	2.43	0.50
26:L2:68:LEU:HD11	26:K2:12:MET:HE3	1.93	0.50
19:e3:324:GLN:O	19:e3:376:TYR:N	2.40	0.50
25:E5:364:TYR:HB2	25:E5:478:MET:HE1	1.93	0.50
1:A:229:ASP:OD1	5:I:70:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:43:ARG:NH1	16:Q:121:GLU:OE1	2.45	0.49
27:d1:125:PHE:CE1	28:e1:25:VAL:HG13	2.47	0.49
24:C2:67:ASP:OD1	25:D2:293:ARG:NH2	2.44	0.49
24:B2:77:LYS:O	24:B2:121:ARG:NH1	2.45	0.49
24:B2:111:ARG:O	25:F2:50:GLN:NE2	2.38	0.49
7:C3:75:LEU:HA	7:C3:79:ALA:HB3	1.93	0.49
8:G3:43:ARG:NH1	16:Q3:121:GLU:OE1	2.44	0.49
26:M4:57:LEU:HD23	26:L4:55:PHE:CE2	2.47	0.49
24:C5:362:ALA:HB2	25:D5:337:THR:HG21	1.94	0.49
25:E5:168:GLY:O	25:E5:317:THR:OG1	2.28	0.49
3:d:122:SER:OG	3:d:123:LYS:N	2.45	0.49
8:g:101:ARG:NH2	8:g:146:LYS:O	2.45	0.49
24:C2:163:LYS:NZ	25:F2:83:ASP:OD2	2.34	0.49
24:B2:279:TYR:OH	24:B2:332:LEU:O	2.28	0.49
6:k3:94:ASN:OD1	6:k3:95:ASP:N	2.45	0.49
1:A3:226:THR:HG21	5:I3:88:PHE:HD2	1.76	0.49
10:J3:72:ASN:ND2	10:J3:95:ASN:OD1	2.40	0.49
7:c:82:ASP:OD1	7:c:83:PHE:N	2.45	0.49
15:p:89:PHE:O	15:p:94:ASN:ND2	2.41	0.49
21:t:137:CYS:O	21:t:283:ASN:ND2	2.40	0.49
27:d1:28:LYS:O	27:d1:29:MET:HB2	2.12	0.49
24:A2:84:VAL:O	24:A2:92:GLY:N	2.46	0.49
1:a3:140:TRP:O	12:m3:219:GLN:NE2	2.39	0.49
3:D3:87:ILE:O	3:D3:88:SER:OG	2.25	0.49
24:C5:98:GLU:OE1	24:C5:101:ASN:ND2	2.42	0.49
24:A5:487:LEU:HD23	24:A5:487:LEU:H	1.77	0.49
3:d:194:ASP:OD2	9:h:128:GLN:N	2.45	0.49
9:h:39:TYR:OH	9:h:42:ARG:NH2	2.45	0.49
26:I1:11:VAL:HG13	26:H1:13:GLY:HA3	1.94	0.49
24:C2:208:ALA:N	33:C2:601:ATP:O1A	2.45	0.49
24:A2:487:LEU:HD23	24:A2:487:LEU:H	1.78	0.49
25:E2:177:ALA:O	25:E2:356:ARG:NH2	2.45	0.49
26:I2:11:VAL:HG13	26:H2:13:GLY:CA	2.42	0.49
24:B4:238:GLY:N	24:B4:265:ALA:O	2.43	0.49
5:i:51:ARG:NH2	17:r:31:GLU:OE2	2.37	0.49
2:B:218:ARG:NH1	3:D:121:SER:OG	2.45	0.49
24:A1:414:MET:HA	24:A1:414:MET:HE3	1.93	0.49
21:t3:253:ILE:CD1	21:t3:263:VAL:HG22	2.41	0.49
24:B5:179:THR:HB	24:B5:213:THR:HG22	1.94	0.49
25:F5:156:ILE:HD12	25:F5:156:ILE:N	2.28	0.49
1:a:383:ILE:HG21	29:B:404:CDL:H601	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:394:PHE:CZ	29:F:302:CDL:H431	2.46	0.49
5:I:79:HIS:NE2	5:I:84:MET:O	2.46	0.49
24:B2:160:VAL:O	24:B2:339:ARG:NH1	2.38	0.49
25:F2:418:GLU:OE1	25:F2:418:GLU:N	2.44	0.49
26:Q2:41:PRO:O	26:Q2:44:THR:HG23	2.13	0.49
11:l3:44:VAL:HG21	26:K4:3:LEU:HB2	1.93	0.49
25:F4:235:ALA:C	25:F4:236:LEU:HD12	2.38	0.49
27:d5:30:GLU:HG3	27:d5:106:THR:HG23	1.95	0.49
1:a:398:SER:HB2	29:F:302:CDL:H412	1.95	0.49
11:l:243:MET:SD	11:l:243:MET:N	2.83	0.49
26:H1:11:VAL:HG13	26:Q1:13:GLY:CA	2.43	0.49
24:A2:178:GLN:O	24:A2:217:GLN:NE2	2.46	0.49
26:J2:47:LEU:HD23	26:I2:37:LEU:HD23	1.93	0.49
1:a3:295:GLY:O	6:k3:54:ARG:NH2	2.42	0.49
24:C4:67:ASP:OD1	25:D4:293:ARG:NH2	2.46	0.49
26:Q5:17:LEU:HB3	26:Q5:18:PRO:HD3	1.95	0.49
24:C1:67:ASP:OD1	25:D1:293:ARG:NH2	2.46	0.49
25:E2:364:TYR:HB2	25:E2:478:MET:HE1	1.95	0.49
26:I4:11:VAL:HG13	26:H4:13:GLY:HA3	1.93	0.49
2:b:117:THR:HG23	29:F:303:CDL:H182	1.95	0.49
2:B:78:HIS:NE2	29:I:301:CDL:OA4	2.44	0.49
32:I:303:UQ8:H25A	32:I:303:UQ8:C28	2.43	0.49
10:J:183:ARG:NH2	12:M:37:ASP:OD2	2.45	0.49
16:Q:122:THR:O	16:Q:125:VAL:HG22	2.13	0.49
19:E:328:HIS:ND1	19:E:330:LYS:O	2.46	0.49
25:F1:156:ILE:N	25:F1:156:ILE:HD12	2.28	0.49
26:L1:71:PHE:O	26:L1:75:ALA:N	2.46	0.49
25:F4:156:ILE:N	25:F4:156:ILE:HD12	2.28	0.49
24:A5:178:GLN:O	24:A5:217:GLN:NE2	2.45	0.49
28:e5:25:VAL:O	28:e5:25:VAL:HG12	2.12	0.49
29:i3:301:CDL:H372	32:i3:303:UQ8:H40	1.95	0.49
4:F3:87:LYS:NZ	29:I3:302:CDL:OA3	2.40	0.49
22:G4:40:GLU:OE1	22:G4:133:LYS:NZ	2.45	0.49
24:B4:446:GLN:O	24:B4:450:ASN:ND2	2.44	0.49
25:D5:205:VAL:HG12	25:D5:251:VAL:HG13	1.95	0.49
25:D1:235:ALA:C	25:D1:236:LEU:HD12	2.38	0.48
26:K2:68:LEU:HD21	26:J2:12:MET:HE3	1.95	0.48
26:I2:17:LEU:HB3	26:I2:18:PRO:HD3	1.94	0.48
5:i3:49:ILE:HD12	29:l3:301:CDL:OB3	2.13	0.48
21:t3:99:HIS:O	21:t3:99:HIS:ND1	2.42	0.48
24:A5:266:THR:N	24:A5:269:ASP:OD2	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:E5:112:ARG:NH2	25:E5:125:GLY:O	2.40	0.48
19:e:51:CYS:O	19:e:55:PHE:N	2.42	0.48
25:D2:235:ALA:C	25:D2:236:LEU:HD12	2.38	0.48
24:B2:485:ASP:OD1	24:B2:486:ALA:N	2.46	0.48
25:F2:156:ILE:HD12	25:F2:156:ILE:N	2.28	0.48
27:d2:130:ILE:HD12	27:d2:130:ILE:H	1.77	0.48
11:L3:243:MET:SD	11:L3:243:MET:N	2.86	0.48
25:F4:67:GLU:OE2	25:F4:136:HIS:NE2	2.44	0.48
26:J5:71:PHE:O	26:J5:75:ALA:N	2.46	0.48
13:n:75:ARG:NH2	17:R:107:GLU:OE2	2.42	0.48
11:L:24:LYS:O	11:L:28:ASN:ND2	2.43	0.48
23:g1:76:LEU:O	23:g1:83:GLN:NE2	2.45	0.48
25:E1:172:GLY:HA3	25:E1:348:LEU:HD13	1.95	0.48
26:I1:2:LEU:O	26:I1:6:ALA:N	2.44	0.48
26:I2:11:VAL:HG13	26:H2:13:GLY:HA3	1.94	0.48
3:d3:86:VAL:HG13	3:d3:87:ILE:N	2.29	0.48
29:B3:404:CDL:OB4	4:F3:76:ARG:NH1	2.45	0.48
8:G3:101:ARG:NH2	8:G3:146:LYS:O	2.46	0.48
27:d4:148:THR:HG21	28:e4:21:SER:HB3	1.95	0.48
26:K5:68:LEU:HD21	26:J5:12:MET:HE3	1.96	0.48
24:C1:209:ILE:HD12	24:C1:383:LEU:HD11	1.95	0.48
27:d2:148:THR:HG21	28:e2:21:SER:HB3	1.95	0.48
1:a3:398:SER:OG	29:a3:502:CDL:H432	2.12	0.48
19:E3:237:GLU:OE1	19:E3:264:ASN:ND2	2.46	0.48
24:B5:485:ASP:OD1	24:B5:486:ALA:N	2.46	0.48
3:D:86:VAL:HG13	3:D:87:ILE:N	2.29	0.48
24:A1:114:LYS:NZ	25:E1:48:LEU:O	2.33	0.48
24:C2:98:GLU:OE1	24:C2:101:ASN:ND2	2.43	0.48
25:D2:157:LYS:NZ	25:D2:432:PHE:O	2.41	0.48
8:g3:260:CYS:SG	8:g3:261:ASP:N	2.86	0.48
25:E4:303:THR:OG1	25:E4:307:ASP:OD2	2.31	0.48
27:d4:28:LYS:O	27:d4:29:MET:HB2	2.13	0.48
25:D5:58:GLN:O	25:D5:92:GLN:NE2	2.46	0.48
25:D5:235:ALA:C	25:D5:236:LEU:HD12	2.38	0.48
24:A5:201:ASP:O	24:A5:206:LYS:NZ	2.44	0.48
26:P5:40:ASN:ND2	26:P5:43:GLU:OE1	2.46	0.48
3:d3:122:SER:OG	3:d3:123:LYS:N	2.46	0.48
4:f3:187:GLN:OE1	4:f3:190:ARG:NH2	2.46	0.48
19:E3:328:HIS:ND1	19:E3:330:LYS:O	2.45	0.48
24:C5:317:ARG:NH1	25:D5:292:GLY:O	2.44	0.48
3:d:86:VAL:HG13	3:d:87:ILE:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:e:316:ASN:OD1	19:e:317:GLY:N	2.47	0.48
3:D:60:LEU:O	3:D:60:LEU:HD13	2.13	0.48
5:I:142:THR:N	11:L:164:CYS:O	2.46	0.48
24:A1:487:LEU:HD23	24:A1:487:LEU:H	1.78	0.48
26:O1:47:LEU:HD23	26:N1:37:LEU:HD23	1.96	0.48
25:F2:154:THR:O	25:F2:191:ASN:ND2	2.43	0.48
25:F2:248:ARG:NH2	25:F2:286:GLU:OE1	2.46	0.48
11:I3:243:MET:SD	11:I3:243:MET:N	2.86	0.48
19:e3:316:ASN:OD1	19:e3:317:GLY:N	2.47	0.48
5:I3:46:VAL:HG23	5:I3:51:ARG:CZ	2.43	0.48
5:I3:64:GLN:OE1	32:I3:304:UQ8:H4MA	2.12	0.48
20:i4:57:LEU:HD12	20:i4:58:LEU:N	2.29	0.48
26:H4:11:VAL:HG13	26:Q4:13:GLY:CA	2.44	0.48
25:D5:54:ALA:O	25:D5:97:THR:OG1	2.30	0.48
8:g:158:ARG:NH1	8:g:173:GLU:OE2	2.39	0.48
10:j:213:ARG:NH1	10:j:220:ASP:OD1	2.46	0.48
21:t:250:LEU:O	21:t:253:ILE:HG22	2.14	0.48
24:A1:138:VAL:N	24:A1:147:ASP:OD2	2.47	0.48
26:O1:45:GLU:OE1	26:O1:45:GLU:N	2.41	0.48
23:g2:93:SER:OG	23:g2:179:ASP:OD1	2.29	0.48
24:A5:138:VAL:N	24:A5:147:ASP:OD2	2.47	0.48
12:m:2:ASP:OD1	13:n:61:THR:N	2.47	0.48
2:B:141:THR:HG22	2:B:141:THR:O	2.13	0.48
25:F1:210:ARG:NH2	25:F1:211:GLU:OE2	2.47	0.48
10:J3:28:ASP:OD1	10:J3:31:THR:N	2.45	0.48
23:g4:125:ARG:O	23:g4:126:SER:OG	2.22	0.48
24:B4:114:LYS:NZ	25:F4:47:GLU:OE2	2.37	0.48
24:B4:485:ASP:OD1	24:B4:486:ALA:N	2.47	0.48
25:F4:303:THR:OG1	25:F4:307:ASP:OD2	2.27	0.48
24:A4:67:ASP:OD1	25:E4:70:GLN:NE2	2.47	0.48
24:A5:438:GLY:O	24:A5:439:SER:OG	2.28	0.48
26:P5:2:LEU:HD13	26:Q5:1:MET:N	2.29	0.48
26:P1:13:GLY:HA3	26:Q1:11:VAL:HG13	1.95	0.48
1:a3:398:SER:HB2	29:a3:502:CDL:H412	1.96	0.48
27:d4:130:ILE:H	27:d4:130:ILE:HD12	1.79	0.48
19:e:281:ASN:O	19:e:285:GLY:N	2.44	0.47
23:g1:202:LEU:HD23	23:g1:202:LEU:H	1.79	0.47
24:B1:485:ASP:OD1	24:B1:486:ALA:N	2.47	0.47
24:A1:58:GLU:OE2	24:A1:76:THR:N	2.47	0.47
25:E1:56:GLU:OE2	25:E1:63:ARG:NH2	2.47	0.47
26:H2:11:VAL:HG13	26:Q2:13:GLY:HA3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:g4:202:LEU:HD23	23:g4:202:LEU:H	1.79	0.47
24:A4:138:VAL:N	24:A4:147:ASP:OD2	2.47	0.47
26:I5:11:VAL:HG13	26:H5:13:GLY:CA	2.44	0.47
6:k:94:ASN:OD1	6:k:95:ASP:N	2.47	0.47
11:L:124:VAL:HG22	29:L:302:CDL:HA62	1.96	0.47
25:D2:68:VAL:HA	25:D2:79:THR:HG22	1.95	0.47
25:D2:416:SER:OG	25:D2:419:ASP:OD1	2.32	0.47
26:O2:68:LEU:HD11	26:N2:12:MET:HE3	1.96	0.47
17:r3:139:VAL:HG21	13:N3:171:VAL:HG11	1.96	0.47
3:D3:86:VAL:HG13	3:D3:87:ILE:N	2.29	0.47
3:D3:183:GLU:OE1	12:M3:103:ARG:NE	2.46	0.47
16:Q3:122:THR:O	16:Q3:125:VAL:HG22	2.13	0.47
20:i4:78:ASN:OD1	20:i4:97:ILE:HG21	2.14	0.47
20:i1:57:LEU:HD12	20:i1:58:LEU:N	2.28	0.47
24:B1:98:GLU:O	25:E1:90:ARG:NH1	2.44	0.47
24:B1:279:TYR:OH	24:B1:332:LEU:O	2.28	0.47
24:A1:201:ASP:O	24:A1:206:LYS:NZ	2.43	0.47
19:e3:56:ASP:O	19:e3:60:HIS:N	2.44	0.47
24:A4:114:LYS:NZ	25:E4:48:LEU:O	2.34	0.47
27:d4:109:ILE:HD12	27:d4:109:ILE:N	2.29	0.47
25:D5:157:LYS:NZ	25:D5:432:PHE:O	2.43	0.47
27:d5:28:LYS:HG3	27:d5:29:MET:N	2.30	0.47
3:d:183:GLU:OE1	12:m:103:ARG:NE	2.48	0.47
29:F:302:CDL:H351	26:I2:53:MET:SD	2.54	0.47
19:E:324:GLN:O	19:E:376:TYR:N	2.42	0.47
18:s3:120:TYR:O	18:s3:124:ILE:HG22	2.14	0.47
5:I3:190:GLN:OE1	5:I3:190:GLN:N	2.47	0.47
24:B4:179:THR:HB	24:B4:213:THR:HG22	1.96	0.47
25:F4:82:MET:HE2	25:F4:82:MET:HA	1.96	0.47
24:A4:438:GLY:O	24:A4:439:SER:OG	2.26	0.47
23:g2:172:SER:OG	23:g2:204:ARG:NH1	2.47	0.47
24:A2:241:ARG:CG	24:A2:266:THR:HG21	2.44	0.47
26:P2:12:MET:HE3	26:Q2:68:LEU:HD11	1.96	0.47
14:o3:57:ASN:OD1	14:o3:58:THR:N	2.48	0.47
23:g4:282:GLN:NE2	25:F4:335:ASP:OD2	2.45	0.47
1:A:392:THR:O	1:A:396:VAL:HG22	2.14	0.47
18:S:112:ASP:OD1	18:S:113:VAL:N	2.47	0.47
25:D1:58:GLN:O	25:D1:92:GLN:NE2	2.45	0.47
24:B1:446:GLN:O	24:B1:450:ASN:ND2	2.46	0.47
26:M1:57:LEU:HD23	26:L1:55:PHE:CE2	2.49	0.47
24:A2:438:GLY:O	24:A2:439:SER:OG	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:E2:153:VAL:O	25:E2:153:VAL:HG23	2.15	0.47
27:d2:74:PRO:HG2	27:d2:148:THR:HG22	1.97	0.47
3:d3:134:PHE:CE2	3:d3:138:ILE:HD11	2.50	0.47
5:i3:156:GLU:O	5:i3:160:ARG:NH1	2.48	0.47
19:e3:205:CYS:SG	36:e3:900:NAD:N7N	2.86	0.47
25:E5:428:LYS:NZ	25:E5:469:ASP:O	2.47	0.47
8:g:223:GLU:OE2	16:q:130:LYS:NZ	2.47	0.47
1:A:446:ASN:ND2	7:C:62:GLN:O	2.45	0.47
12:M:3:ASN:ND2	12:M:40:GLU:OE2	2.47	0.47
24:B1:160:VAL:O	24:B1:339:ARG:NH1	2.40	0.47
24:A1:438:GLY:O	24:A1:439:SER:OG	2.27	0.47
26:J1:71:PHE:O	26:J1:75:ALA:N	2.47	0.47
27:d1:109:ILE:HD12	27:d1:109:ILE:N	2.29	0.47
27:d2:28:LYS:HG3	27:d2:29:MET:N	2.29	0.47
27:d2:126:GLU:C	27:d2:130:ILE:HD11	2.40	0.47
7:c3:49:TRP:N	7:c3:50:PRO:CD	2.78	0.47
11:l3:206:ILE:N	11:l3:207:PRO:CD	2.78	0.47
3:D3:180:GLU:OE2	3:D3:192:LYS:NZ	2.48	0.47
5:I3:16:SER:OG	5:I3:20:ASN:ND2	2.48	0.47
21:t3:250:LEU:O	21:t3:253:ILE:HG22	2.14	0.47
25:E4:172:GLY:HA3	25:E4:348:LEU:HD13	1.95	0.47
26:M4:71:PHE:O	26:M4:75:ALA:N	2.48	0.47
26:H5:53:MET:HE1	26:Q5:52:LEU:HD21	1.96	0.47
3:d3:60:LEU:O	3:d3:60:LEU:HD13	2.15	0.47
26:O4:47:LEU:HD23	26:N4:37:LEU:HD23	1.97	0.47
25:E5:153:VAL:HG23	25:E5:153:VAL:O	2.15	0.47
4:f:187:GLN:OE1	4:f:190:ARG:NH2	2.48	0.47
7:c:49:TRP:N	7:c:50:PRO:CD	2.78	0.47
25:E1:112:ARG:NH2	25:E1:125:GLY:O	2.41	0.47
25:E1:153:VAL:HG23	25:E1:153:VAL:O	2.15	0.47
25:F2:131:LYS:C	25:F2:132:LEU:HD12	2.40	0.47
9:h3:190:GLU:OE1	9:h3:190:GLU:N	2.46	0.47
11:l3:186:GLU:OE1	13:N3:169:ARG:NH1	2.47	0.47
8:G3:158:ARG:NH1	8:G3:173:GLU:OE2	2.42	0.47
25:D4:208:ARG:O	25:D4:240:GLN:NE2	2.47	0.47
24:A4:487:LEU:HD23	24:A4:487:LEU:H	1.78	0.47
26:Q5:41:PRO:O	26:Q5:44:THR:HG23	2.14	0.47
5:i:84:MET:SD	9:h:77:ARG:NH2	2.88	0.47
5:I:61:MET:HE1	12:M:97:ASN:HB2	1.95	0.47
10:J:11:TYR:OH	11:L:67:LEU:O	2.23	0.47
27:d1:130:ILE:H	27:d1:130:ILE:HD12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:D2:205:VAL:HG12	25:D2:251:VAL:HG13	1.96	0.47
24:C4:517:SER:OG	24:C4:519:ASP:OD1	2.21	0.47
5:i:194:LEU:HD23	10:j:196:VAL:HB	1.97	0.46
8:g:260:CYS:SG	8:g:261:ASP:N	2.87	0.46
9:h:190:GLU:OE1	9:h:190:GLU:N	2.46	0.46
1:A:178:ILE:CG2	29:L:302:CDL:H473	2.46	0.46
7:C:61:SER:OG	7:C:63:GLU:OE2	2.31	0.46
11:L:193:ARG:NH2	17:R:106:THR:O	2.48	0.46
11:L:206:ILE:N	11:L:207:PRO:CD	2.78	0.46
23:g4:76:LEU:O	23:g4:83:GLN:NE2	2.43	0.46
25:F5:275:ASP:OD1	25:F5:276:ASN:N	2.47	0.46
29:f:304:CDL:OA4	2:B:113:LYS:NZ	2.36	0.46
11:l:74:LEU:HD21	11:L3:58:GLU:OE1	2.15	0.46
7:C:49:TRP:N	7:C:50:PRO:CD	2.78	0.46
24:B2:222:ASN:OD1	24:B2:258:LYS:NZ	2.44	0.46
25:E2:56:GLU:OE2	25:E2:63:ARG:NH2	2.48	0.46
26:Q2:17:LEU:HB3	26:Q2:18:PRO:HD3	1.95	0.46
3:d3:60:LEU:HD13	3:d3:60:LEU:C	2.40	0.46
16:q3:116:TYR:OH	16:q3:140:GLU:OE2	2.32	0.46
29:B3:404:CDL:OB3	4:F3:75:LYS:NZ	2.41	0.46
28:e4:57:ILE:N	28:e4:57:ILE:HD12	2.30	0.46
24:B5:160:VAL:O	24:B5:339:ARG:NH1	2.40	0.46
27:d5:109:ILE:N	27:d5:109:ILE:HD12	2.30	0.46
19:E:376:TYR:OH	19:E:379:PHE:O	2.29	0.46
26:L1:12:MET:HE1	26:L1:70:PHE:CE2	2.51	0.46
26:I2:56:ALA:O	26:I2:60:THR:OG1	2.33	0.46
3:d3:129:GLU:O	3:d3:133:SER:OG	2.24	0.46
2:B3:141:THR:HG22	2:B3:141:THR:O	2.15	0.46
24:B4:159:ARG:NH1	24:B4:162:ILE:HG22	2.30	0.46
25:E4:202:PHE:O	25:E4:237:ILE:N	2.41	0.46
25:E5:68:VAL:HA	25:E5:79:THR:HG22	1.97	0.46
27:d5:28:LYS:O	27:d5:63:ASN:ND2	2.48	0.46
3:D:231:MET:SD	26:Q1:56:ALA:HB2	2.55	0.46
24:B1:159:ARG:NH1	24:B1:162:ILE:HG22	2.31	0.46
24:C2:71:ARG:NH1	24:C2:98:GLU:OE2	2.48	0.46
24:B2:241:ARG:HE	24:B2:266:THR:HG21	1.80	0.46
27:d2:109:ILE:N	27:d2:109:ILE:HD12	2.30	0.46
1:a3:158:GLU:OE1	11:l3:176:ARG:NH1	2.42	0.46
2:b3:141:THR:O	2:b3:141:THR:HG22	2.16	0.46
18:S3:118:LYS:O	18:S3:122:HIS:ND1	2.48	0.46
24:B5:241:ARG:HE	24:B5:266:THR:HG21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:I5:11:VAL:HG13	26:H5:13:GLY:HA3	1.96	0.46
2:b:229:GLU:OE2	2:b:232:ARG:NH2	2.41	0.46
8:g:47:LYS:NZ	8:g:151:ASP:OD2	2.41	0.46
9:h:255:ARG:NH2	21:t:428:ILE:O	2.44	0.46
13:n:124:GLY:O	13:n:125:LEU:HD22	2.16	0.46
18:s:120:TYR:O	18:s:124:ILE:HG22	2.16	0.46
5:I:190:GLN:OE1	5:I:190:GLN:N	2.49	0.46
18:S:145:ILE:C	18:S:145:ILE:HD12	2.41	0.46
25:F1:82:MET:HE2	25:F1:82:MET:HA	1.96	0.46
28:e1:57:ILE:N	28:e1:57:ILE:HD12	2.30	0.46
25:E2:235:ALA:C	25:E2:236:LEU:HD12	2.41	0.46
27:d2:30:GLU:HG3	27:d2:106:THR:HG23	1.97	0.46
9:h3:132:ASP:OD1	9:h3:133:GLN:NE2	2.48	0.46
3:D3:60:LEU:O	3:D3:60:LEU:HD13	2.15	0.46
25:D4:441:GLU:O	25:D4:445:GLY:N	2.48	0.46
24:B4:98:GLU:O	25:E4:90:ARG:NH1	2.42	0.46
25:F4:210:ARG:NH2	25:F4:211:GLU:OE2	2.49	0.46
25:E4:317:THR:HG23	25:E4:322:SER:HA	1.98	0.46
23:g5:184:ILE:HD12	23:g5:184:ILE:N	2.31	0.46
25:E5:80:ILE:HD12	25:E5:80:ILE:N	2.31	0.46
5:I:79:HIS:ND1	5:I:84:MET:SD	2.88	0.46
25:D1:441:GLU:O	25:D1:445:GLY:N	2.47	0.46
26:P2:27:GLY:CA	26:Q2:58:ILE:HD11	2.45	0.46
26:K2:17:LEU:HB3	26:K2:18:PRO:HD3	1.98	0.46
25:D4:58:GLN:O	25:D4:92:GLN:NE2	2.44	0.46
25:D5:248:ARG:NH2	25:D5:286:GLU:OE1	2.48	0.46
25:F5:131:LYS:C	25:F5:132:LEU:HD12	2.40	0.46
9:h3:139:GLU:O	9:h3:143:VAL:HG23	2.14	0.46
22:G4:51:LEU:HD22	22:G4:114:LEU:HD22	1.97	0.46
25:F4:441:GLU:O	25:F4:445:GLY:N	2.46	0.46
26:L5:68:LEU:HD11	26:K5:12:MET:HE3	1.98	0.46
26:J5:47:LEU:HD23	26:I5:37:LEU:HD23	1.98	0.46
14:o:104:LEU:HD12	15:p:143:ARG:HG3	1.96	0.46
18:s:134:GLU:OE2	18:s:137:ARG:NH2	2.46	0.46
3:D:129:GLU:O	3:D:133:SER:OG	2.26	0.46
26:Q1:1:MET:HE2	26:Q1:1:MET:HA	1.98	0.46
25:D2:58:GLN:O	25:D2:92:GLN:NE2	2.46	0.46
25:E2:329:ILE:HD12	25:E2:329:ILE:N	2.31	0.46
29:a3:502:CDL:H351	26:I5:53:MET:SD	2.56	0.46
6:k3:12:ASN:OD1	33:g3:301:ATP:N6	2.49	0.46
18:s3:145:ILE:C	18:s3:145:ILE:HD12	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D3:231:MET:SD	26:Q4:56:ALA:HB2	2.56	0.46
10:J3:130:GLN:NE2	12:M3:59:THR:OG1	2.49	0.46
26:P4:13:GLY:HA3	26:Q4:11:VAL:HG13	1.98	0.46
24:A5:84:VAL:O	24:A5:92:GLY:N	2.47	0.46
26:O5:68:LEU:HD11	26:N5:12:MET:HE3	1.98	0.46
26:H5:17:LEU:HB3	26:H5:18:PRO:HD3	1.98	0.46
14:o:57:ASN:OD1	14:o:58:THR:N	2.49	0.46
11:L:113:ARG:NH2	29:L:302:CDL:OB4	2.41	0.46
19:E:165:ASN:ND2	19:E:205:CYS:SG	2.85	0.46
23:g2:184:ILE:N	23:g2:184:ILE:HD12	2.31	0.46
1:A3:226:THR:HG23	1:A3:231:TYR:HD2	1.81	0.46
7:C3:49:TRP:N	7:C3:50:PRO:CD	2.79	0.46
18:S3:145:ILE:C	18:S3:145:ILE:HD12	2.41	0.46
25:F4:363:ILE:HD11	25:F4:431:LYS:HD3	1.97	0.46
26:Q4:1:MET:HE2	26:Q4:1:MET:HA	1.96	0.46
25:E5:231:GLU:O	25:E5:232:SER:OG	2.25	0.46
1:a:398:SER:CB	29:F:302:CDL:H432	2.45	0.46
11:l:206:ILE:N	11:l:207:PRO:CD	2.79	0.46
16:Q:65:GLU:OE1	16:Q:65:GLU:N	2.46	0.46
21:t:167:ASN:ND2	21:t:174:HIS:O	2.38	0.46
25:D1:208:ARG:O	25:D1:240:GLN:NE2	2.49	0.46
25:E2:80:ILE:HD12	25:E2:80:ILE:N	2.31	0.46
26:H2:57:LEU:HD23	26:Q2:55:PHE:CD2	2.50	0.46
1:a3:226:THR:HG23	1:a3:231:TYR:HD2	1.81	0.46
11:l3:32:LYS:NZ	29:l3:303:CDL:O1	2.35	0.46
16:q3:87:LEU:HD12	16:q3:91:SER:CB	2.46	0.46
3:D3:72:VAL:HG13	3:D3:72:VAL:O	2.16	0.46
9:H3:253:GLU:OE1	9:H3:255:ARG:NH2	2.48	0.46
13:N3:107:ILE:HG23	13:N3:110:HIS:HB3	1.98	0.46
20:i5:57:LEU:HD12	20:i5:58:LEU:N	2.31	0.46
26:H4:11:VAL:HG13	26:Q4:13:GLY:HA3	1.98	0.46
10:j:44:ILE:C	10:j:44:ILE:HD12	2.41	0.45
11:L:16:GLU:OE1	11:L:16:GLU:N	2.46	0.45
26:H2:17:LEU:HB3	26:H2:18:PRO:HD3	1.98	0.45
22:G4:141:LEU:O	22:G4:141:LEU:HD13	2.16	0.45
24:C4:113:ILE:HD12	24:C4:113:ILE:C	2.41	0.45
24:C4:182:LYS:NZ	24:C4:458:MET:O	2.38	0.45
25:F4:131:LYS:C	25:F4:132:LEU:HD12	2.42	0.45
26:N4:17:LEU:HB3	26:N4:18:PRO:HD3	1.99	0.45
24:B5:279:TYR:OH	24:B5:332:LEU:O	2.34	0.45
25:F5:275:ASP:OD1	25:F5:276:ASN:ND2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:E5:235:ALA:C	25:E5:236:LEU:HD12	2.41	0.45
18:s:145:ILE:C	18:s:145:ILE:HD12	2.42	0.45
20:i2:57:LEU:HD12	20:i2:58:LEU:N	2.31	0.45
24:B2:159:ARG:NH1	24:B2:162:ILE:HG22	2.31	0.45
26:J2:17:LEU:HB3	26:J2:18:PRO:HD3	1.99	0.45
1:a3:394:PHE:CZ	29:a3:502:CDL:H431	2.51	0.45
10:j3:168:ARG:NH1	17:r3:120:ASP:OD1	2.48	0.45
19:e3:365:ARG:NE	19:e3:371:THR:O	2.49	0.45
2:B3:187:HIS:NE2	3:D3:156:TYR:O	2.47	0.45
27:d4:130:ILE:HD12	27:d4:130:ILE:N	2.31	0.45
18:s:22:LEU:HD23	18:s:22:LEU:N	2.31	0.45
2:B:305:ASP:OD2	22:G1:206:ARG:NE	2.49	0.45
24:C1:165:PRO:O	24:C1:170:ARG:NH1	2.46	0.45
25:E1:317:THR:HG23	25:E1:322:SER:HA	1.98	0.45
26:I1:17:LEU:HB3	26:I1:18:PRO:HD3	1.99	0.45
27:d1:50:ILE:HG12	27:d1:79:ILE:HG22	1.98	0.45
22:G2:141:LEU:O	22:G2:141:LEU:HD13	2.17	0.45
25:F2:54:ALA:O	25:F2:97:THR:OG1	2.27	0.45
25:F2:363:ILE:HD11	25:F2:431:LYS:HD3	1.97	0.45
2:b3:117:THR:HG23	29:F3:302:CDL:H182	1.98	0.45
6:k3:96:MET:HA	6:k3:96:MET:HE3	1.98	0.45
8:G3:98:ARG:NH1	8:G3:149:ASP:OD1	2.49	0.45
23:g4:75:MET:HE3	27:d4:69:LEU:HD21	1.97	0.45
27:d5:126:GLU:C	27:d5:130:ILE:HD11	2.40	0.45
27:d5:148:THR:HG21	28:e5:21:SER:HB3	1.97	0.45
13:n:169:ARG:NH1	11:L:186:GLU:OE1	2.44	0.45
18:s:37:MET:SD	21:t:407:ARG:NH2	2.89	0.45
3:D:60:LEU:HD13	3:D:60:LEU:C	2.41	0.45
25:E2:172:GLY:HA3	25:E2:348:LEU:HD13	1.99	0.45
26:N2:17:LEU:HB3	26:N2:18:PRO:HD3	1.99	0.45
26:N2:57:LEU:HD23	26:M2:55:PHE:CD2	2.52	0.45
27:d2:27:GLN:O	27:d2:28:LYS:C	2.58	0.45
11:L3:206:ILE:N	11:L3:207:PRO:CD	2.79	0.45
26:H5:11:VAL:HG13	26:Q5:13:GLY:HA3	1.98	0.45
15:p:2:SER:OG	15:p:27:GLN:OE1	2.35	0.45
29:F:302:CDL:H402	26:I2:57:LEU:HD11	1.99	0.45
22:G1:141:LEU:O	22:G1:141:LEU:HD13	2.16	0.45
25:E1:80:ILE:N	25:E1:80:ILE:HD12	2.32	0.45
25:F2:275:ASP:OD1	25:F2:276:ASN:ND2	2.50	0.45
1:a3:399:GLN:HE22	29:a3:502:CDL:H452	1.81	0.45
6:k3:37:ALA:N	29:k3:201:CDL:OA4	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:F5:303:THR:OG1	25:F5:307:ASP:OD2	2.24	0.45
28:e5:57:ILE:HD12	28:e5:57:ILE:N	2.32	0.45
1:a:254:MET:HE1	29:a:501:CDL:H521	1.98	0.45
3:d:87:ILE:O	3:d:88:SER:OG	2.24	0.45
24:B1:179:THR:HB	24:B1:213:THR:HG22	1.98	0.45
24:B1:507:HIS:ND1	24:B1:527:GLU:OE2	2.50	0.45
27:d1:130:ILE:HD12	27:d1:130:ILE:N	2.31	0.45
25:F2:82:MET:HA	25:F2:82:MET:HE2	1.99	0.45
27:d2:28:LYS:O	27:d2:105:ASN:ND2	2.50	0.45
1:a3:446:ASN:ND2	7:c3:62:GLN:O	2.45	0.45
32:i3:303:UQ8:H7A	32:i3:303:UQ8:H10	1.76	0.45
11:I3:180:VAL:HG21	17:R3:110:ALA:HB2	1.99	0.45
29:I3:301:CDL:H722	11:L3:110:LEU:HD13	1.98	0.45
32:I3:304:UQ8:H30A	11:L3:110:LEU:HD11	1.98	0.45
25:F4:335:ASP:OD1	25:F4:337:THR:OG1	2.34	0.45
25:E4:235:ALA:C	25:E4:236:LEU:HD12	2.41	0.45
26:M4:11:VAL:HG13	26:L4:13:GLY:HA3	1.98	0.45
26:I4:2:LEU:O	26:I4:6:ALA:N	2.45	0.45
25:E5:329:ILE:HD12	25:E5:329:ILE:N	2.31	0.45
26:N5:17:LEU:HB3	26:N5:18:PRO:HD3	1.99	0.45
3:d:44:LEU:HD13	3:d:44:LEU:C	2.42	0.45
5:i:46:VAL:HG23	5:i:51:ARG:CZ	2.46	0.45
32:I:303:UQ8:H30A	11:L:110:LEU:HD11	1.98	0.45
6:K:37:ALA:N	29:K:201:CDL:OA4	2.45	0.45
11:L:32:LYS:NZ	29:L:301:CDL:O1	2.39	0.45
25:F1:131:LYS:C	25:F1:132:LEU:HD12	2.42	0.45
25:E1:68:VAL:HA	25:E1:79:THR:HG22	1.98	0.45
25:E1:235:ALA:C	25:E1:236:LEU:HD12	2.42	0.45
25:F2:441:GLU:O	25:F2:445:GLY:N	2.46	0.45
18:s3:45:PRO:O	21:t3:354:ARG:NH1	2.50	0.45
1:A3:420:ILE:HG22	9:H3:67:PRO:HA	1.99	0.45
29:I3:302:CDL:HA62	11:L3:124:VAL:HG22	1.99	0.45
9:H3:190:GLU:OE1	9:H3:190:GLU:N	2.49	0.45
19:E3:189:ASP:OD1	19:E3:229:THR:OG1	2.34	0.45
19:E3:210:VAL:HG12	19:E3:387:GLY:O	2.16	0.45
25:E4:80:ILE:N	25:E4:80:ILE:HD12	2.32	0.45
26:O4:17:LEU:HB3	26:O4:18:PRO:HD3	1.99	0.45
26:L4:57:LEU:HD23	26:K4:55:PHE:CE2	2.51	0.45
24:C5:165:PRO:O	24:C5:170:ARG:NH1	2.46	0.45
25:D5:208:ARG:O	25:D5:240:GLN:NE2	2.49	0.45
25:F5:82:MET:HE2	25:F5:82:MET:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:60:LEU:O	3:d:60:LEU:HD13	2.17	0.45
6:k:96:MET:HE3	6:k:96:MET:HA	1.98	0.45
9:h:139:GLU:O	9:h:143:VAL:HG23	2.17	0.45
1:A:226:THR:HG23	1:A:231:TYR:HD2	1.81	0.45
29:B:402:CDL:H742	7:C:43:THR:HG21	1.98	0.45
3:D:72:VAL:O	3:D:72:VAL:HG13	2.16	0.45
22:G1:161:GLN:NE2	22:G1:165:GLN:OE1	2.50	0.45
25:D1:205:VAL:HG12	25:D1:251:VAL:HG13	1.98	0.45
1:a3:205:GLU:OE2	2:b3:173:ARG:NE	2.49	0.45
5:i3:79:HIS:NE2	5:i3:84:MET:O	2.50	0.45
8:G3:153:LYS:NZ	33:G3:301:ATP:O1A	2.33	0.45
24:B4:241:ARG:HE	24:B4:266:THR:HG21	1.82	0.45
26:P4:17:LEU:HB3	26:P4:18:PRO:HD3	1.99	0.45
24:B5:182:LYS:NZ	24:B5:458:MET:O	2.42	0.45
26:N5:12:MET:HE1	26:N5:70:PHE:CE2	2.51	0.45
26:M5:57:LEU:HD22	26:L5:30:PHE:CE2	2.52	0.45
26:J5:17:LEU:HB3	26:J5:18:PRO:HD3	1.99	0.45
1:a:158:GLU:OE1	11:l:176:ARG:NH1	2.45	0.45
17:r:110:ALA:HB2	11:L:180:VAL:HG21	1.99	0.45
17:r:139:VAL:HG21	13:N:171:VAL:HG11	1.99	0.45
32:I:303:UQ8:H27A	32:I:303:UQ8:H30	1.75	0.45
9:h3:240:ASP:OD1	21:t3:457:LEU:HD21	2.17	0.45
5:I3:61:MET:HE1	12:M3:97:ASN:HB2	1.98	0.45
12:M3:144:ALA:O	12:M3:148:VAL:HG23	2.16	0.45
19:E3:281:ASN:O	19:E3:285:GLY:N	2.43	0.45
20:i4:89:HIS:O	20:i4:89:HIS:ND1	2.50	0.45
25:E4:153:VAL:HG23	25:E4:153:VAL:O	2.15	0.45
24:A5:58:GLU:OE2	24:A5:76:THR:N	2.50	0.45
25:E5:172:GLY:HA3	25:E5:348:LEU:HD13	1.98	0.45
20:i2:99:GLU:OE1	20:i1:87:ARG:NH1	2.50	0.45
26:O1:17:LEU:HB3	26:O1:18:PRO:HD3	1.99	0.45
26:M2:17:LEU:HB3	26:M2:18:PRO:HD3	1.98	0.45
26:H2:53:MET:HE3	26:Q2:52:LEU:HD21	1.99	0.45
19:E3:325:THR:O	19:E3:362:ASN:ND2	2.50	0.45
25:F4:31:GLN:O	25:F4:43:GLN:N	2.42	0.45
25:D5:329:ILE:HD12	25:D5:329:ILE:N	2.32	0.45
27:d5:27:GLN:O	27:d5:28:LYS:C	2.60	0.45
2:b:112:ARG:NH1	4:f:74:ASN:O	2.50	0.44
21:t:144:ILE:O	21:t:148:THR:OG1	2.30	0.44
25:F1:335:ASP:OD1	25:F1:337:THR:OG1	2.33	0.44
26:N1:17:LEU:HB3	26:N1:18:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:D2:329:ILE:HD12	25:D2:329:ILE:N	2.32	0.44
9:H3:244:PRO:O	21:t3:241:LYS:NZ	2.34	0.44
22:G5:141:LEU:O	22:G5:141:LEU:HD13	2.17	0.44
25:D5:231:GLU:O	25:D5:232:SER:OG	2.24	0.44
24:A5:241:ARG:HG2	24:A5:266:THR:HG21	1.97	0.44
26:K5:17:LEU:HB3	26:K5:18:PRO:HD3	1.98	0.44
1:a:226:THR:HG23	1:a:231:TYR:HD2	1.82	0.44
16:Q:45:LEU:HD12	16:Q:45:LEU:N	2.31	0.44
23:g1:75:MET:HE3	27:d1:69:LEU:HD21	1.99	0.44
7:c3:17:LEU:C	7:c3:17:LEU:HD12	2.42	0.44
18:s3:49:ARG:NH2	21:t3:409:GLU:OE2	2.51	0.44
12:M3:13:LEU:HD21	12:M3:18:LEU:HG	1.99	0.44
25:E4:329:ILE:HD12	25:E4:329:ILE:N	2.32	0.44
25:F5:441:GLU:O	25:F5:445:GLY:N	2.46	0.44
26:M5:71:PHE:O	26:M5:75:ALA:N	2.50	0.44
27:d5:74:PRO:HG2	27:d5:148:THR:HG22	2.00	0.44
1:a:399:GLN:HE22	29:F:302:CDL:H452	1.83	0.44
1:a:420:ILE:HG22	9:h:67:PRO:HA	1.99	0.44
4:f:71:ASP:OD1	21:t:418:ARG:NH2	2.49	0.44
5:i:138:LEU:O	5:i:141:ARG:NH2	2.49	0.44
18:s:56:ILE:HG22	18:s:58:GLU:HG3	1.99	0.44
24:C1:113:ILE:HD12	24:C1:113:ILE:C	2.41	0.44
24:C1:380:GLN:OE1	24:C1:380:GLN:N	2.51	0.44
25:E1:329:ILE:HD12	25:E1:329:ILE:N	2.32	0.44
23:g2:261:ASN:OD1	23:g2:265:ASN:ND2	2.50	0.44
25:F2:275:ASP:OD1	25:F2:276:ASN:N	2.47	0.44
26:J2:57:LEU:HD23	26:I2:55:PHE:CE2	2.53	0.44
3:d3:231:MET:SD	26:Q5:56:ALA:HB2	2.57	0.44
18:s3:22:LEU:N	18:s3:22:LEU:HD23	2.32	0.44
19:e3:90:LYS:NZ	19:e3:172:ARG:O	2.51	0.44
29:B3:402:CDL:H742	7:C3:43:THR:HG21	1.99	0.44
19:E3:346:THR:OG1	19:E3:396:HIS:NE2	2.33	0.44
26:L4:17:LEU:HB3	26:L4:18:PRO:HD3	2.00	0.44
25:E5:207:GLU:HA	25:E5:241:MET:HE3	2.00	0.44
2:b:333:LEU:HD13	24:A2:36:THR:HB	1.99	0.44
23:g1:221:GLU:HB2	23:g1:222:PRO:CD	2.48	0.44
24:B2:441:LEU:HD13	24:B2:445:THR:HG21	2.00	0.44
4:f3:43:GLU:OE2	21:t3:319:VAL:HG13	2.17	0.44
10:j3:168:ARG:NH2	17:r3:120:ASP:OD1	2.49	0.44
3:D3:188:ILE:HG21	3:D3:212:ILE:HG12	1.99	0.44
10:J3:44:ILE:C	10:J3:44:ILE:HD12	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:E3:166:ARG:NH2	19:E3:169:GLU:OE2	2.50	0.44
23:g4:221:GLU:HB2	23:g4:222:PRO:CD	2.47	0.44
26:K4:17:LEU:HB3	26:K4:18:PRO:HD3	1.99	0.44
26:J4:17:LEU:HB3	26:J4:18:PRO:HD3	1.99	0.44
7:C:17:LEU:C	7:C:17:LEU:HD12	2.41	0.44
26:J1:17:LEU:HB3	26:J1:18:PRO:HD3	1.99	0.44
27:d1:74:PRO:HG2	27:d1:148:THR:HG22	1.98	0.44
28:e2:57:ILE:HD12	28:e2:57:ILE:N	2.32	0.44
11:L3:63:ASP:HB2	13:N3:125:LEU:HD23	2.00	0.44
7:c:17:LEU:C	7:c:17:LEU:HD12	2.43	0.44
9:h:93:ARG:NH1	16:q:111:GLU:OE2	2.51	0.44
24:B1:182:LYS:NZ	24:B1:458:MET:O	2.38	0.44
26:K1:17:LEU:HB3	26:K1:18:PRO:HD3	2.00	0.44
26:J1:57:LEU:HD23	26:I1:55:PHE:CG	2.53	0.44
22:G2:155:LEU:HD12	22:G2:155:LEU:N	2.33	0.44
25:D2:172:GLY:HA3	25:D2:348:LEU:HD13	2.00	0.44
12:m3:13:LEU:HD21	12:m3:18:LEU:HG	2.00	0.44
7:C3:61:SER:OG	7:C3:63:GLU:OE2	2.35	0.44
19:E3:108:GLU:OE2	19:E3:110:LEU:HD12	2.18	0.44
25:D4:304:LEU:HD23	25:D4:304:LEU:C	2.43	0.44
25:D5:304:LEU:HD23	25:D5:304:LEU:C	2.43	0.44
24:A5:81:GLY:N	24:A5:94:ALA:O	2.43	0.44
2:b:141:THR:O	2:b:141:THR:HG22	2.18	0.44
3:d:60:LEU:HD13	3:d:60:LEU:C	2.42	0.44
16:Q:116:TYR:OH	16:Q:140:GLU:OE2	2.35	0.44
20:i1:89:HIS:O	20:i1:89:HIS:ND1	2.51	0.44
24:B1:114:LYS:NZ	25:F1:47:GLU:OE2	2.42	0.44
25:F1:275:ASP:OD1	25:F1:276:ASN:N	2.46	0.44
26:N2:57:LEU:HD23	26:M2:55:PHE:CE2	2.52	0.44
7:C3:17:LEU:C	7:C3:17:LEU:HD12	2.42	0.44
12:M3:205:ASN:ND2	12:M3:208:ASP:OD1	2.50	0.44
16:Q3:65:GLU:OE1	16:Q3:65:GLU:N	2.46	0.44
18:S3:121:VAL:HG23	18:S3:122:HIS:HD1	1.82	0.44
24:A4:58:GLU:OE2	24:A4:76:THR:N	2.50	0.44
1:a:211:ASP:OD2	3:d:198:ARG:NH2	2.45	0.44
9:h:42:ARG:NH1	4:F:46:GLU:OE2	2.47	0.44
23:g1:125:ARG:O	23:g1:126:SER:OG	2.23	0.44
23:g1:153:ILE:HD12	23:g1:153:ILE:N	2.33	0.44
25:D1:172:GLY:HA3	25:D1:348:LEU:HD13	2.00	0.44
25:D1:208:ARG:NH2	24:A1:375:SER:O	2.51	0.44
26:O2:17:LEU:HB3	26:O2:18:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:K2:47:LEU:HD23	26:J2:37:LEU:HD23	1.99	0.44
3:d3:155:GLU:OE2	9:h3:231:ARG:NH1	2.50	0.44
13:N3:124:GLY:O	13:N3:125:LEU:HD22	2.18	0.44
16:Q3:45:LEU:N	16:Q3:45:LEU:HD12	2.33	0.44
21:t3:134:THR:HG22	21:t3:135:GLU:N	2.33	0.44
24:C5:231:TYR:O	24:C5:296:LEU:N	2.41	0.44
26:H5:41:PRO:O	26:H5:44:THR:OG1	2.32	0.44
7:C:75:LEU:HA	7:C:79:ALA:HB3	2.00	0.44
25:D1:304:LEU:HD23	25:D1:304:LEU:C	2.43	0.44
25:F1:275:ASP:OD1	25:F1:276:ASN:ND2	2.51	0.44
26:H1:11:VAL:HG13	26:Q1:13:GLY:HA3	2.00	0.44
22:G2:183:ASP:N	22:G2:184:PRO:HD3	2.33	0.44
26:H2:53:MET:HE1	26:Q2:52:LEU:HD21	1.99	0.44
8:G3:40:TYR:OH	16:Q3:111:GLU:OE1	2.32	0.44
21:t3:126:ASP:OD1	21:t3:126:ASP:N	2.49	0.44
21:t3:345:THR:HG23	21:t3:362:ILE:HD13	1.99	0.44
24:C4:380:GLN:OE1	24:C4:380:GLN:N	2.51	0.44
25:D4:380:ILE:HD12	25:D4:380:ILE:N	2.33	0.44
25:F4:275:ASP:OD1	25:F4:276:ASN:N	2.46	0.44
26:L4:12:MET:HE1	26:L4:70:PHE:CE2	2.52	0.44
26:H4:41:PRO:O	26:H4:44:THR:OG1	2.31	0.44
27:d4:133:LEU:HD11	28:e4:60:LEU:HD13	1.99	0.44
26:M5:17:LEU:HB3	26:M5:18:PRO:HD3	1.99	0.44
1:a:412:LEU:O	1:a:416:THR:OG1	2.23	0.43
8:g:197:GLU:OE1	8:g:197:GLU:N	2.46	0.43
16:q:82:THR:OG1	18:s:103:SER:O	2.33	0.43
1:A:323:GLN:OE1	1:A:326:ARG:NE	2.38	0.43
8:G:180:ASP:OD1	8:G:181:TYR:N	2.51	0.43
24:B1:207:THR:N	33:B1:1003:ATP:O2B	2.50	0.43
25:F1:248:ARG:NH2	25:F1:286:GLU:OE1	2.51	0.43
24:A2:138:VAL:N	24:A2:147:ASP:OD2	2.51	0.43
9:h3:88:TYR:OH	9:h3:121:PHE:O	2.36	0.43
10:j3:44:ILE:C	10:j3:44:ILE:HD12	2.43	0.43
12:m3:23:ASP:OD1	12:m3:27:GLN:NE2	2.51	0.43
8:G3:47:LYS:NZ	8:G3:151:ASP:OD2	2.42	0.43
21:t3:248:ASN:O	21:t3:251:THR:OG1	2.28	0.43
22:G4:127:LEU:C	22:G4:127:LEU:HD13	2.43	0.43
25:D4:172:GLY:HA3	25:D4:348:LEU:HD13	2.00	0.43
22:G5:155:LEU:HD12	22:G5:155:LEU:N	2.34	0.43
25:D5:380:ILE:HD12	25:D5:380:ILE:N	2.33	0.43
26:N5:57:LEU:HD23	26:M5:55:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:253:GLU:OE1	9:H:255:ARG:NH2	2.50	0.43
21:t:250:LEU:HD11	21:t:271:ILE:HD11	2.00	0.43
22:G1:183:ASP:N	22:G1:184:PRO:HD3	2.33	0.43
23:g1:172:SER:OG	23:g1:204:ARG:NH1	2.50	0.43
23:g1:184:ILE:N	23:g1:184:ILE:HD12	2.33	0.43
24:A1:247:LEU:HD23	24:A1:247:LEU:C	2.43	0.43
24:A2:96:ASN:OD1	24:A2:318:ARG:NH2	2.46	0.43
26:P2:2:LEU:HD13	26:Q2:1:MET:N	2.33	0.43
35:a3:503:PEE:H60	29:B3:404:CDL:H391	2.01	0.43
5:i3:194:LEU:HD23	10:j3:196:VAL:HB	2.00	0.43
19:e3:185:PHE:O	19:e3:224:LEU:HD13	2.18	0.43
19:e3:410:ASN:OD1	19:e3:411:ASN:N	2.52	0.43
1:A3:446:ASN:ND2	7:C3:62:GLN:O	2.47	0.43
24:B4:211:ILE:HG21	24:B4:464:TYR:CE2	2.53	0.43
24:A4:247:LEU:HD23	24:A4:247:LEU:C	2.43	0.43
24:A4:386:GLU:OE1	24:A4:386:GLU:N	2.46	0.43
33:B5:1003:ATP:O3'	25:F5:375:ARG:O	2.36	0.43
3:d:34:GLN:NE2	3:d:68:ASN:O	2.50	0.43
3:d:231:MET:SD	26:Q2:56:ALA:HB2	2.58	0.43
7:c:75:LEU:HA	7:c:79:ALA:HB3	1.99	0.43
29:B:404:CDL:OB3	4:F:75:LYS:NZ	2.43	0.43
3:D:86:VAL:HG13	3:D:87:ILE:H	1.84	0.43
26:O1:71:PHE:O	26:O1:75:ALA:N	2.49	0.43
26:L1:57:LEU:HD23	26:K1:55:PHE:CE2	2.54	0.43
24:A2:58:GLU:OE2	24:A2:76:THR:N	2.51	0.43
16:q3:122:THR:O	16:q3:125:VAL:HG22	2.19	0.43
3:D3:44:LEU:HD13	3:D3:44:LEU:C	2.43	0.43
5:I3:79:HIS:NE2	5:I3:84:MET:O	2.51	0.43
22:G4:155:LEU:HD12	22:G4:155:LEU:N	2.32	0.43
23:g4:184:ILE:N	23:g4:184:ILE:HD12	2.33	0.43
29:a:501:CDL:H392	32:i:302:UQ8:H15	2.00	0.43
8:G:66:LYS:HZ3	8:G:69:ASP:CG	2.26	0.43
26:I1:4:VAL:HG23	26:H1:2:LEU:HD11	2.00	0.43
23:g2:75:MET:SD	23:g2:76:LEU:N	2.92	0.43
25:D2:304:LEU:HD23	25:D2:304:LEU:C	2.43	0.43
24:B2:211:ILE:HG21	24:B2:464:TYR:CE2	2.53	0.43
4:f3:37:THR:OG1	29:F3:302:CDL:OB4	2.36	0.43
26:I4:17:LEU:HB3	26:I4:18:PRO:HD3	2.00	0.43
27:d4:27:GLN:O	27:d4:28:LYS:C	2.61	0.43
25:F5:67:GLU:OE2	25:F5:136:HIS:NE2	2.50	0.43
16:q:122:THR:O	16:q:125:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:GLU:OE1	18:S:49:ARG:NH1	2.51	0.43
5:I:46:VAL:HG23	5:I:51:ARG:CZ	2.48	0.43
5:I:169:ILE:HG21	5:I:203:LEU:CD2	2.48	0.43
22:G1:127:LEU:C	22:G1:127:LEU:HD13	2.43	0.43
22:G1:155:LEU:HD12	22:G1:155:LEU:N	2.32	0.43
24:C1:231:TYR:O	24:C1:296:LEU:N	2.41	0.43
25:D1:380:ILE:N	25:D1:380:ILE:HD12	2.33	0.43
23:g2:230:TYR:OH	28:e2:3:ILE:O	2.36	0.43
26:L2:12:MET:HE1	26:L2:70:PHE:CE2	2.54	0.43
22:G4:183:ASP:N	22:G4:184:PRO:HD3	2.33	0.43
24:C4:76:THR:HG22	24:C4:77:LYS:N	2.34	0.43
24:C4:209:ILE:HD12	24:C4:383:LEU:HD11	2.00	0.43
25:D4:133:TYR:OH	25:D4:265:GLU:OE2	2.35	0.43
24:B4:365:VAL:O	24:B4:365:VAL:HG12	2.19	0.43
26:P4:12:MET:HE1	26:P4:70:PHE:CE2	2.53	0.43
26:P4:27:GLY:CA	26:Q4:58:ILE:HD11	2.49	0.43
26:M4:17:LEU:HB3	26:M4:18:PRO:HD3	2.01	0.43
26:K4:47:LEU:HD23	26:J4:37:LEU:HD23	2.00	0.43
24:B5:159:ARG:NH1	24:B5:162:ILE:HG22	2.32	0.43
26:O5:17:LEU:HB3	26:O5:18:PRO:HD3	2.01	0.43
26:L5:12:MET:HE1	26:L5:70:PHE:CD2	2.54	0.43
27:d5:50:ILE:HG12	27:d5:79:ILE:HG22	2.01	0.43
4:f:43:GLU:N	4:f:43:GLU:OE2	2.51	0.43
10:j:271:LEU:HD12	6:K:160:LYS:HD2	2.01	0.43
24:A1:96:ASN:OD1	24:A1:318:ARG:NH2	2.51	0.43
24:A2:247:LEU:HD23	24:A2:247:LEU:C	2.43	0.43
11:L3:16:GLU:OE1	11:L3:16:GLU:N	2.46	0.43
22:G4:105:THR:HG22	22:G4:106:ASN:N	2.34	0.43
25:D4:157:LYS:NZ	25:D4:432:PHE:O	2.44	0.43
25:D4:231:GLU:O	25:D4:232:SER:OG	2.25	0.43
25:F4:157:LYS:NZ	25:F4:432:PHE:O	2.43	0.43
25:F4:201:VAL:O	25:F4:273:PHE:N	2.47	0.43
22:G5:105:THR:HG22	22:G5:106:ASN:N	2.34	0.43
22:G5:183:ASP:N	22:G5:184:PRO:HD3	2.33	0.43
24:A5:247:LEU:HD23	24:A5:247:LEU:C	2.44	0.43
32:I:303:UQ8:H31	11:L:110:LEU:HD11	2.01	0.43
6:K:94:ASN:OD1	6:K:95:ASP:N	2.52	0.43
7:C:95:LYS:HD2	9:H:216:ILE:HD13	2.01	0.43
21:t:126:ASP:OD1	21:t:126:ASP:N	2.50	0.43
21:t:332:PHE:O	21:t:364:TYR:HA	2.19	0.43
25:D1:329:ILE:N	25:D1:329:ILE:HD12	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B1:241:ARG:HE	24:B1:266:THR:HG21	1.83	0.43
24:A1:62:VAL:O	24:A1:62:VAL:HG23	2.18	0.43
22:G2:127:LEU:HD13	22:G2:127:LEU:C	2.43	0.43
22:G2:141:LEU:HD13	22:G2:141:LEU:C	2.44	0.43
23:g2:75:MET:HE3	27:d2:69:LEU:HD21	1.99	0.43
23:g2:210:LEU:C	23:g2:210:LEU:HD23	2.43	0.43
1:a3:226:THR:HG21	5:i3:88:PHE:CD2	2.54	0.43
4:f3:43:GLU:OE2	4:f3:43:GLU:N	2.52	0.43
8:G3:180:ASP:OD1	8:G3:181:TYR:N	2.51	0.43
18:S3:112:ASP:OD1	18:S3:113:VAL:N	2.47	0.43
25:D4:329:ILE:N	25:D4:329:ILE:HD12	2.34	0.43
24:B4:173:VAL:O	24:B4:173:VAL:HG23	2.19	0.43
24:B4:507:HIS:ND1	24:B4:527:GLU:OE2	2.52	0.43
24:A4:62:VAL:O	24:A4:62:VAL:HG23	2.19	0.43
22:G5:127:LEU:HD13	22:G5:127:LEU:C	2.43	0.43
24:A5:125:ILE:HG22	24:A5:126:VAL:N	2.34	0.43
27:d5:130:ILE:HD12	27:d5:130:ILE:N	2.33	0.43
2:b:356:LEU:HD12	18:s:136:VAL:HG22	2.01	0.43
3:d:86:VAL:HG13	3:d:87:ILE:H	1.84	0.43
10:J:44:ILE:HD12	10:J:44:ILE:C	2.44	0.43
22:G1:189:GLY:C	22:G1:190:LEU:HD22	2.44	0.43
26:M1:47:LEU:HD23	26:L1:37:LEU:HD23	2.00	0.43
25:D2:380:ILE:HD12	25:D2:380:ILE:N	2.34	0.43
24:B2:206:LYS:HG2	24:B2:383:LEU:HD12	2.00	0.43
24:B2:317:ARG:NH1	25:F2:292:GLY:O	2.51	0.43
24:A2:125:ILE:HG22	24:A2:126:VAL:N	2.34	0.43
26:N2:12:MET:HE1	26:N2:70:PHE:CE2	2.54	0.43
26:M2:57:LEU:HD23	26:L2:55:PHE:CE2	2.53	0.43
27:d2:130:ILE:HD12	27:d2:130:ILE:N	2.33	0.43
1:A3:137:GLU:O	12:M3:163:TYR:OH	2.27	0.43
2:B3:136:TRP:O	2:B3:140:SER:OG	2.36	0.43
2:B3:202:LYS:NZ	3:D3:143:TYR:OH	2.47	0.43
25:D4:205:VAL:HG12	25:D4:251:VAL:HG13	2.01	0.43
24:A4:125:ILE:HG22	24:A4:126:VAL:N	2.34	0.43
26:K4:68:LEU:HD23	26:K4:68:LEU:O	2.19	0.43
26:O5:47:LEU:HD23	26:N5:37:LEU:HD23	2.00	0.43
27:d5:115:PHE:CZ	28:e5:29:LEU:HD22	2.54	0.43
2:b:187:HIS:NE2	3:d:156:TYR:O	2.46	0.43
2:b:365:ASN:O	2:b:368:ASN:ND2	2.51	0.43
3:d:55:SER:O	3:d:58:THR:OG1	2.26	0.43
21:t:130:MET:N	21:t:159:ASN:O	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:M1:11:VAL:HG13	26:L1:13:GLY:HA3	2.00	0.43
27:d1:115:PHE:CZ	28:e1:29:LEU:HD22	2.54	0.43
22:G2:95:GLN:HB3	22:G2:119:ILE:HD12	2.00	0.43
33:B2:1003:ATP:O3'	25:F2:375:ARG:O	2.37	0.43
24:A2:279:TYR:OH	24:A2:332:LEU:O	2.33	0.43
26:J2:68:LEU:HD11	26:I2:12:MET:CE	2.49	0.43
2:b3:333:LEU:HD13	24:A5:36:THR:HB	2.01	0.43
2:b3:356:LEU:HD12	18:s3:136:VAL:HG22	2.00	0.43
3:d3:86:VAL:HG13	3:d3:87:ILE:H	1.84	0.43
10:j3:142:GLU:OE1	10:j3:142:GLU:N	2.43	0.43
2:B3:107:SER:OG	2:B3:110:MET:SD	2.73	0.43
8:G3:38:ASN:O	8:G3:42:LYS:NZ	2.47	0.43
25:E4:421:LEU:HD23	25:E4:421:LEU:C	2.44	0.43
23:g5:153:ILE:N	23:g5:153:ILE:HD12	2.34	0.43
24:C5:167:ILE:O	25:F5:213:ASN:ND2	2.46	0.43
26:P5:17:LEU:HB3	26:P5:18:PRO:HD3	2.01	0.43
26:P5:37:LEU:HD11	26:P5:44:THR:CG2	2.47	0.43
2:B:112:ARG:NH1	4:F:74:ASN:O	2.51	0.43
29:B:404:CDL:H391	35:L:303:PEE:H60	2.01	0.43
8:G:38:ASN:O	8:G:42:LYS:NZ	2.49	0.43
10:J:183:ARG:O	12:M:34:LYS:NZ	2.48	0.43
24:C1:76:THR:HG22	24:C1:77:LYS:N	2.34	0.43
25:D1:182:THR:CB	37:D1:501:ADP:O1B	2.46	0.43
24:A1:279:TYR:OH	24:A1:332:LEU:O	2.32	0.43
26:P1:11:VAL:HG13	26:O1:13:GLY:HA3	2.00	0.43
25:D2:441:GLU:O	25:D2:445:GLY:N	2.52	0.43
25:F2:421:LEU:C	25:F2:421:LEU:HD23	2.44	0.43
25:E2:157:LYS:NZ	25:E2:432:PHE:O	2.48	0.43
25:E2:207:GLU:HA	25:E2:241:MET:HE3	1.99	0.43
25:E2:303:THR:OG1	25:E2:307:ASP:OD2	2.25	0.43
28:e2:47:LYS:O	28:e2:48:GLU:C	2.61	0.43
5:I3:72:SER:O	5:I3:86:ARG:NH2	2.52	0.43
10:J3:60:PHE:CE2	11:L3:97:THR:HG22	2.54	0.43
23:g4:153:ILE:HD12	23:g4:153:ILE:N	2.33	0.43
25:D5:441:GLU:O	25:D5:445:GLY:N	2.52	0.43
1:A:430:LYS:NZ	16:Q:100:GLU:OE1	2.32	0.42
24:B1:82:GLU:OE2	24:B1:123:GLY:N	2.52	0.42
27:d1:102:HIS:HE2	27:d1:108:GLU:CD	2.26	0.42
27:d1:133:LEU:HD11	28:e1:60:LEU:HD13	2.00	0.42
26:O2:47:LEU:HD23	26:N2:37:LEU:HD23	2.01	0.42
26:L2:17:LEU:HB3	26:L2:18:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:n3:124:GLY:O	13:n3:125:LEU:HD22	2.18	0.42
1:A3:254:MET:HE1	29:A3:501:CDL:H522	1.99	0.42
22:G4:149:ILE:HD12	22:G4:149:ILE:N	2.34	0.42
28:e4:47:LYS:O	28:e4:48:GLU:C	2.62	0.42
10:J:57:ARG:NH1	35:J:303:PEE:O1P	2.41	0.42
19:E:72:PRO:O	19:E:97:SER:N	2.44	0.42
19:E:108:GLU:OE2	19:E:110:LEU:HD12	2.18	0.42
24:C1:486:ALA:O	24:C1:544:LYS:N	2.40	0.42
26:J2:68:LEU:HD11	26:I2:12:MET:HE3	2.01	0.42
10:j3:155:CYS:O	17:r3:141:LYS:NZ	2.50	0.42
4:F3:43:GLU:N	4:F3:43:GLU:OE2	2.51	0.42
21:t3:259:SER:O	21:t3:263:VAL:HG23	2.18	0.42
24:B4:82:GLU:OE2	24:B4:123:GLY:N	2.52	0.42
32:i:302:UQ8:H7A	32:i:302:UQ8:H10	1.73	0.42
1:A:205:GLU:OE2	2:B:173:ARG:NE	2.51	0.42
3:D:44:LEU:C	3:D:44:LEU:HD13	2.45	0.42
8:G:52:TYR:HB3	8:G:54:THR:O	2.19	0.42
20:i1:57:LEU:HD12	20:i1:57:LEU:C	2.45	0.42
22:G1:141:LEU:HD13	22:G1:141:LEU:C	2.44	0.42
24:B1:173:VAL:HG23	24:B1:173:VAL:O	2.19	0.42
27:d1:32:THR:HG22	27:d1:42:ALA:O	2.19	0.42
27:d1:114:LEU:HD23	27:d1:114:LEU:C	2.45	0.42
23:g2:101:SER:OG	23:g2:110:ASN:ND2	2.45	0.42
25:D2:90:ARG:NH1	24:A2:98:GLU:O	2.51	0.42
25:D2:213:ASN:ND2	24:A2:167:ILE:O	2.45	0.42
25:F2:157:LYS:NZ	25:F2:432:PHE:O	2.48	0.42
26:P2:17:LEU:HB3	26:P2:18:PRO:HD3	2.00	0.42
7:C3:75:LEU:HD21	9:H3:163:PHE:HZ	1.85	0.42
25:E4:157:LYS:NZ	25:E4:479:LYS:O	2.40	0.42
22:G5:141:LEU:HD13	22:G5:141:LEU:C	2.44	0.42
24:C5:76:THR:HG22	24:C5:77:LYS:N	2.34	0.42
25:D5:213:ASN:ND2	24:A5:167:ILE:O	2.47	0.42
25:E5:304:LEU:C	25:E5:304:LEU:HD23	2.44	0.42
26:P5:27:GLY:CA	26:Q5:58:ILE:HD11	2.48	0.42
26:L5:17:LEU:HB3	26:L5:18:PRO:HD3	2.01	0.42
19:e:410:ASN:OD1	19:e:411:ASN:N	2.52	0.42
2:B:179:ILE:HG23	7:C:54:PHE:CE1	2.54	0.42
24:C2:76:THR:HG22	24:C2:77:LYS:N	2.34	0.42
24:C2:113:ILE:HD12	24:C2:113:ILE:C	2.43	0.42
25:E2:141:SER:OG	25:E2:144:ASP:OD1	2.14	0.42
26:L2:57:LEU:HD23	26:K2:55:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a3:398:SER:CB	29:a3:502:CDL:H432	2.49	0.42
29:a3:502:CDL:H402	26:I5:57:LEU:HD11	2.01	0.42
1:A3:213:LEU:HD21	30:D3:301:PC1:H3I2	2.02	0.42
3:D3:60:LEU:HD13	3:D3:60:LEU:C	2.43	0.42
6:K3:94:ASN:OD1	6:K3:95:ASP:N	2.53	0.42
23:g4:259:MET:N	23:g4:259:MET:HE2	2.35	0.42
24:C5:209:ILE:HD12	24:C5:383:LEU:HD11	2.01	0.42
25:E5:494:LEU:C	25:E5:494:LEU:HD23	2.45	0.42
27:d5:114:LEU:HD23	27:d5:114:LEU:C	2.45	0.42
3:D:130:ASN:OD1	18:S:89:ARG:NH2	2.52	0.42
7:C:76:LYS:O	18:S:79:GLN:NE2	2.52	0.42
21:t:134:THR:HG22	21:t:135:GLU:N	2.35	0.42
22:G2:105:THR:HG22	22:G2:106:ASN:N	2.34	0.42
9:h3:256:ARG:NE	21:t3:431:ASP:OD2	2.47	0.42
2:B3:229:GLU:OE2	2:B3:232:ARG:NH2	2.43	0.42
29:I3:302:CDL:OB4	11:L3:113:ARG:NH2	2.44	0.42
25:F4:275:ASP:OD1	25:F4:276:ASN:ND2	2.51	0.42
25:D5:172:GLY:HA3	25:D5:348:LEU:HD13	2.01	0.42
25:D5:202:PHE:O	25:D5:237:ILE:N	2.45	0.42
25:E5:32:VAL:O	25:E5:91:GLY:N	2.39	0.42
25:E5:406:ILE:HG22	25:E5:410:LEU:HD11	2.02	0.42
28:e5:37:LEU:O	28:e5:58:LYS:NZ	2.52	0.42
16:q:87:LEU:HD12	16:q:91:SER:CB	2.49	0.42
9:H:145:GLN:OE1	9:H:148:ARG:NH2	2.51	0.42
24:C1:134:MET:HG2	24:C1:152:LEU:HD11	2.02	0.42
25:F1:112:ARG:NH2	25:F1:125:GLY:O	2.44	0.42
24:A1:289:ARG:NH1	24:A1:339:ARG:O	2.52	0.42
26:M1:17:LEU:HB3	26:M1:18:PRO:HD3	2.01	0.42
26:L1:17:LEU:HB3	26:L1:18:PRO:HD3	2.00	0.42
26:I1:4:VAL:CG2	26:H1:2:LEU:HD11	2.50	0.42
28:e1:47:LYS:O	28:e1:48:GLU:C	2.62	0.42
22:G2:149:ILE:HD12	22:G2:149:ILE:N	2.35	0.42
24:C2:362:ALA:HB2	25:D2:337:THR:HG21	2.01	0.42
24:A2:201:ASP:O	24:A2:206:LYS:NZ	2.46	0.42
3:d3:92:LEU:HD23	3:d3:92:LEU:C	2.45	0.42
19:e3:353:TRP:CE3	19:e3:356:ILE:HD11	2.54	0.42
3:D3:86:VAL:HG13	3:D3:87:ILE:H	1.84	0.42
8:G3:96:TRP:O	8:G3:99:ARG:NH2	2.47	0.42
20:i5:79:LEU:HD12	20:i5:79:LEU:N	2.35	0.42
20:i4:57:LEU:HD12	20:i4:57:LEU:C	2.45	0.42
27:d4:114:LEU:HD23	27:d4:114:LEU:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:g5:75:MET:SD	23:g5:76:LEU:N	2.92	0.42
24:B5:441:LEU:HD13	24:B5:445:THR:HG21	2.02	0.42
28:e5:47:LYS:O	28:e5:48:GLU:C	2.61	0.42
1:a:205:GLU:OE2	2:b:173:ARG:NE	2.46	0.42
3:d:30:ALA:O	3:d:70:GLN:NE2	2.48	0.42
29:F:302:CDL:H451	26:I2:60:THR:HG21	2.01	0.42
24:C1:510:LEU:C	24:C1:510:LEU:HD13	2.45	0.42
25:D1:263:ARG:NH1	25:D1:316:THR:O	2.53	0.42
27:d1:126:GLU:C	27:d1:130:ILE:HD11	2.44	0.42
23:g2:210:LEU:HD23	23:g2:210:LEU:O	2.19	0.42
25:E2:68:VAL:HA	25:E2:79:THR:HG22	2.01	0.42
25:E2:304:LEU:C	25:E2:304:LEU:HD23	2.44	0.42
3:d3:44:LEU:HD13	3:d3:44:LEU:C	2.43	0.42
9:h3:267:THR:HB	21:t3:431:ASP:N	2.35	0.42
2:B3:356:LEU:HD12	18:S3:136:VAL:HG22	2.02	0.42
8:G3:62:THR:OG1	8:G3:63:GLU:OE1	2.27	0.42
24:A4:449:LEU:C	24:A4:449:LEU:HD13	2.45	0.42
25:E4:58:GLN:O	25:E4:92:GLN:NE2	2.52	0.42
26:L4:47:LEU:HD23	26:K4:37:LEU:HD23	2.02	0.42
26:J4:57:LEU:HD23	26:I4:55:PHE:CG	2.55	0.42
26:K5:47:LEU:HD23	26:J5:37:LEU:HD23	2.02	0.42
26:J5:57:LEU:HD23	26:I5:55:PHE:CE2	2.54	0.42
17:r:98:GLN:OE1	17:r:101:ARG:NH1	2.52	0.42
19:e:391:LEU:C	19:e:391:LEU:HD12	2.45	0.42
4:F:187:GLN:OE1	4:F:190:ARG:NH2	2.52	0.42
21:t:203:HIS:NE2	21:t:374:HIS:O	2.53	0.42
22:G1:105:THR:HG22	22:G1:106:ASN:N	2.34	0.42
25:D1:168:GLY:N	25:D1:324:THR:OG1	2.52	0.42
25:D1:428:LYS:NZ	25:D1:469:ASP:O	2.53	0.42
24:B1:162:ILE:HD11	24:B1:286:GLU:OE1	2.19	0.42
24:B1:192:ARG:NH2	24:B1:228:LYS:O	2.48	0.42
25:F1:441:GLU:O	25:F1:445:GLY:N	2.46	0.42
24:A1:125:ILE:HG22	24:A1:126:VAL:N	2.34	0.42
28:e1:57:ILE:HG22	28:e1:59:THR:H	1.84	0.42
22:G2:189:GLY:C	22:G2:190:LEU:HD22	2.45	0.42
25:F2:407:ILE:CG2	25:F2:415:LEU:HD11	2.50	0.42
24:A2:386:GLU:OE1	24:A2:386:GLU:N	2.47	0.42
26:I2:65:SER:O	26:I2:69:GLY:N	2.46	0.42
2:b3:218:ARG:NH2	3:d3:117:ILE:O	2.52	0.42
24:C4:543:LEU:N	24:C4:543:LEU:HD23	2.35	0.42
25:D4:68:VAL:HA	25:D4:79:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:D4:112:ARG:NH2	25:D4:125:GLY:O	2.43	0.42
26:M4:47:LEU:HD23	26:L4:37:LEU:HD23	2.01	0.42
24:C5:113:ILE:HD12	24:C5:113:ILE:C	2.43	0.42
24:A5:62:VAL:HG23	24:A5:62:VAL:O	2.20	0.42
2:B:196:ASN:OD1	2:B:199:ARG:NH2	2.48	0.42
3:D:92:LEU:HD23	3:D:92:LEU:C	2.45	0.42
12:M:49:MET:HG2	12:M:50:PRO:HD2	2.00	0.42
23:g1:259:MET:HE2	23:g1:259:MET:N	2.35	0.42
24:A1:449:LEU:C	24:A1:449:LEU:HD13	2.45	0.42
26:L1:47:LEU:HD23	26:K1:37:LEU:HD23	2.02	0.42
26:H1:17:LEU:HB3	26:H1:18:PRO:HD3	2.02	0.42
27:d1:27:GLN:O	27:d1:28:LYS:C	2.62	0.42
24:B2:76:THR:HG22	24:B2:77:LYS:N	2.34	0.42
25:E2:494:LEU:C	25:E2:494:LEU:HD23	2.45	0.42
27:d2:114:LEU:HD23	27:d2:114:LEU:C	2.44	0.42
1:A3:178:ILE:CG2	29:I3:302:CDL:H473	2.49	0.42
22:G4:141:LEU:HD13	22:G4:141:LEU:C	2.44	0.42
25:E4:207:GLU:HA	25:E4:241:MET:HE3	2.01	0.42
26:K4:11:VAL:HG13	26:J4:13:GLY:HA3	2.01	0.42
24:C5:163:LYS:HZ3	25:F5:83:ASP:CG	2.18	0.42
25:F5:421:LEU:C	25:F5:421:LEU:HD23	2.44	0.42
24:C1:543:LEU:HD23	24:C1:543:LEU:N	2.34	0.42
24:B1:342:LYS:NZ	24:B1:349:GLY:O	2.40	0.42
25:F1:157:LYS:NZ	25:F1:432:PHE:O	2.42	0.42
26:P1:17:LEU:HB3	26:P1:18:PRO:HD3	2.00	0.42
26:M2:57:LEU:HD22	26:L2:30:PHE:CE2	2.54	0.42
1:A3:39:ASP:OD1	1:A3:40:ILE:N	2.53	0.42
10:J3:168:ARG:NH2	17:R3:120:ASP:OD1	2.44	0.42
11:L3:66:GLU:OE2	11:L3:69:ARG:NH1	2.53	0.42
21:t3:267:LEU:CD1	21:t3:281:THR:HG22	2.50	0.42
22:G4:189:GLY:C	22:G4:190:LEU:HD22	2.44	0.42
25:E4:168:GLY:O	25:E4:317:THR:OG1	2.34	0.42
25:E4:494:LEU:HD23	25:E4:494:LEU:C	2.45	0.42
26:M4:11:VAL:HG13	26:L4:13:GLY:CA	2.50	0.42
27:d4:74:PRO:HG2	27:d4:148:THR:HG22	2.00	0.42
4:f:77:ARG:NH2	31:f:301:PO4:O2	2.45	0.41
10:j:60:PHE:CE2	11:l:97:THR:HG22	2.55	0.41
11:l:32:LYS:NZ	29:l:302:CDL:O1	2.38	0.41
10:J:168:ARG:NH2	17:R:120:ASP:OD1	2.45	0.41
25:E1:421:LEU:HD23	25:E1:421:LEU:C	2.44	0.41
24:C2:534:LEU:HD23	24:C2:534:LEU:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:D2:67:GLU:OE2	25:D2:136:HIS:NE2	2.51	0.41
24:B2:510:LEU:C	24:B2:510:LEU:HD13	2.45	0.41
26:P2:37:LEU:HD11	26:P2:44:THR:CG2	2.48	0.41
26:I2:57:LEU:HA	26:I2:60:THR:OG1	2.20	0.41
1:a3:226:THR:HG23	1:a3:231:TYR:CD2	2.55	0.41
3:d3:145:ASP:OD2	7:c3:76:LYS:NZ	2.46	0.41
5:i3:46:VAL:HG23	5:i3:51:ARG:CZ	2.50	0.41
10:J3:25:ILE:HG22	13:N3:132:PRO:HD3	2.02	0.41
20:i4:99:GLU:O	20:i4:103:TRP:N	2.49	0.41
21:t3:332:PHE:O	21:t3:364:TYR:HA	2.19	0.41
24:B4:76:THR:HG22	24:B4:77:LYS:N	2.35	0.41
24:B4:510:LEU:C	24:B4:510:LEU:HD13	2.45	0.41
24:A4:446:GLN:OE1	24:A4:450:ASN:ND2	2.51	0.41
25:E4:304:LEU:HD23	25:E4:304:LEU:C	2.45	0.41
26:Q4:17:LEU:HB3	26:Q4:18:PRO:HD3	2.02	0.41
23:g5:210:LEU:C	23:g5:210:LEU:HD23	2.45	0.41
1:a:330:MET:SD	1:a:399:GLN:HB2	2.60	0.41
6:k:47:VAL:HG12	29:g:305:CDL:HA61	2.02	0.41
20:i1:99:GLU:O	20:i1:103:TRP:N	2.48	0.41
24:B1:76:THR:HG22	24:B1:77:LYS:N	2.35	0.41
24:B1:365:VAL:O	24:B1:365:VAL:HG12	2.19	0.41
25:F1:201:VAL:O	25:F1:273:PHE:N	2.49	0.41
28:e1:16:ARG:NH1	28:e1:64:PHE:O	2.53	0.41
24:B2:192:ARG:NH2	24:B2:228:LYS:O	2.52	0.41
24:A2:62:VAL:HG23	24:A2:62:VAL:O	2.20	0.41
1:a3:85:ALA:HB1	11:l3:60:PHE:HE1	1.86	0.41
29:a3:502:CDL:H402	26:l5:57:LEU:CD1	2.51	0.41
9:h3:124:PRO:HA	9:h3:131:THR:HG21	2.02	0.41
18:s3:56:ILE:HG22	18:s3:58:GLU:HG3	2.01	0.41
23:g4:80:SER:OG	26:O4:42:GLU:OE1	2.38	0.41
24:C4:510:LEU:C	24:C4:510:LEU:HD13	2.45	0.41
25:D4:428:LYS:NZ	25:D4:469:ASP:O	2.53	0.41
24:B4:162:ILE:HD11	24:B4:286:GLU:OE1	2.19	0.41
27:d4:126:GLU:C	27:d4:130:ILE:HD11	2.45	0.41
23:g5:75:MET:HE3	27:d5:69:LEU:HD21	2.01	0.41
1:A:205:GLU:CD	2:B:173:ARG:HE	2.29	0.41
7:C:82:ASP:OD1	7:C:83:PHE:N	2.53	0.41
20:i1:29:ARG:NH2	20:i1:32:GLU:OE2	2.53	0.41
23:g2:101:SER:HG	23:g2:106:CYS:HG	1.62	0.41
24:C2:543:LEU:N	24:C2:543:LEU:HD23	2.35	0.41
26:I2:57:LEU:HB3	26:H2:26:THR:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:g4:82:VAL:O	23:g4:86:LYS:N	2.53	0.41
24:C4:534:LEU:HD23	24:C4:534:LEU:C	2.45	0.41
24:B4:207:THR:N	33:B4:1003:ATP:O2B	2.52	0.41
22:G5:149:ILE:HD12	22:G5:149:ILE:N	2.35	0.41
22:G5:189:GLY:C	22:G5:190:LEU:HD22	2.45	0.41
24:B5:173:VAL:HG23	24:B5:173:VAL:O	2.20	0.41
1:a:239:ALA:O	1:a:243:GLY:N	2.50	0.41
5:i:141:ARG:NE	12:m:66:ASP:O	2.45	0.41
4:F:43:GLU:OE2	4:F:43:GLU:N	2.51	0.41
22:G1:149:ILE:N	22:G1:149:ILE:HD12	2.35	0.41
24:C1:534:LEU:HD23	24:C1:534:LEU:C	2.45	0.41
26:Q1:17:LEU:HB3	26:Q1:18:PRO:HD3	2.02	0.41
23:g2:153:ILE:N	23:g2:153:ILE:HD12	2.35	0.41
23:g2:259:MET:HE2	23:g2:259:MET:HA	2.02	0.41
24:C2:206:LYS:HG2	24:C2:383:LEU:HD12	2.03	0.41
25:E2:421:LEU:C	25:E2:421:LEU:HD23	2.46	0.41
27:d2:125:PHE:CE1	28:e2:25:VAL:HG13	2.55	0.41
3:D3:92:LEU:HD23	3:D3:92:LEU:C	2.45	0.41
16:Q3:88:ASN:OD1	16:Q3:90:ASN:N	2.48	0.41
19:E3:391:LEU:HD12	19:E3:391:LEU:C	2.45	0.41
24:C5:510:LEU:HD13	24:C5:510:LEU:C	2.45	0.41
25:E5:202:PHE:O	25:E5:237:ILE:N	2.42	0.41
26:O5:11:VAL:HG13	26:N5:13:GLY:HA3	2.02	0.41
26:J5:68:LEU:HD11	26:I5:12:MET:CE	2.50	0.41
5:I:173:SER:OG	5:I:201:ASN:ND2	2.54	0.41
25:E1:304:LEU:HD23	25:E1:304:LEU:C	2.45	0.41
26:M1:12:MET:HE1	26:M1:70:PHE:CE2	2.56	0.41
26:K1:68:LEU:HD23	26:K1:68:LEU:O	2.20	0.41
23:g2:202:LEU:H	23:g2:202:LEU:HD23	1.86	0.41
24:A2:43:LEU:HD23	24:A2:43:LEU:C	2.46	0.41
3:d3:113:ILE:HD12	3:d3:113:ILE:N	2.35	0.41
6:K3:146:ASN:OD1	6:K3:150:GLN:NE2	2.53	0.41
21:t3:200:LEU:HD13	21:t3:213:VAL:HB	2.03	0.41
24:C4:134:MET:HG2	24:C4:152:LEU:HD11	2.02	0.41
25:F4:421:LEU:HD23	25:F4:421:LEU:C	2.45	0.41
24:C5:534:LEU:HD23	24:C5:534:LEU:C	2.45	0.41
24:A5:96:ASN:OD1	24:A5:318:ARG:NH2	2.46	0.41
25:E5:56:GLU:OE2	25:E5:63:ARG:NH2	2.53	0.41
26:J5:11:VAL:HG13	26:I5:13:GLY:HA3	2.03	0.41
1:a:44:GLY:H	14:o:58:THR:HB	1.85	0.41
2:b:356:LEU:HD12	18:s:136:VAL:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:98:ARG:NH1	8:G:149:ASP:OD1	2.51	0.41
20:i2:104:LYS:NZ	20:i1:104:LYS:O	2.54	0.41
25:F1:421:LEU:HD23	25:F1:421:LEU:C	2.45	0.41
25:E1:207:GLU:HA	25:E1:241:MET:HE3	2.02	0.41
24:B2:365:VAL:O	24:B2:365:VAL:HG12	2.21	0.41
24:A2:317:ARG:NH1	25:E2:292:GLY:O	2.53	0.41
1:a3:239:ALA:O	1:a3:243:GLY:N	2.51	0.41
12:m3:210:LEU:HD21	1:A3:24:PHE:HB2	2.02	0.41
32:I3:304:UQ8:H27A	32:I3:304:UQ8:H30	1.76	0.41
11:L3:32:LYS:NZ	29:L3:301:CDL:O1	2.44	0.41
18:S3:97:VAL:HA	18:S3:101:ILE:HD12	2.02	0.41
26:O4:35:VAL:HG13	26:O4:36:ALA:N	2.35	0.41
26:L4:68:LEU:HD11	26:K4:12:MET:HE3	2.02	0.41
24:B5:76:THR:HG22	24:B5:77:LYS:N	2.35	0.41
24:B5:211:ILE:HG21	24:B5:464:TYR:CE2	2.56	0.41
26:L5:57:LEU:HD23	26:K5:55:PHE:CE2	2.54	0.41
27:d5:32:THR:HG22	27:d5:42:ALA:O	2.20	0.41
18:S:120:TYR:O	18:S:124:ILE:HG22	2.20	0.41
25:E1:494:LEU:HD23	25:E1:494:LEU:C	2.45	0.41
26:M1:57:LEU:HD22	26:L1:30:PHE:CE2	2.56	0.41
26:H1:7:VAL:HG11	26:Q1:9:VAL:HG13	2.03	0.41
27:d1:91:ASP:OD2	27:d1:117:ARG:NE	2.54	0.41
25:E2:62:HIS:O	25:E2:63:ARG:C	2.64	0.41
19:e3:143:HIS:CE1	36:e3:900:NAD:H4N	2.55	0.41
22:G4:151:SER:HB3	22:G4:155:LEU:HD11	2.02	0.41
26:J4:47:LEU:HD23	26:I4:37:LEU:HD23	2.02	0.41
27:d4:26:LYS:NZ	27:d4:30:GLU:OE2	2.54	0.41
26:I5:57:LEU:HB3	26:H5:26:THR:HG21	2.02	0.41
1:a:240:TYR:OH	1:a:251:TRP:NE1	2.48	0.41
3:d:92:LEU:HD23	3:d:92:LEU:C	2.45	0.41
19:e:295:LEU:HD23	19:e:296:TYR:N	2.35	0.41
32:I:303:UQ8:H7A	32:I:303:UQ8:H10	1.83	0.41
21:t:347:PRO:HA	21:t:350:LYS:HB3	2.03	0.41
23:g1:75:MET:SD	23:g1:76:LEU:N	2.94	0.41
25:E1:173:LEU:HD12	25:E1:185:ILE:HD11	2.03	0.41
26:P1:47:LEU:HD23	26:O1:37:LEU:HD23	2.03	0.41
24:C2:510:LEU:HD13	24:C2:510:LEU:C	2.45	0.41
6:k3:47:VAL:HG12	29:g3:305:CDL:HA61	2.03	0.41
8:g3:111:LEU:HB2	8:g3:112:PRO:HD3	2.03	0.41
10:J3:228:GLN:OE1	10:J3:232:ASN:ND2	2.54	0.41
24:B4:342:LYS:NZ	24:B4:349:GLY:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:J4:11:VAL:HG13	26:I4:13:GLY:CA	2.51	0.41
22:G5:168:LYS:O	22:G5:172:ALA:N	2.53	0.41
24:B5:137:ARG:NH2	24:B5:150:GLY:O	2.44	0.41
25:E5:393:VAL:HG13	25:E5:429:VAL:HG11	2.03	0.41
25:E5:421:LEU:HD23	25:E5:421:LEU:C	2.46	0.41
1:a:226:THR:HG23	1:a:231:TYR:CD2	2.56	0.41
1:a:446:ASN:ND2	7:c:62:GLN:O	2.49	0.41
10:j:168:ARG:NH2	17:r:120:ASP:OD1	2.49	0.41
2:B:356:LEU:HD12	18:S:136:VAL:HG22	2.01	0.41
29:B:404:CDL:OB4	4:F:76:ARG:NH1	2.52	0.41
4:F:137:THR:HG23	11:L:184:ILE:HD11	2.03	0.41
29:F:302:CDL:H402	26:I2:57:LEU:CD1	2.51	0.41
8:G:158:ARG:NH1	8:G:173:GLU:OE2	2.50	0.41
18:S:144:LEU:O	18:S:145:ILE:C	2.64	0.41
21:t:134:THR:HG23	21:t:143:TRP:CD1	2.56	0.41
21:t:139:LEU:HD11	21:t:282:ASN:CB	2.50	0.41
24:B1:441:LEU:HD13	24:B1:445:THR:HG21	2.03	0.41
26:N1:57:LEU:HD22	26:M1:30:PHE:CE2	2.56	0.41
26:Q1:71:PHE:O	26:Q1:75:ALA:N	2.54	0.41
26:J2:11:VAL:O	26:J2:14:GLY:N	2.53	0.41
2:b3:356:LEU:HD12	18:s3:136:VAL:CG2	2.51	0.41
8:g3:236:PRO:O	8:g3:281:PRO:HA	2.21	0.41
18:s3:97:VAL:HA	18:s3:101:ILE:HD12	2.03	0.41
18:s3:144:LEU:O	18:s3:145:ILE:C	2.64	0.41
5:I3:169:ILE:HG21	5:I3:203:LEU:CD2	2.51	0.41
29:I3:301:CDL:H861	29:I3:302:CDL:H472	2.03	0.41
18:S3:21:THR:O	18:S3:24:TRP:NE1	2.54	0.41
21:t3:144:ILE:N	21:t3:145:PRO:HD2	2.36	0.41
23:g4:198:HIS:ND1	23:g4:198:HIS:O	2.54	0.41
25:E4:62:HIS:O	25:E4:63:ARG:C	2.64	0.41
25:E4:275:ASP:O	25:E4:276:ASN:C	2.64	0.41
28:e4:57:ILE:HG22	28:e4:59:THR:H	1.85	0.41
25:D5:68:VAL:HA	25:D5:79:THR:HG22	2.03	0.41
24:B5:510:LEU:HD13	24:B5:510:LEU:C	2.46	0.41
26:N5:57:LEU:HD23	26:M5:55:PHE:CE2	2.55	0.41
26:I5:7:VAL:HG23	26:H5:9:VAL:HG11	2.02	0.41
4:f:76:ARG:H	29:f:303:CDL:H1O1	1.64	0.41
4:F:197:LYS:NZ	17:R:77:ASN:OD1	2.47	0.41
8:G:236:PRO:O	8:G:281:PRO:HA	2.21	0.41
9:H:190:GLU:OE1	9:H:190:GLU:N	2.49	0.41
19:E:440:LEU:N	19:E:440:LEU:HD12	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:t:253:ILE:CD1	21:t:263:VAL:HG22	2.45	0.41
25:D1:157:LYS:NZ	25:D1:432:PHE:O	2.47	0.41
24:B1:211:ILE:HG21	24:B1:464:TYR:CE2	2.56	0.41
24:A1:458:MET:HE3	24:A1:476:ILE:HD13	2.01	0.41
26:O1:12:MET:HE1	26:O1:70:PHE:CD2	2.56	0.41
26:N1:11:VAL:HG13	26:M1:13:GLY:HA3	2.02	0.41
25:E2:406:ILE:HG22	25:E2:410:LEU:HD11	2.02	0.41
26:L2:12:MET:HE1	26:L2:70:PHE:CD2	2.56	0.41
1:a3:420:ILE:HG22	9:h3:67:PRO:HA	2.03	0.41
6:K3:106:ARG:NH2	6:K3:155:SER:O	2.53	0.41
7:C3:82:ASP:OD1	7:C3:83:PHE:N	2.53	0.41
25:F4:214:ASP:O	25:F4:218:GLU:N	2.50	0.41
27:d4:50:ILE:HG12	27:d4:79:ILE:HG22	2.02	0.41
24:B5:98:GLU:O	25:E5:90:ARG:NH1	2.46	0.41
1:a:229:ASP:OD1	5:i:70:ARG:NH2	2.54	0.40
3:d:113:ILE:HD12	3:d:113:ILE:N	2.35	0.40
7:C:43:THR:HG22	7:C:47:LEU:HD12	2.02	0.40
21:t:305:ASN:ND2	21:t:312:ASP:O	2.45	0.40
25:D1:363:ILE:HD12	25:D1:363:ILE:N	2.36	0.40
24:B1:510:LEU:C	24:B1:510:LEU:HD13	2.45	0.40
25:D2:475:CYS:O	25:D2:479:LYS:NZ	2.49	0.40
24:B2:114:LYS:NZ	25:F2:47:GLU:OE2	2.48	0.40
24:A2:449:LEU:HD13	24:A2:449:LEU:C	2.46	0.40
26:L2:1:MET:N	26:K2:2:LEU:HD21	2.36	0.40
2:B3:356:LEU:HD12	18:S3:136:VAL:CG2	2.51	0.40
22:G4:95:GLN:HB3	22:G4:119:ILE:HD12	2.03	0.40
23:g4:75:MET:SD	23:g4:76:LEU:N	2.94	0.40
23:g4:210:LEU:HD23	23:g4:210:LEU:C	2.45	0.40
23:g4:259:MET:HE2	23:g4:259:MET:HA	2.03	0.40
25:D4:168:GLY:N	25:D4:324:THR:OG1	2.51	0.40
24:A4:238:GLY:N	24:A4:265:ALA:O	2.43	0.40
24:C5:543:LEU:N	24:C5:543:LEU:HD23	2.35	0.40
25:F5:173:LEU:HD23	25:F5:173:LEU:C	2.46	0.40
26:P5:13:GLY:CA	26:Q5:11:VAL:HG13	2.51	0.40
10:j:142:GLU:OE1	10:j:142:GLU:N	2.44	0.40
12:M:144:ALA:O	12:M:148:VAL:HG23	2.21	0.40
19:E:166:ARG:NH2	19:E:169:GLU:OE2	2.54	0.40
22:G1:168:LYS:O	22:G1:172:ALA:N	2.54	0.40
24:A1:222:ASN:OD1	24:A1:258:LYS:NZ	2.43	0.40
8:g3:52:TYR:HB3	8:g3:54:THR:O	2.21	0.40
11:l3:56:PRO:O	11:l3:61:LYS:NZ	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:g4:49:VAL:HG13	24:C4:440:ASP:HB3	2.03	0.40
24:C4:179:THR:OG1	24:C4:185:ASP:OD1	2.39	0.40
24:C5:241:ARG:CG	24:C5:266:THR:HG21	2.51	0.40
25:D5:363:ILE:N	25:D5:363:ILE:HD12	2.36	0.40
24:B5:365:VAL:O	24:B5:365:VAL:HG12	2.21	0.40
1:a:171:ILE:HD12	1:a:171:ILE:N	2.37	0.40
3:d:63:LEU:HD13	18:s:124:ILE:HG23	2.03	0.40
4:f:43:GLU:HB3	21:t:323:ILE:HG13	2.02	0.40
3:D:113:ILE:N	3:D:113:ILE:HD12	2.36	0.40
24:C1:125:ILE:HG22	24:C1:126:VAL:N	2.36	0.40
24:A1:215:LEU:HD23	24:A1:256:CYS:SG	2.62	0.40
25:E1:406:ILE:HG22	25:E1:410:LEU:HD11	2.03	0.40
26:O1:35:VAL:HG13	26:O1:36:ALA:N	2.36	0.40
26:H1:11:VAL:HG13	26:Q1:13:GLY:HA2	2.04	0.40
24:B2:173:VAL:O	24:B2:173:VAL:HG23	2.20	0.40
24:B2:342:LYS:NZ	24:B2:349:GLY:O	2.44	0.40
25:F2:173:LEU:C	25:F2:173:LEU:HD23	2.46	0.40
26:I2:16:MET:HA	26:I2:19:ILE:HD12	2.02	0.40
29:a3:502:CDL:H831	29:a3:502:CDL:H362	2.03	0.40
6:k3:106:ARG:NH2	6:k3:155:SER:O	2.54	0.40
9:h3:237:PRO:O	17:r3:20:ARG:NH2	2.53	0.40
19:e3:295:LEU:HD23	19:e3:296:TYR:N	2.36	0.40
6:K3:48:ARG:NH2	29:K3:202:CDL:OA4	2.55	0.40
12:M3:49:MET:HG2	12:M3:50:PRO:HD2	2.02	0.40
18:S3:144:LEU:O	18:S3:145:ILE:C	2.64	0.40
19:E3:239:PHE:N	19:E3:247:ASP:OD2	2.52	0.40
21:t3:134:THR:HG23	21:t3:143:TRP:CD1	2.56	0.40
24:B4:160:VAL:O	24:B4:339:ARG:NH1	2.43	0.40
24:B4:441:LEU:HD13	24:B4:445:THR:HG21	2.02	0.40
26:N4:12:MET:HE1	26:N4:70:PHE:CD2	2.57	0.40
23:g5:259:MET:HE2	23:g5:259:MET:HA	2.03	0.40
25:E5:410:LEU:O	25:E5:410:LEU:HD12	2.22	0.40
15:P:119:LYS:NZ	17:R:78:GLY:O	2.51	0.40
23:g1:198:HIS:O	23:g1:198:HIS:ND1	2.54	0.40
25:F1:173:LEU:HD23	25:F1:173:LEU:C	2.47	0.40
24:A1:130:ILE:HG22	24:A1:284:ILE:HA	2.03	0.40
25:E1:62:HIS:O	25:E1:63:ARG:C	2.64	0.40
24:C2:167:ILE:O	25:F2:213:ASN:ND2	2.48	0.40
24:B2:82:GLU:OE2	24:B2:123:GLY:N	2.55	0.40
26:M2:12:MET:HE1	26:M2:70:PHE:CE2	2.57	0.40
15:P3:24:GLU:OE1	15:P3:24:GLU:N	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:N4:57:LEU:HD22	26:M4:30:PHE:CE2	2.57	0.40
23:g5:202:LEU:HD23	23:g5:202:LEU:H	1.87	0.40
24:A5:446:GLN:OE1	24:A5:450:ASN:ND2	2.52	0.40
1:a:140:TRP:O	12:m:219:GLN:NE2	2.47	0.40
2:b:81:LEU:HD21	9:h:157:THR:HG22	2.04	0.40
5:i:95:LEU:HB2	5:i:96:PRO:HD3	2.04	0.40
19:E:143:HIS:CE1	36:E:900:NAD:H4N	2.57	0.40
20:i1:78:ASN:OD1	20:i1:97:ILE:HG21	2.21	0.40
23:g1:225:GLU:OE2	26:H1:39:ARG:NH1	2.49	0.40
24:A1:177:MET:HE1	24:A1:179:THR:HG22	2.04	0.40
24:A1:300:ASP:O	24:A1:301:ASP:C	2.65	0.40
26:P1:27:GLY:CA	26:Q1:58:ILE:HD11	2.52	0.40
26:L1:12:MET:HE1	26:L1:70:PHE:CD2	2.55	0.40
26:J2:11:VAL:HG13	26:I2:13:GLY:CA	2.51	0.40
26:J2:11:VAL:HG13	26:I2:13:GLY:HA3	2.03	0.40
1:a3:326:ARG:NH2	29:a3:502:CDL:C47	2.85	0.40
29:a3:502:CDL:H451	26:I5:60:THR:HG21	2.04	0.40
3:D3:113:ILE:N	3:D3:113:ILE:HD12	2.36	0.40
26:N4:68:LEU:HD11	26:M4:12:MET:HE3	2.04	0.40
27:d4:49:ARG:HE	27:d4:62:GLN:NE2	2.20	0.40
25:E5:335:ASP:OD1	25:E5:337:THR:OG1	2.36	0.40
26:L5:12:MET:HE1	26:L5:70:PHE:CE2	2.56	0.40

There are no symmetry-related clashes.

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	A3	431/446 (97%)	426 (99%)	5 (1%)	0	100	100
1	a	431/446 (97%)	423 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a3	431/446 (97%)	421 (98%)	10 (2%)	0	100	100
2	B	352/381 (92%)	341 (97%)	11 (3%)	0	100	100
2	B3	352/381 (92%)	341 (97%)	11 (3%)	0	100	100
2	b	352/381 (92%)	340 (97%)	12 (3%)	0	100	100
2	b3	352/381 (92%)	339 (96%)	13 (4%)	0	100	100
3	D	204/234 (87%)	199 (98%)	5 (2%)	0	100	100
3	D3	204/234 (87%)	198 (97%)	6 (3%)	0	100	100
3	d	204/234 (87%)	198 (97%)	6 (3%)	0	100	100
3	d3	204/234 (87%)	198 (97%)	6 (3%)	0	100	100
4	F	198/204 (97%)	197 (100%)	1 (0%)	0	100	100
4	F3	198/204 (97%)	197 (100%)	1 (0%)	0	100	100
4	f	198/204 (97%)	197 (100%)	1 (0%)	0	100	100
4	f3	198/204 (97%)	196 (99%)	2 (1%)	0	100	100
5	I	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
5	I3	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
5	i	207/209 (99%)	202 (98%)	5 (2%)	0	100	100
5	i3	207/209 (99%)	202 (98%)	5 (2%)	0	100	100
6	K	177/179 (99%)	166 (94%)	11 (6%)	0	100	100
6	K3	177/179 (99%)	166 (94%)	11 (6%)	0	100	100
6	k	177/179 (99%)	169 (96%)	8 (4%)	0	100	100
6	k3	177/179 (99%)	169 (96%)	8 (4%)	0	100	100
7	C	94/100 (94%)	90 (96%)	4 (4%)	0	100	100
7	C3	94/100 (94%)	90 (96%)	4 (4%)	0	100	100
7	c	94/100 (94%)	90 (96%)	4 (4%)	0	100	100
7	c3	94/100 (94%)	90 (96%)	4 (4%)	0	100	100
8	G	254/286 (89%)	245 (96%)	9 (4%)	0	100	100
8	G3	254/286 (89%)	246 (97%)	8 (3%)	0	100	100
8	g	254/286 (89%)	243 (96%)	11 (4%)	0	100	100
8	g3	254/286 (89%)	244 (96%)	10 (4%)	0	100	100
9	H	229/268 (85%)	226 (99%)	3 (1%)	0	100	100
9	H3	229/268 (85%)	225 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	h	229/268 (85%)	225 (98%)	4 (2%)	0	100	100
9	h3	229/268 (85%)	226 (99%)	3 (1%)	0	100	100
10	J	267/273 (98%)	261 (98%)	6 (2%)	0	100	100
10	J3	267/273 (98%)	261 (98%)	6 (2%)	0	100	100
10	j	267/273 (98%)	263 (98%)	4 (2%)	0	100	100
10	j3	267/273 (98%)	262 (98%)	5 (2%)	0	100	100
11	L	244/247 (99%)	239 (98%)	5 (2%)	0	100	100
11	L3	244/247 (99%)	239 (98%)	5 (2%)	0	100	100
11	l	244/247 (99%)	241 (99%)	3 (1%)	0	100	100
11	l3	244/247 (99%)	241 (99%)	3 (1%)	0	100	100
12	M	219/221 (99%)	219 (100%)	0	0	100	100
12	M3	219/221 (99%)	219 (100%)	0	0	100	100
12	m	219/221 (99%)	218 (100%)	1 (0%)	0	100	100
12	m3	219/221 (99%)	217 (99%)	2 (1%)	0	100	100
13	N	117/179 (65%)	114 (97%)	3 (3%)	0	100	100
13	N3	117/179 (65%)	114 (97%)	3 (3%)	0	100	100
13	n	117/179 (65%)	115 (98%)	2 (2%)	0	100	100
13	n3	117/179 (65%)	115 (98%)	2 (2%)	0	100	100
14	O	97/154 (63%)	95 (98%)	2 (2%)	0	100	100
14	O3	97/154 (63%)	95 (98%)	2 (2%)	0	100	100
14	o	97/154 (63%)	96 (99%)	1 (1%)	0	100	100
14	o3	97/154 (63%)	96 (99%)	1 (1%)	0	100	100
15	P	148/152 (97%)	140 (95%)	8 (5%)	0	100	100
15	P3	148/152 (97%)	140 (95%)	8 (5%)	0	100	100
15	p	148/152 (97%)	139 (94%)	9 (6%)	0	100	100
15	p3	148/152 (97%)	138 (93%)	10 (7%)	0	100	100
16	Q	106/152 (70%)	105 (99%)	1 (1%)	0	100	100
16	Q3	106/152 (70%)	105 (99%)	1 (1%)	0	100	100
16	q	106/152 (70%)	105 (99%)	1 (1%)	0	100	100
16	q3	106/152 (70%)	105 (99%)	1 (1%)	0	100	100
17	R	138/149 (93%)	136 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	R3	138/149 (93%)	136 (99%)	2 (1%)	0	100	100
17	r	143/149 (96%)	142 (99%)	1 (1%)	0	100	100
17	r3	143/149 (96%)	142 (99%)	1 (1%)	0	100	100
18	S	123/145 (85%)	118 (96%)	5 (4%)	0	100	100
18	S3	123/145 (85%)	121 (98%)	2 (2%)	0	100	100
18	s	122/145 (84%)	122 (100%)	0	0	100	100
18	s3	122/145 (84%)	122 (100%)	0	0	100	100
19	E	415/480 (86%)	407 (98%)	8 (2%)	0	100	100
19	E3	415/480 (86%)	406 (98%)	9 (2%)	0	100	100
19	e	415/480 (86%)	405 (98%)	10 (2%)	0	100	100
19	e3	415/480 (86%)	403 (97%)	12 (3%)	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
20	i4	64/108 (59%)	64 (100%)	0	0	100	100
20	i5	60/108 (56%)	60 (100%)	0	0	100	100
21	t	363/460 (79%)	360 (99%)	3 (1%)	0	100	100
21	t3	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
22	G4	186/219 (85%)	176 (95%)	10 (5%)	0	100	100
22	G5	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
23	g4	273/299 (91%)	265 (97%)	8 (3%)	0	100	100
23	g5	273/299 (91%)	264 (97%)	9 (3%)	0	100	100
24	A1	510/546 (93%)	504 (99%)	6 (1%)	0	100	100
24	A2	510/546 (93%)	502 (98%)	8 (2%)	0	100	100
24	A4	510/546 (93%)	503 (99%)	7 (1%)	0	100	100
24	A5	510/546 (93%)	502 (98%)	8 (2%)	0	100	100
24	B1	509/546 (93%)	498 (98%)	10 (2%)	1 (0%)	43	73
24	B2	509/546 (93%)	500 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	B4	509/546 (93%)	498 (98%)	10 (2%)	1 (0%)	43	73
24	B5	509/546 (93%)	499 (98%)	10 (2%)	0	100	100
24	C1	511/546 (94%)	509 (100%)	2 (0%)	0	100	100
24	C2	511/546 (94%)	508 (99%)	3 (1%)	0	100	100
24	C4	511/546 (94%)	509 (100%)	2 (0%)	0	100	100
24	C5	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	D4	468/497 (94%)	461 (98%)	7 (2%)	0	100	100
25	D5	468/497 (94%)	462 (99%)	6 (1%)	0	100	100
25	E1	468/497 (94%)	458 (98%)	10 (2%)	0	100	100
25	E2	468/497 (94%)	459 (98%)	9 (2%)	0	100	100
25	E4	468/497 (94%)	458 (98%)	10 (2%)	0	100	100
25	E5	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
25	F4	467/497 (94%)	454 (97%)	13 (3%)	0	100	100
25	F5	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	H4	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	H5	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	I1	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	I2	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	I4	73/76 (96%)	73 (100%)	0	0	100	100
26	I5	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	J1	73/76 (96%)	73 (100%)	0	0	100	100
26	J2	73/76 (96%)	73 (100%)	0	0	100	100
26	J4	73/76 (96%)	73 (100%)	0	0	100	100
26	J5	73/76 (96%)	73 (100%)	0	0	100	100
26	K1	73/76 (96%)	73 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	K2	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	K4	73/76 (96%)	73 (100%)	0	0	100	100
26	K5	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	L4	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	L5	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	M4	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	M5	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%)	72 (99%)	1 (1%)	0	100	100
26	N4	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	N5	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%)	73 (100%)	0	0	100	100
26	O4	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	O5	73/76 (96%)	71 (97%)	2 (3%)	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	P4	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	P5	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
26	Q4	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	Q5	73/76 (96%)	70 (96%)	3 (4%)	0	100	100
27	d1	132/158 (84%)	127 (96%)	5 (4%)	0	100	100
27	d2	132/158 (84%)	127 (96%)	5 (4%)	0	100	100
27	d4	132/158 (84%)	127 (96%)	5 (4%)	0	100	100
27	d5	132/158 (84%)	127 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	e1	66/71 (93%)	60 (91%)	6 (9%)	0	100	100
28	e2	66/71 (93%)	60 (91%)	6 (9%)	0	100	100
28	e4	66/71 (93%)	60 (91%)	6 (9%)	0	100	100
28	e5	66/71 (93%)	60 (91%)	6 (9%)	0	100	100
All	All	34342/37732 (91%)	33598 (98%)	742 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	B1	55	ASP
24	B4	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%)	396 (100%)	1 (0%)	86	87
1	A3	397/409 (97%)	395 (100%)	2 (0%)	81	85
1	a	397/409 (97%)	396 (100%)	1 (0%)	86	87
1	a3	397/409 (97%)	395 (100%)	2 (0%)	81	85
2	B	306/331 (92%)	306 (100%)	0	100	100
2	B3	306/331 (92%)	306 (100%)	0	100	100
2	b	306/331 (92%)	306 (100%)	0	100	100
2	b3	306/331 (92%)	306 (100%)	0	100	100
3	D	183/206 (89%)	183 (100%)	0	100	100
3	D3	183/206 (89%)	183 (100%)	0	100	100
3	d	183/206 (89%)	182 (100%)	1 (0%)	81	85
3	d3	183/206 (89%)	182 (100%)	1 (0%)	81	85
4	F	175/178 (98%)	173 (99%)	2 (1%)	65	78
4	F3	175/178 (98%)	173 (99%)	2 (1%)	65	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	f	175/178 (98%)	174 (99%)	1 (1%)	78	83
4	f3	175/178 (98%)	173 (99%)	2 (1%)	65	78
5	I	182/182 (100%)	180 (99%)	2 (1%)	65	78
5	I3	182/182 (100%)	180 (99%)	2 (1%)	65	78
5	i	182/182 (100%)	181 (100%)	1 (0%)	81	85
5	i3	182/182 (100%)	182 (100%)	0	100	100
6	K	152/152 (100%)	152 (100%)	0	100	100
6	K3	152/152 (100%)	152 (100%)	0	100	100
6	k	152/152 (100%)	152 (100%)	0	100	100
6	k3	152/152 (100%)	152 (100%)	0	100	100
7	C	93/97 (96%)	93 (100%)	0	100	100
7	C3	93/97 (96%)	93 (100%)	0	100	100
7	c	93/97 (96%)	93 (100%)	0	100	100
7	c3	93/97 (96%)	93 (100%)	0	100	100
8	G	235/262 (90%)	234 (100%)	1 (0%)	84	86
8	G3	235/262 (90%)	234 (100%)	1 (0%)	84	86
8	g	235/262 (90%)	234 (100%)	1 (0%)	84	86
8	g3	235/262 (90%)	234 (100%)	1 (0%)	84	86
9	H	208/245 (85%)	208 (100%)	0	100	100
9	H3	208/245 (85%)	208 (100%)	0	100	100
9	h	208/245 (85%)	208 (100%)	0	100	100
9	h3	208/245 (85%)	208 (100%)	0	100	100
10	J	235/239 (98%)	235 (100%)	0	100	100
10	J3	235/239 (98%)	235 (100%)	0	100	100
10	j	235/239 (98%)	235 (100%)	0	100	100
10	j3	235/239 (98%)	235 (100%)	0	100	100
11	L	219/220 (100%)	218 (100%)	1 (0%)	81	85
11	L3	219/220 (100%)	218 (100%)	1 (0%)	81	85
11	l	219/220 (100%)	218 (100%)	1 (0%)	81	85
11	l3	219/220 (100%)	218 (100%)	1 (0%)	81	85
12	M	202/202 (100%)	202 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	M3	202/202 (100%)	202 (100%)	0	100	100
12	m	202/202 (100%)	201 (100%)	1 (0%)	81	85
12	m3	202/202 (100%)	201 (100%)	1 (0%)	81	85
13	N	104/162 (64%)	104 (100%)	0	100	100
13	N3	104/162 (64%)	104 (100%)	0	100	100
13	n	104/162 (64%)	104 (100%)	0	100	100
13	n3	104/162 (64%)	104 (100%)	0	100	100
14	O	89/142 (63%)	89 (100%)	0	100	100
14	O3	89/142 (63%)	89 (100%)	0	100	100
14	o	89/142 (63%)	89 (100%)	0	100	100
14	o3	89/142 (63%)	89 (100%)	0	100	100
15	P	131/133 (98%)	131 (100%)	0	100	100
15	P3	131/133 (98%)	131 (100%)	0	100	100
15	p	131/133 (98%)	131 (100%)	0	100	100
15	p3	131/133 (98%)	131 (100%)	0	100	100
16	Q	97/135 (72%)	97 (100%)	0	100	100
16	Q3	97/135 (72%)	97 (100%)	0	100	100
16	q	97/135 (72%)	97 (100%)	0	100	100
16	q3	97/135 (72%)	97 (100%)	0	100	100
17	R	120/129 (93%)	119 (99%)	1 (1%)	73	81
17	R3	120/129 (93%)	119 (99%)	1 (1%)	73	81
17	r	125/129 (97%)	124 (99%)	1 (1%)	73	81
17	r3	125/129 (97%)	124 (99%)	1 (1%)	73	81
18	S	112/131 (86%)	112 (100%)	0	100	100
18	S3	112/131 (86%)	112 (100%)	0	100	100
18	s	111/131 (85%)	108 (97%)	3 (3%)	39	67
18	s3	111/131 (85%)	108 (97%)	3 (3%)	39	67
19	E	359/414 (87%)	359 (100%)	0	100	100
19	E3	359/414 (87%)	359 (100%)	0	100	100
19	e	359/414 (87%)	359 (100%)	0	100	100
19	e3	359/414 (87%)	359 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	i1	64/101 (63%)	64 (100%)	0	100	100
20	i2	61/101 (60%)	61 (100%)	0	100	100
20	i4	64/101 (63%)	64 (100%)	0	100	100
20	i5	61/101 (60%)	61 (100%)	0	100	100
21	t	325/414 (78%)	321 (99%)	4 (1%)	63	78
21	t3	325/414 (78%)	321 (99%)	4 (1%)	63	78
22	G1	166/195 (85%)	166 (100%)	0	100	100
22	G2	166/195 (85%)	166 (100%)	0	100	100
22	G4	166/195 (85%)	166 (100%)	0	100	100
22	G5	166/195 (85%)	166 (100%)	0	100	100
23	g1	234/254 (92%)	233 (100%)	1 (0%)	84	86
23	g2	234/254 (92%)	232 (99%)	2 (1%)	70	80
23	g4	234/254 (92%)	232 (99%)	2 (1%)	70	80
23	g5	234/254 (92%)	232 (99%)	2 (1%)	70	80
24	A1	422/453 (93%)	420 (100%)	2 (0%)	81	85
24	A2	422/453 (93%)	420 (100%)	2 (0%)	81	85
24	A4	422/453 (93%)	420 (100%)	2 (0%)	81	85
24	A5	422/453 (93%)	420 (100%)	2 (0%)	81	85
24	B1	422/453 (93%)	422 (100%)	0	100	100
24	B2	422/453 (93%)	422 (100%)	0	100	100
24	B4	422/453 (93%)	422 (100%)	0	100	100
24	B5	422/453 (93%)	422 (100%)	0	100	100
24	C1	424/453 (94%)	423 (100%)	1 (0%)	87	89
24	C2	424/453 (94%)	423 (100%)	1 (0%)	87	89
24	C4	424/453 (94%)	423 (100%)	1 (0%)	87	89
24	C5	424/453 (94%)	423 (100%)	1 (0%)	87	89
25	D1	381/402 (95%)	380 (100%)	1 (0%)	86	87
25	D2	381/402 (95%)	380 (100%)	1 (0%)	86	87
25	D4	381/402 (95%)	380 (100%)	1 (0%)	86	87
25	D5	381/402 (95%)	380 (100%)	1 (0%)	86	87
25	E1	381/402 (95%)	380 (100%)	1 (0%)	86	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	E2	381/402 (95%)	381 (100%)	0	100	100
25	E4	381/402 (95%)	381 (100%)	0	100	100
25	E5	381/402 (95%)	380 (100%)	1 (0%)	86	87
25	F1	380/402 (94%)	380 (100%)	0	100	100
25	F2	380/402 (94%)	380 (100%)	0	100	100
25	F4	380/402 (94%)	380 (100%)	0	100	100
25	F5	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	H4	59/59 (100%)	59 (100%)	0	100	100
26	H5	59/59 (100%)	59 (100%)	0	100	100
26	I1	59/59 (100%)	58 (98%)	1 (2%)	53	74
26	I2	59/59 (100%)	59 (100%)	0	100	100
26	I4	59/59 (100%)	58 (98%)	1 (2%)	53	74
26	I5	59/59 (100%)	59 (100%)	0	100	100
26	J1	59/59 (100%)	59 (100%)	0	100	100
26	J2	59/59 (100%)	59 (100%)	0	100	100
26	J4	59/59 (100%)	59 (100%)	0	100	100
26	J5	59/59 (100%)	59 (100%)	0	100	100
26	K1	59/59 (100%)	59 (100%)	0	100	100
26	K2	59/59 (100%)	59 (100%)	0	100	100
26	K4	59/59 (100%)	59 (100%)	0	100	100
26	K5	59/59 (100%)	59 (100%)	0	100	100
26	L1	59/59 (100%)	59 (100%)	0	100	100
26	L2	59/59 (100%)	59 (100%)	0	100	100
26	L4	59/59 (100%)	59 (100%)	0	100	100
26	L5	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	M4	59/59 (100%)	59 (100%)	0	100	100
26	M5	59/59 (100%)	59 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	N1	59/59 (100%)	59 (100%)	0	100	100
26	N2	59/59 (100%)	59 (100%)	0	100	100
26	N4	59/59 (100%)	59 (100%)	0	100	100
26	N5	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	O4	59/59 (100%)	59 (100%)	0	100	100
26	O5	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	P4	59/59 (100%)	59 (100%)	0	100	100
26	P5	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
26	Q4	59/59 (100%)	59 (100%)	0	100	100
26	Q5	59/59 (100%)	59 (100%)	0	100	100
27	d1	117/139 (84%)	115 (98%)	2 (2%)	53	74
27	d2	117/139 (84%)	116 (99%)	1 (1%)	70	80
27	d4	117/139 (84%)	116 (99%)	1 (1%)	70	80
27	d5	117/139 (84%)	115 (98%)	2 (2%)	53	74
28	e1	57/60 (95%)	57 (100%)	0	100	100
28	e2	57/60 (95%)	57 (100%)	0	100	100
28	e4	57/60 (95%)	57 (100%)	0	100	100
28	e5	57/60 (95%)	57 (100%)	0	100	100
All	All	29600/32320 (92%)	29519 (100%)	81 (0%)	84	87

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	364	LEU
3	d	128	ILE
4	f	37	THR
5	i	26	ARG
8	g	217	PHE

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Mol	Chain	Res	Type
11	l	205	TRP
12	m	49	MET
17	r	28	GLN
18	s	36	VAL
18	s	44	VAL
18	s	67	LEU
1	A	364	LEU
4	F	12	LEU
4	F	31	TYR
5	I	90	HIS
5	I	124	LEU
8	G	217	PHE
11	L	205	TRP
17	R	19	LEU
21	t	140	THR
21	t	158	ARG
21	t	193	GLN
21	t	232	MET
23	g1	194	TYR
24	C1	247	LEU
25	D1	437	PHE
24	A1	221	PHE
24	A1	414	MET
25	E1	27	LYS
26	I1	24	LEU
27	d1	28	LYS
27	d1	126	GLU
23	g2	194	TYR
23	g2	242	ASN
24	C2	247	LEU
25	D2	437	PHE
24	A2	221	PHE
24	A2	414	MET
27	d2	126	GLU
1	a3	64	TYR
1	a3	364	LEU
3	d3	128	ILE
4	f3	7	MET
4	f3	37	THR
8	g3	217	PHE
11	l3	205	TRP
12	m3	49	MET

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Mol	Chain	Res	Type
17	r3	28	GLN
18	s3	36	VAL
18	s3	44	VAL
18	s3	67	LEU
1	A3	64	TYR
1	A3	364	LEU
4	F3	12	LEU
4	F3	31	TYR
5	I3	90	HIS
5	I3	124	LEU
8	G3	217	PHE
11	L3	205	TRP
17	R3	19	LEU
21	t3	140	THR
21	t3	158	ARG
21	t3	193	GLN
21	t3	232	MET
23	g4	83	GLN
23	g4	194	TYR
24	C4	247	LEU
25	D4	437	PHE
24	A4	221	PHE
24	A4	414	MET
26	I4	53	MET
27	d4	126	GLU
23	g5	194	TYR
23	g5	242	ASN
24	C5	247	LEU
25	D5	437	PHE
24	A5	221	PHE
24	A5	414	MET
25	E5	27	LYS
27	d5	28	LYS
27	d5	126	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (204) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	124	HIS
1	a	399	GLN
2	b	104	HIS
2	b	332	ASN

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Mol	Chain	Res	Type
2	b	359	GLN
4	f	4	HIS
6	k	80	ASN
6	k	84	GLN
9	h	83	HIS
9	h	171	HIS
9	h	260	HIS
10	j	130	GLN
10	j	157	ASN
11	l	28	ASN
11	l	46	ASN
11	l	50	GLN
11	l	217	HIS
12	m	3	ASN
12	m	16	GLN
12	m	97	ASN
12	m	150	GLN
12	m	215	HIS
13	n	73	GLN
13	n	76	ASN
13	n	154	GLN
14	o	97	GLN
15	p	57	ASN
16	q	55	ASN
16	q	146	ASN
17	r	116	GLN
17	r	122	HIS
19	e	74	ASN
19	e	220	HIS
19	e	264	ASN
19	e	320	ASN
1	A	202	ASN
1	A	391	HIS
2	B	104	HIS
2	B	255	ASN
2	B	332	ASN
2	B	359	GLN
5	I	20	ASN
5	I	201	ASN
5	I	209	GLN
8	G	93	ASN
9	H	101	GLN

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Mol	Chain	Res	Type
9	H	200	GLN
10	J	149	GLN
10	J	211	HIS
10	J	232	ASN
11	L	50	GLN
11	L	217	HIS
11	L	221	HIS
12	M	3	ASN
12	M	97	ASN
14	O	63	HIS
15	P	150	GLN
16	Q	55	ASN
16	Q	58	GLN
16	Q	69	GLN
17	R	122	HIS
18	S	48	GLN
19	E	220	HIS
19	E	320	ASN
20	i2	83	ASN
21	t	164	ASN
21	t	340	HIS
22	G1	161	GLN
22	G1	165	GLN
22	G1	191	GLN
23	g1	110	ASN
25	D1	50	GLN
24	B1	380	GLN
24	B1	448	GLN
24	A1	436	GLN
25	E1	92	GLN
26	K1	40	ASN
26	I1	50	ASN
22	G2	106	ASN
22	G2	161	GLN
22	G2	165	GLN
22	G2	191	GLN
23	g2	83	GLN
23	g2	229	ASN
23	g2	242	ASN
25	D2	276	ASN
25	D2	312	GLN
25	D2	327	GLN

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Mol	Chain	Res	Type
24	B2	380	GLN
24	B2	448	GLN
24	A2	171	GLN
24	A2	239	GLN
24	A2	502	HIS
24	A2	506	ASN
25	E2	92	GLN
25	E2	213	ASN
25	E2	217	HIS
25	E2	398	GLN
25	E2	452	ASN
26	I2	40	ASN
1	a3	202	ASN
1	a3	399	GLN
1	a3	443	ASN
2	b3	332	ASN
2	b3	368	ASN
4	f3	4	HIS
4	f3	81	ASN
5	i3	139	ASN
5	i3	201	ASN
6	k3	80	ASN
6	k3	84	GLN
8	g3	100	HIS
9	h3	58	HIS
9	h3	183	GLN
9	h3	260	HIS
10	j3	130	GLN
11	l3	28	ASN
11	l3	46	ASN
11	l3	50	GLN
11	l3	183	ASN
11	l3	217	HIS
11	l3	221	HIS
11	l3	245	GLN
12	m3	16	GLN
12	m3	27	GLN
12	m3	97	ASN
12	m3	150	GLN
12	m3	215	HIS
13	n3	73	GLN
13	n3	76	ASN

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Mol	Chain	Res	Type
15	p3	150	GLN
16	q3	55	ASN
18	s3	48	GLN
19	e3	221	HIS
19	e3	264	ASN
19	e3	320	ASN
1	A3	124	HIS
1	A3	391	HIS
2	B3	82	ASN
2	B3	104	HIS
2	B3	255	ASN
2	B3	359	GLN
3	D3	230	ASN
5	I3	20	ASN
5	I3	201	ASN
5	I3	209	GLN
8	G3	93	ASN
9	H3	61	ASN
9	H3	83	HIS
9	H3	101	GLN
9	H3	183	GLN
9	H3	200	GLN
10	J3	149	GLN
10	J3	211	HIS
10	J3	232	ASN
11	L3	50	GLN
11	L3	90	HIS
11	L3	181	GLN
11	L3	217	HIS
11	L3	221	HIS
12	M3	97	ASN
14	O3	63	HIS
15	P3	150	GLN
16	Q3	55	ASN
16	Q3	69	GLN
18	S3	48	GLN
19	E3	320	ASN
21	t3	164	ASN
21	t3	340	HIS
22	G4	161	GLN
22	G4	165	GLN
22	G4	191	GLN

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Mol	Chain	Res	Type
23	g4	110	ASN
23	g4	242	ASN
23	g4	265	ASN
25	D4	145	GLN
24	B4	380	GLN
24	B4	448	GLN
24	B4	463	GLN
24	A4	436	GLN
25	E4	92	GLN
25	E4	195	HIS
25	E4	398	GLN
25	E4	452	ASN
26	M4	40	ASN
26	I4	40	ASN
26	I4	50	ASN
22	G5	161	GLN
22	G5	165	GLN
22	G5	191	GLN
23	g5	83	GLN
23	g5	229	ASN
23	g5	242	ASN
25	D5	276	ASN
24	B5	380	GLN
24	B5	448	GLN
25	F5	435	GLN
24	A5	171	GLN
24	A5	239	GLN
24	A5	506	ASN
25	E5	92	GLN
25	E5	213	ASN
25	E5	217	HIS
26	Q5	49	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 140 ligands modelled in this entry, 24 are monoatomic - leaving 116 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
32	UQ8	I	303	-	53,53,53	1.85	7 (13%)	66,67,67	1.66	16 (24%)
35	PEE	L	303	-	47,47,50	1.19	6 (12%)	50,52,55	1.19	5 (10%)
29	CDL	B3	401	-	99,99,99	0.89	8 (8%)	105,111,111	0.99	4 (3%)
33	ATP	G	301	34	32,33,33	3.54	13 (40%)	48,52,52	2.22	14 (29%)
29	CDL	f	303	-	99,99,99	0.89	8 (8%)	105,111,111	1.09	5 (4%)
30	PC1	G3	304	-	53,53,53	0.96	4 (7%)	59,61,61	1.01	2 (3%)
36	NAD	e3	900	-	46,48,48	4.06	21 (45%)	64,73,73	2.10	13 (20%)
33	ATP	C5	601	34	32,33,33	3.59	13 (40%)	48,52,52	2.20	12 (25%)
29	CDL	b3	401	-	99,99,99	0.89	8 (8%)	105,111,111	1.13	4 (3%)
29	CDL	K3	202	-	99,99,99	0.89	8 (8%)	105,111,111	1.10	5 (4%)
29	CDL	A	502	-	99,99,99	0.90	8 (8%)	105,111,111	1.11	4 (3%)
35	PEE	m	301	-	50,50,50	1.16	6 (12%)	53,55,55	1.12	5 (9%)
32	UQ8	i3	303	-	53,53,53	1.85	7 (13%)	66,67,67	1.60	16 (24%)
30	PC1	g	304	-	53,53,53	0.97	4 (7%)	59,61,61	0.96	3 (5%)
33	ATP	A4	601	34	32,33,33	3.59	13 (40%)	48,52,52	2.20	13 (27%)
29	CDL	I3	303	-	99,99,99	0.90	8 (8%)	105,111,111	1.05	4 (3%)
37	ADP	B1	1002	34	28,29,29	3.43	10 (35%)	43,45,45	3.27	17 (39%)
29	CDL	j3	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.03	4 (3%)
29	CDL	A3	501	-	99,99,99	0.90	8 (8%)	105,111,111	1.09	4 (3%)
29	CDL	J	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.03	4 (3%)
29	CDL	F	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.02	5 (4%)
29	CDL	L	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.05	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CDL	i	301	-	99,99,99	0.90	7 (7%)	105,111,111	1.08	4 (3%)
29	CDL	l3	303	-	99,99,99	0.90	8 (8%)	105,111,111	1.03	4 (3%)
29	CDL	a	501	-	99,99,99	0.90	8 (8%)	105,111,111	1.07	5 (4%)
29	CDL	B	401	-	99,99,99	0.89	8 (8%)	105,111,111	0.98	4 (3%)
33	ATP	g3	301	34	32,33,33	3.54	13 (40%)	48,52,52	2.22	14 (29%)
33	ATP	g	301	34	32,33,33	3.55	13 (40%)	48,52,52	2.21	13 (27%)
37	ADP	D5	501	34	28,29,29	3.42	10 (35%)	43,45,45	3.26	15 (34%)
29	CDL	I	301	-	99,99,99	0.89	8 (8%)	105,111,111	0.99	4 (3%)
33	ATP	G3	301	34	32,33,33	3.54	13 (40%)	48,52,52	2.22	13 (27%)
29	CDL	r	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.05	4 (3%)
29	CDL	J3	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.03	4 (3%)
29	CDL	i3	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.07	4 (3%)
29	CDL	k3	201	-	99,99,99	0.90	8 (8%)	105,111,111	1.02	4 (3%)
30	PC1	D3	301	-	53,53,53	0.95	4 (7%)	59,61,61	1.10	2 (3%)
29	CDL	f3	303	-	99,99,99	0.89	8 (8%)	105,111,111	1.08	4 (3%)
29	CDL	f	304	-	99,99,99	0.89	8 (8%)	105,111,111	1.06	4 (3%)
30	PC1	g3	303	-	53,53,53	0.97	4 (7%)	59,61,61	1.01	2 (3%)
35	PEE	A	501	-	47,47,50	1.20	6 (12%)	50,52,55	1.23	4 (8%)
29	CDL	p	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.04	4 (3%)
29	CDL	j	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.03	4 (3%)
29	CDL	I3	301	-	99,99,99	0.89	8 (8%)	105,111,111	1.03	4 (3%)
30	PC1	g	303	-	53,53,53	0.97	4 (7%)	59,61,61	0.99	2 (3%)
33	ATP	C4	601	34	32,33,33	3.58	13 (40%)	48,52,52	2.19	13 (27%)
29	CDL	i3	301	-	99,99,99	0.88	8 (8%)	105,111,111	1.05	4 (3%)
37	ADP	B5	1002	34	28,29,29	3.43	10 (35%)	43,45,45	3.28	16 (37%)
29	CDL	a3	502	-	99,99,99	0.89	8 (8%)	105,111,111	1.04	5 (4%)
35	PEE	l3	302	-	47,47,50	1.19	6 (12%)	50,52,55	1.23	4 (8%)
29	CDL	K	202	-	99,99,99	0.89	8 (8%)	105,111,111	1.10	4 (3%)
31	PO4	f	301	-	4,4,4	1.01	0	6,6,6	0.44	0
29	CDL	B	403	-	99,99,99	0.89	8 (8%)	105,111,111	1.03	4 (3%)
29	CDL	f3	304	-	99,99,99	0.89	8 (8%)	105,111,111	1.07	4 (3%)
30	PC1	g3	304	-	53,53,53	0.97	4 (7%)	59,61,61	0.93	2 (3%)
31	PO4	F	301	-	4,4,4	1.03	0	6,6,6	0.48	0
29	CDL	B3	404	-	99,99,99	0.90	8 (8%)	105,111,111	1.12	5 (4%)
33	ATP	B5	1003	34	32,33,33	3.59	13 (40%)	48,52,52	2.21	14 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	ATP	B4	1003	34	32,33,33	3.59	13 (40%)	48,52,52	2.20	14 (29%)
29	CDL	B3	402	-	99,99,99	0.88	8 (8%)	105,111,111	1.13	5 (4%)
36	NAD	E3	900	-	46,48,48	4.06	21 (45%)	64,73,73	2.11	13 (20%)
29	CDL	g	305	-	99,99,99	0.90	8 (8%)	105,111,111	1.09	4 (3%)
29	CDL	I3	302	-	99,99,99	0.90	8 (8%)	105,111,111	1.03	4 (3%)
30	PC1	G	304	-	53,53,53	0.96	4 (7%)	59,61,61	0.99	2 (3%)
29	CDL	b	401	-	99,99,99	0.88	7 (7%)	105,111,111	1.11	5 (4%)
37	ADP	D2	501	34	28,29,29	3.43	10 (35%)	43,45,45	3.25	15 (34%)
29	CDL	j	301	-	99,99,99	0.90	8 (8%)	105,111,111	1.05	4 (3%)
29	CDL	I	302	-	99,99,99	0.89	7 (7%)	105,111,111	1.06	4 (3%)
33	ATP	B1	1003	34	32,33,33	3.59	13 (40%)	48,52,52	2.19	14 (29%)
36	NAD	e	900	-	46,48,48	4.06	21 (45%)	64,73,73	2.12	13 (20%)
29	CDL	f	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.02	4 (3%)
29	CDL	l	302	-	99,99,99	0.90	8 (8%)	105,111,111	1.04	4 (3%)
30	PC1	d3	301	-	53,53,53	0.96	4 (7%)	59,61,61	1.08	2 (3%)
33	ATP	A5	601	34	32,33,33	3.59	13 (40%)	48,52,52	2.20	12 (25%)
29	CDL	l	301	-	99,99,99	0.89	8 (8%)	105,111,111	1.05	4 (3%)
29	CDL	J	301	-	99,99,99	0.90	7 (7%)	105,111,111	1.06	4 (3%)
29	CDL	L	301	-	99,99,99	0.90	8 (8%)	105,111,111	1.02	4 (3%)
33	ATP	B2	1003	34	32,33,33	3.59	13 (40%)	48,52,52	2.21	14 (29%)
29	CDL	B	404	-	99,99,99	0.90	8 (8%)	105,111,111	1.09	5 (4%)
29	CDL	P	201	-	99,99,99	0.89	7 (7%)	105,111,111	1.03	5 (4%)
29	CDL	P3	201	-	99,99,99	0.89	7 (7%)	105,111,111	1.04	5 (4%)
35	PEE	L3	302	-	50,50,50	1.17	6 (12%)	53,55,55	1.17	4 (7%)
30	PC1	G	303	-	53,53,53	0.97	4 (7%)	59,61,61	1.01	2 (3%)
33	ATP	A1	601	34	32,33,33	3.59	13 (40%)	48,52,52	2.20	12 (25%)
30	PC1	d	301	-	53,53,53	0.95	4 (7%)	59,61,61	1.08	2 (3%)
29	CDL	l3	301	-	99,99,99	0.89	8 (8%)	105,111,111	1.06	5 (4%)
29	CDL	J3	301	-	99,99,99	0.90	8 (8%)	105,111,111	1.04	4 (3%)
29	CDL	B	402	-	99,99,99	0.88	8 (8%)	105,111,111	1.13	6 (5%)
29	CDL	g3	305	-	99,99,99	0.89	8 (8%)	105,111,111	1.11	4 (3%)
29	CDL	K	201	-	99,99,99	0.90	8 (8%)	105,111,111	1.04	4 (3%)
29	CDL	B3	403	-	99,99,99	0.89	8 (8%)	105,111,111	1.02	4 (3%)
29	CDL	F	303	-	99,99,99	0.88	8 (8%)	105,111,111	1.09	4 (3%)
33	ATP	C2	601	34	32,33,33	3.58	13 (40%)	48,52,52	2.20	13 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CDL	f3	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.02	4 (3%)
37	ADP	B2	1002	34	28,29,29	3.43	10 (35%)	43,45,45	3.28	17 (39%)
29	CDL	p3	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.05	4 (3%)
37	ADP	D1	501	34	28,29,29	3.42	11 (39%)	43,45,45	3.46	16 (37%)
31	PO4	F3	301	-	4,4,4	1.01	0	6,6,6	0.46	0
29	CDL	K3	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.06	4 (3%)
29	CDL	F3	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.08	4 (3%)
35	PEE	a3	503	-	47,47,50	1.20	6 (12%)	50,52,55	1.19	5 (10%)
32	UQ8	I3	304	-	53,53,53	1.87	7 (13%)	66,67,67	1.63	16 (24%)
33	ATP	C1	601	34	32,33,33	3.59	13 (40%)	48,52,52	2.18	12 (25%)
35	PEE	j3	303	-	50,50,50	1.16	6 (12%)	53,55,55	1.11	5 (9%)
36	NAD	E	900	-	46,48,48	4.06	21 (45%)	64,73,73	2.09	13 (20%)
29	CDL	L3	301	-	99,99,99	0.90	8 (8%)	105,111,111	1.00	4 (3%)
29	CDL	j3	301	-	99,99,99	0.89	8 (8%)	105,111,111	1.07	4 (3%)
32	UQ8	i	302	-	53,53,53	1.86	7 (13%)	66,67,67	1.59	17 (25%)
37	ADP	D4	501	34	28,29,29	3.43	11 (39%)	43,45,45	3.46	15 (34%)
29	CDL	k	201	-	99,99,99	0.90	8 (8%)	105,111,111	1.02	4 (3%)
37	ADP	B4	1002	34	28,29,29	3.43	10 (35%)	43,45,45	3.28	17 (39%)
29	CDL	a3	501	-	99,99,99	0.90	8 (8%)	105,111,111	1.04	5 (4%)
35	PEE	J	303	-	50,50,50	1.17	6 (12%)	53,55,55	1.17	5 (9%)
30	PC1	G3	303	-	53,53,53	0.97	4 (7%)	59,61,61	1.00	2 (3%)
33	ATP	A2	601	34	32,33,33	3.59	13 (40%)	48,52,52	2.20	13 (27%)
31	PO4	f3	301	-	4,4,4	1.03	0	6,6,6	0.48	0
30	PC1	D	301	-	53,53,53	0.95	4 (7%)	59,61,61	1.09	2 (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
32	UQ8	I	303	-	-	9/51/75/75	0/1/1/1
35	PEE	L	303	-	-	21/51/51/54	-
29	CDL	B3	401	-	-	44/110/110/110	-
33	ATP	G	301	34	-	0/22/38/38	0/3/3/3
29	CDL	f	303	-	-	42/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PC1	G3	304	-	-	19/57/57/57	-
36	NAD	e3	900	-	-	9/30/62/62	0/5/5/5
33	ATP	C5	601	34	-	4/22/38/38	0/3/3/3
29	CDL	b3	401	-	-	43/110/110/110	-
29	CDL	K3	202	-	-	35/110/110/110	-
29	CDL	A	502	-	-	46/110/110/110	-
35	PEE	m	301	-	-	24/54/54/54	-
32	UQ8	i3	303	-	-	8/51/75/75	0/1/1/1
30	PC1	g	304	-	-	19/57/57/57	-
33	ATP	A4	601	34	-	5/22/38/38	0/3/3/3
29	CDL	I3	303	-	-	38/110/110/110	-
37	ADP	B1	1002	34	-	1/16/32/32	0/3/3/3
29	CDL	j3	302	-	-	41/110/110/110	-
29	CDL	A3	501	-	-	45/110/110/110	-
29	CDL	J	302	-	-	37/110/110/110	-
29	CDL	F	302	-	-	38/110/110/110	-
29	CDL	L	302	-	-	44/110/110/110	-
29	CDL	i	301	-	-	38/110/110/110	-
29	CDL	l3	303	-	-	40/110/110/110	-
29	CDL	a	501	-	-	34/110/110/110	-
29	CDL	B	401	-	-	44/110/110/110	-
33	ATP	g3	301	34	-	0/22/38/38	0/3/3/3
33	ATP	g	301	34	-	0/22/38/38	0/3/3/3
37	ADP	D5	501	34	-	1/16/32/32	0/3/3/3
29	CDL	I	301	-	-	45/110/110/110	-
33	ATP	G3	301	34	-	0/22/38/38	0/3/3/3
29	CDL	r	201	-	-	36/110/110/110	-
29	CDL	J3	302	-	-	40/110/110/110	-
29	CDL	i3	302	-	-	37/110/110/110	-
29	CDL	k3	201	-	-	36/110/110/110	-
30	PC1	D3	301	-	-	22/57/57/57	-
29	CDL	f3	303	-	-	42/110/110/110	-
29	CDL	f	304	-	-	47/110/110/110	-
30	PC1	g3	303	-	-	20/57/57/57	-
35	PEE	A	501	-	-	20/51/51/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CDL	p	201	-	-	44/110/110/110	-
29	CDL	j	302	-	-	41/110/110/110	-
29	CDL	I3	301	-	-	43/110/110/110	-
30	PC1	g	303	-	-	20/57/57/57	-
33	ATP	C4	601	34	-	5/22/38/38	0/3/3/3
29	CDL	i3	301	-	-	36/110/110/110	-
37	ADP	B5	1002	34	-	2/16/32/32	0/3/3/3
29	CDL	a3	502	-	-	38/110/110/110	-
35	PEE	l3	302	-	-	20/51/51/54	-
29	CDL	K	202	-	-	34/110/110/110	-
29	CDL	B	403	-	-	33/110/110/110	-
29	CDL	f3	304	-	-	47/110/110/110	-
30	PC1	g3	304	-	-	17/57/57/57	-
29	CDL	B3	404	-	-	44/110/110/110	-
33	ATP	B5	1003	34	-	1/22/38/38	0/3/3/3
33	ATP	B4	1003	34	-	1/22/38/38	0/3/3/3
29	CDL	B3	402	-	-	39/110/110/110	-
36	NAD	E3	900	-	-	7/30/62/62	0/5/5/5
29	CDL	g	305	-	-	34/110/110/110	-
29	CDL	I3	302	-	-	44/110/110/110	-
30	PC1	G	304	-	-	19/57/57/57	-
29	CDL	b	401	-	-	44/110/110/110	-
37	ADP	D2	501	34	-	1/16/32/32	0/3/3/3
29	CDL	j	301	-	-	38/110/110/110	-
29	CDL	I	302	-	-	38/110/110/110	-
33	ATP	B1	1003	34	-	1/22/38/38	0/3/3/3
36	NAD	e	900	-	-	8/30/62/62	0/5/5/5
29	CDL	f	302	-	-	53/110/110/110	-
29	CDL	l	302	-	-	40/110/110/110	-
30	PC1	d3	301	-	-	23/57/57/57	-
33	ATP	A5	601	34	-	6/22/38/38	0/3/3/3
29	CDL	l	301	-	-	38/110/110/110	-
29	CDL	J	301	-	-	40/110/110/110	-
29	CDL	L	301	-	-	37/110/110/110	-
33	ATP	B2	1003	34	-	1/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CDL	B	404	-	-	45/110/110/110	-
29	CDL	P	201	-	-	36/110/110/110	-
29	CDL	P3	201	-	-	36/110/110/110	-
35	PEE	L3	302	-	-	28/54/54/54	-
30	PC1	G	303	-	-	28/57/57/57	-
33	ATP	A1	601	34	-	5/22/38/38	0/3/3/3
30	PC1	d	301	-	-	23/57/57/57	-
29	CDL	l3	301	-	-	38/110/110/110	-
29	CDL	J3	301	-	-	41/110/110/110	-
29	CDL	B	402	-	-	38/110/110/110	-
29	CDL	g3	305	-	-	34/110/110/110	-
29	CDL	K	201	-	-	28/110/110/110	-
29	CDL	B3	403	-	-	32/110/110/110	-
29	CDL	F	303	-	-	46/110/110/110	-
33	ATP	C2	601	34	-	4/22/38/38	0/3/3/3
29	CDL	f3	302	-	-	53/110/110/110	-
37	ADP	B2	1002	34	-	2/16/32/32	0/3/3/3
29	CDL	p3	201	-	-	43/110/110/110	-
37	ADP	D1	501	34	-	3/16/32/32	0/3/3/3
29	CDL	K3	201	-	-	28/110/110/110	-
29	CDL	F3	302	-	-	45/110/110/110	-
35	PEE	a3	503	-	-	21/51/51/54	-
32	UQ8	I3	304	-	-	9/51/75/75	0/1/1/1
33	ATP	C1	601	34	-	5/22/38/38	0/3/3/3
35	PEE	j3	303	-	-	24/54/54/54	-
36	NAD	E	900	-	-	8/30/62/62	0/5/5/5
29	CDL	L3	301	-	-	37/110/110/110	-
29	CDL	j3	301	-	-	39/110/110/110	-
32	UQ8	i	302	-	-	8/51/75/75	0/1/1/1
37	ADP	D4	501	34	-	3/16/32/32	0/3/3/3
29	CDL	k	201	-	-	36/110/110/110	-
37	ADP	B4	1002	34	-	1/16/32/32	0/3/3/3
29	CDL	a3	501	-	-	34/110/110/110	-
35	PEE	J	303	-	-	28/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PC1	G3	303	-	-	28/57/57/57	-
33	ATP	A2	601	34	-	6/22/38/38	0/3/3/3
30	PC1	D	301	-	-	22/57/57/57	-

All (972) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	D2	501	ADP	C2'-C3'	-10.64	1.24	1.53
37	D5	501	ADP	C2'-C3'	-10.59	1.24	1.53
37	B2	1002	ADP	C2'-C3'	-10.58	1.24	1.53
37	D1	501	ADP	C2'-C3'	-10.58	1.24	1.53
37	B4	1002	ADP	C2'-C3'	-10.56	1.24	1.53
37	D4	501	ADP	C2'-C3'	-10.54	1.24	1.53
37	B1	1002	ADP	C2'-C3'	-10.53	1.24	1.53
37	B5	1002	ADP	C2'-C3'	-10.51	1.24	1.53
36	e	900	NAD	O4D-C1D	-10.34	1.27	1.40
36	E3	900	NAD	O4D-C1D	-10.30	1.27	1.40
36	e3	900	NAD	O4D-C1D	-10.23	1.27	1.40
36	E	900	NAD	O4D-C1D	-10.22	1.27	1.40
32	I3	304	UQ8	C6-C1	10.02	1.53	1.35
32	i	302	UQ8	C6-C1	10.01	1.53	1.35
36	e	900	NAD	PN-O3	9.95	1.70	1.59
36	E	900	NAD	PN-O3	9.95	1.70	1.59
36	E3	900	NAD	PN-O3	9.91	1.70	1.59
36	e3	900	NAD	PN-O3	9.90	1.70	1.59
32	i3	303	UQ8	C6-C1	9.87	1.52	1.35
32	I	303	UQ8	C6-C1	9.83	1.52	1.35
33	g3	301	ATP	C3'-C4'	-9.67	1.28	1.53
33	G	301	ATP	C3'-C4'	-9.63	1.28	1.53
33	g	301	ATP	C3'-C4'	-9.62	1.28	1.53
33	G3	301	ATP	C3'-C4'	-9.60	1.28	1.53
33	A4	601	ATP	C3'-C4'	-9.58	1.28	1.53
33	A2	601	ATP	C3'-C4'	-9.56	1.28	1.53
33	A1	601	ATP	C3'-C4'	-9.55	1.28	1.53
33	A5	601	ATP	C3'-C4'	-9.54	1.28	1.53
33	C4	601	ATP	C3'-C4'	-9.54	1.28	1.53
33	C1	601	ATP	C3'-C4'	-9.49	1.28	1.53
33	C2	601	ATP	C3'-C4'	-9.48	1.29	1.53
33	B1	1003	ATP	C3'-C4'	-9.47	1.29	1.53
33	B4	1003	ATP	C3'-C4'	-9.45	1.29	1.53
33	C5	601	ATP	C3'-C4'	-9.45	1.29	1.53
33	B5	1003	ATP	C3'-C4'	-9.45	1.29	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	B2	1003	ATP	C3'-C4'	-9.42	1.29	1.53
36	E3	900	NAD	C3B-C4B	-9.22	1.29	1.53
36	e	900	NAD	C3B-C4B	-9.17	1.29	1.53
36	E	900	NAD	C3B-C4B	-9.17	1.29	1.53
36	e3	900	NAD	C3B-C4B	-9.17	1.29	1.53
36	e	900	NAD	C7N-N7N	8.80	1.49	1.33
36	e3	900	NAD	C7N-N7N	8.77	1.49	1.33
36	E3	900	NAD	C7N-N7N	8.76	1.49	1.33
36	E	900	NAD	C7N-N7N	8.73	1.49	1.33
36	e3	900	NAD	C3D-C4D	-8.47	1.31	1.53
36	E	900	NAD	C3D-C4D	-8.46	1.31	1.53
36	E3	900	NAD	C3D-C4D	-8.42	1.31	1.53
36	e	900	NAD	C3D-C4D	-8.39	1.31	1.53
33	C5	601	ATP	C2'-C1'	-8.24	1.27	1.53
33	B2	1003	ATP	C2'-C1'	-8.24	1.27	1.53
33	A1	601	ATP	C2'-C1'	-8.23	1.27	1.53
33	A5	601	ATP	C2'-C1'	-8.21	1.27	1.53
33	B5	1003	ATP	C2'-C1'	-8.19	1.27	1.53
33	B1	1003	ATP	C2'-C1'	-8.19	1.27	1.53
33	C2	601	ATP	C2'-C1'	-8.19	1.27	1.53
33	A4	601	ATP	C2'-C1'	-8.17	1.27	1.53
33	g	301	ATP	C2'-C1'	-8.17	1.27	1.53
33	C1	601	ATP	C2'-C1'	-8.16	1.27	1.53
33	A2	601	ATP	C2'-C1'	-8.16	1.27	1.53
33	B4	1003	ATP	C2'-C1'	-8.16	1.27	1.53
33	g3	301	ATP	C2'-C1'	-8.12	1.28	1.53
33	G3	301	ATP	C2'-C1'	-8.12	1.28	1.53
33	G	301	ATP	C2'-C1'	-8.11	1.28	1.53
33	C4	601	ATP	C2'-C1'	-8.11	1.28	1.53
36	e3	900	NAD	O4B-C4B	7.73	1.62	1.45
36	E	900	NAD	O4B-C4B	7.68	1.62	1.45
36	e	900	NAD	O4B-C4B	7.67	1.62	1.45
36	E3	900	NAD	O4B-C4B	7.63	1.62	1.45
36	E	900	NAD	O4D-C4D	7.48	1.61	1.45
36	e3	900	NAD	O4D-C4D	7.46	1.61	1.45
36	e	900	NAD	O4D-C4D	7.44	1.61	1.45
36	E3	900	NAD	O4D-C4D	7.41	1.61	1.45
33	A2	601	ATP	O4'-C1'	6.55	1.57	1.42
33	A1	601	ATP	O4'-C1'	6.54	1.57	1.42
33	A5	601	ATP	O4'-C1'	6.54	1.57	1.42
33	C1	601	ATP	O4'-C1'	6.52	1.57	1.42
33	C4	601	ATP	O4'-C1'	6.50	1.57	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	g3	301	ATP	O4'-C1'	6.49	1.57	1.42
37	B5	1002	ADP	O4'-C4'	-6.49	1.30	1.45
37	B4	1002	ADP	O4'-C4'	-6.49	1.30	1.45
37	B2	1002	ADP	O4'-C4'	-6.49	1.30	1.45
33	A4	601	ATP	O4'-C1'	6.48	1.57	1.42
37	B1	1002	ADP	O4'-C4'	-6.46	1.30	1.45
33	B1	1003	ATP	O4'-C1'	6.46	1.56	1.42
33	C2	601	ATP	O4'-C1'	6.46	1.56	1.42
33	B5	1003	ATP	O4'-C1'	6.46	1.56	1.42
33	G	301	ATP	O4'-C1'	6.46	1.56	1.42
33	B4	1003	ATP	O4'-C1'	6.45	1.56	1.42
33	g	301	ATP	O4'-C1'	6.44	1.56	1.42
33	B2	1003	ATP	O4'-C1'	6.44	1.56	1.42
37	D1	501	ADP	O4'-C4'	-6.43	1.30	1.45
33	C5	601	ATP	O4'-C1'	6.43	1.56	1.42
37	D4	501	ADP	O4'-C4'	-6.42	1.30	1.45
33	G3	301	ATP	O4'-C1'	6.41	1.56	1.42
37	D5	501	ADP	O4'-C4'	-6.33	1.30	1.45
37	D2	501	ADP	O4'-C4'	-6.27	1.31	1.45
33	B5	1003	ATP	PB-O3A	6.26	1.66	1.59
33	B1	1003	ATP	PB-O3A	6.25	1.66	1.59
33	B4	1003	ATP	PB-O3A	6.25	1.66	1.59
33	B2	1003	ATP	PB-O3A	6.23	1.66	1.59
33	A2	601	ATP	PB-O3A	6.17	1.66	1.59
33	C1	601	ATP	PA-O3A	6.15	1.66	1.59
33	C4	601	ATP	PB-O3A	6.14	1.66	1.59
33	B5	1003	ATP	PA-O3A	6.14	1.66	1.59
33	C5	601	ATP	PB-O3A	6.13	1.66	1.59
33	B4	1003	ATP	PA-O3A	6.11	1.66	1.59
33	C2	601	ATP	PB-O3A	6.10	1.66	1.59
33	C1	601	ATP	PB-O3A	6.08	1.66	1.59
33	C4	601	ATP	PA-O3A	6.08	1.66	1.59
33	A4	601	ATP	PB-O3A	6.07	1.66	1.59
33	B2	1003	ATP	PA-O3A	6.07	1.66	1.59
33	A5	601	ATP	PB-O3A	6.07	1.66	1.59
33	B1	1003	ATP	PA-O3A	6.05	1.66	1.59
33	C2	601	ATP	PA-O3A	6.04	1.66	1.59
33	A1	601	ATP	PB-O3A	6.03	1.66	1.59
33	A4	601	ATP	PA-O3A	6.03	1.66	1.59
33	A5	601	ATP	PA-O3A	6.02	1.66	1.59
33	C5	601	ATP	PA-O3A	6.01	1.66	1.59
33	A2	601	ATP	PA-O3A	6.00	1.66	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	D5	501	ADP	C3'-C4'	5.99	1.68	1.53
36	E	900	NAD	C6A-N6A	5.99	1.49	1.34
36	e3	900	NAD	C6A-N6A	5.99	1.49	1.34
37	D2	501	ADP	C3'-C4'	5.98	1.68	1.53
33	g	301	ATP	PA-O3A	5.98	1.66	1.59
36	e	900	NAD	C6A-N6A	5.95	1.49	1.34
33	A1	601	ATP	PA-O3A	5.95	1.65	1.59
33	G3	301	ATP	PA-O3A	5.93	1.65	1.59
36	E3	900	NAD	C6A-N6A	5.93	1.49	1.34
37	D4	501	ADP	C3'-C4'	5.91	1.68	1.53
37	D1	501	ADP	C3'-C4'	5.85	1.67	1.53
37	B5	1002	ADP	C3'-C4'	5.84	1.67	1.53
33	g3	301	ATP	PA-O3A	5.84	1.65	1.59
33	g3	301	ATP	PB-O3A	5.84	1.65	1.59
33	G	301	ATP	PA-O3A	5.82	1.65	1.59
37	B4	1002	ADP	C3'-C4'	5.82	1.67	1.53
37	B1	1002	ADP	C3'-C4'	5.82	1.67	1.53
37	B2	1002	ADP	C3'-C4'	5.80	1.67	1.53
33	G3	301	ATP	PB-O3A	5.80	1.65	1.59
33	G	301	ATP	PB-O3A	5.76	1.65	1.59
33	g	301	ATP	PB-O3A	5.75	1.65	1.59
33	C2	601	ATP	PB-O3B	5.49	1.65	1.59
33	A4	601	ATP	PB-O3B	5.49	1.65	1.59
33	A1	601	ATP	PB-O3B	5.47	1.65	1.59
33	C1	601	ATP	PB-O3B	5.47	1.65	1.59
33	A5	601	ATP	PB-O3B	5.47	1.65	1.59
33	C5	601	ATP	PB-O3B	5.45	1.65	1.59
33	B2	1003	ATP	PB-O3B	5.44	1.65	1.59
33	C4	601	ATP	PB-O3B	5.44	1.65	1.59
33	A2	601	ATP	PB-O3B	5.43	1.65	1.59
33	B4	1003	ATP	PB-O3B	5.43	1.65	1.59
33	B1	1003	ATP	PB-O3B	5.42	1.65	1.59
33	B5	1003	ATP	PB-O3B	5.41	1.65	1.59
33	G	301	ATP	PB-O3B	5.22	1.65	1.59
33	g	301	ATP	PB-O3B	5.22	1.65	1.59
37	D1	501	ADP	C1'-N9	-5.20	1.32	1.46
37	D4	501	ADP	C1'-N9	-5.20	1.32	1.46
33	G3	301	ATP	PB-O3B	5.19	1.65	1.59
33	g3	301	ATP	PB-O3B	5.16	1.65	1.59
36	E	900	NAD	PA-O3	5.09	1.65	1.59
36	e3	900	NAD	PA-O3	5.06	1.65	1.59
36	E3	900	NAD	PA-O3	5.04	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	e	900	NAD	PA-O3	5.03	1.64	1.59
37	B1	1002	ADP	C1'-N9	-4.90	1.32	1.46
37	B2	1002	ADP	C1'-N9	-4.89	1.32	1.46
36	E3	900	NAD	C3N-C7N	4.89	1.57	1.50
37	B5	1002	ADP	C1'-N9	-4.87	1.32	1.46
37	D5	501	ADP	C1'-N9	-4.87	1.32	1.46
37	B4	1002	ADP	C1'-N9	-4.86	1.32	1.46
37	D2	501	ADP	C1'-N9	-4.86	1.32	1.46
33	B5	1003	ATP	C2'-C3'	4.86	1.66	1.53
33	B1	1003	ATP	C2'-C3'	4.84	1.66	1.53
36	e	900	NAD	C3N-C7N	4.82	1.57	1.50
36	e3	900	NAD	C3N-C7N	4.82	1.57	1.50
33	B2	1003	ATP	C2'-C3'	4.82	1.66	1.53
33	B4	1003	ATP	C2'-C3'	4.82	1.66	1.53
36	E	900	NAD	C3N-C7N	4.81	1.57	1.50
33	A2	601	ATP	C2'-C3'	4.81	1.66	1.53
33	C2	601	ATP	C2'-C3'	4.81	1.66	1.53
33	C5	601	ATP	C2'-C3'	4.80	1.66	1.53
33	C1	601	ATP	C2'-C3'	4.79	1.66	1.53
33	A4	601	ATP	C2'-C3'	4.78	1.66	1.53
33	C4	601	ATP	C2'-C3'	4.77	1.66	1.53
33	C5	601	ATP	O4'-C4'	4.77	1.55	1.45
33	B2	1003	ATP	O4'-C4'	4.77	1.55	1.45
33	A5	601	ATP	C2'-C3'	4.76	1.66	1.53
33	A4	601	ATP	O4'-C4'	4.75	1.55	1.45
33	A1	601	ATP	O4'-C4'	4.74	1.55	1.45
33	A1	601	ATP	C2'-C3'	4.74	1.66	1.53
33	B1	1003	ATP	O4'-C4'	4.74	1.55	1.45
33	G	301	ATP	C2'-C3'	4.73	1.66	1.53
33	C2	601	ATP	O4'-C4'	4.72	1.55	1.45
33	B4	1003	ATP	O4'-C4'	4.72	1.55	1.45
33	G3	301	ATP	C2'-C3'	4.72	1.66	1.53
33	A5	601	ATP	O4'-C4'	4.72	1.55	1.45
33	g	301	ATP	C2'-C3'	4.71	1.66	1.53
33	B5	1003	ATP	O4'-C4'	4.71	1.55	1.45
33	C1	601	ATP	O4'-C4'	4.69	1.55	1.45
33	C4	601	ATP	O4'-C4'	4.68	1.55	1.45
33	A2	601	ATP	O4'-C4'	4.68	1.55	1.45
33	g3	301	ATP	C2'-C3'	4.67	1.66	1.53
33	A4	601	ATP	C6-N6	4.66	1.46	1.34
32	I	303	UQ8	C4-C3	4.65	1.53	1.36
37	D2	501	ADP	PA-O3A	4.65	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C1	601	ATP	C6-N6	4.65	1.46	1.34
33	A1	601	ATP	C6-N6	4.65	1.46	1.34
33	A2	601	ATP	C6-N6	4.64	1.46	1.34
33	B2	1003	ATP	C6-N6	4.64	1.46	1.34
33	A5	601	ATP	C6-N6	4.64	1.46	1.34
33	B5	1003	ATP	C6-N6	4.63	1.46	1.34
33	C5	601	ATP	C6-N6	4.63	1.46	1.34
32	i3	303	UQ8	C4-C3	4.63	1.53	1.36
37	B5	1002	ADP	PA-O3A	4.63	1.64	1.59
33	B1	1003	ATP	C6-N6	4.62	1.46	1.34
33	B4	1003	ATP	C6-N6	4.62	1.46	1.34
33	C4	601	ATP	C6-N6	4.62	1.46	1.34
37	B1	1002	ADP	PA-O3A	4.61	1.64	1.59
37	D4	501	ADP	PA-O3A	4.60	1.64	1.59
33	C2	601	ATP	C6-N6	4.59	1.45	1.34
32	I3	304	UQ8	C4-C3	4.58	1.52	1.36
37	B4	1002	ADP	PA-O3A	4.58	1.64	1.59
33	g3	301	ATP	C6-N6	4.58	1.45	1.34
33	G	301	ATP	C6-N6	4.58	1.45	1.34
32	i	302	UQ8	C4-C3	4.56	1.52	1.36
33	G3	301	ATP	C6-N6	4.55	1.45	1.34
37	B2	1002	ADP	PA-O3A	4.55	1.64	1.59
33	g	301	ATP	C6-N6	4.55	1.45	1.34
33	g	301	ATP	O4'-C4'	4.52	1.55	1.45
37	D5	501	ADP	PA-O3A	4.52	1.64	1.59
33	G3	301	ATP	O4'-C4'	4.50	1.55	1.45
37	B5	1002	ADP	C6-N6	4.49	1.45	1.34
37	B1	1002	ADP	C6-N6	4.49	1.45	1.34
37	D2	501	ADP	C6-N6	4.48	1.45	1.34
37	B2	1002	ADP	C6-N6	4.47	1.45	1.34
37	B4	1002	ADP	C6-N6	4.47	1.45	1.34
33	g3	301	ATP	O4'-C4'	4.47	1.54	1.45
37	D5	501	ADP	C6-N6	4.46	1.45	1.34
33	G	301	ATP	O4'-C4'	4.45	1.54	1.45
37	D4	501	ADP	C6-N6	4.44	1.45	1.34
37	D1	501	ADP	C6-N6	4.42	1.45	1.34
37	D1	501	ADP	PA-O3A	4.42	1.64	1.59
37	B2	1002	ADP	O4'-C1'	4.41	1.52	1.42
37	B5	1002	ADP	O4'-C1'	4.40	1.52	1.42
37	B4	1002	ADP	O4'-C1'	4.39	1.52	1.42
37	B1	1002	ADP	O4'-C1'	4.37	1.52	1.42
37	D5	501	ADP	O4'-C1'	4.37	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	D2	501	ADP	O4'-C1'	4.36	1.52	1.42
36	e3	900	NAD	O3D-C3D	4.33	1.53	1.43
36	E3	900	NAD	O3D-C3D	4.33	1.53	1.43
36	E	900	NAD	O3D-C3D	4.32	1.53	1.43
36	e	900	NAD	O3D-C3D	4.30	1.53	1.43
37	D1	501	ADP	O4'-C1'	4.25	1.51	1.42
37	D4	501	ADP	O4'-C1'	4.25	1.51	1.42
36	E3	900	NAD	O4B-C1B	-4.20	1.32	1.42
36	e	900	NAD	O4B-C1B	-4.18	1.32	1.42
36	E	900	NAD	O4B-C1B	-4.17	1.32	1.42
36	e3	900	NAD	O4B-C1B	-4.15	1.32	1.42
37	D2	501	ADP	C5-C4	-3.81	1.32	1.39
37	B1	1002	ADP	C5-C4	-3.81	1.32	1.39
35	J	303	PEE	C18-C19	3.81	1.53	1.31
37	B5	1002	ADP	C5-C4	-3.80	1.32	1.39
35	m	301	PEE	C18-C19	3.79	1.53	1.31
35	j3	303	PEE	C18-C19	3.79	1.53	1.31
37	D5	501	ADP	C5-C4	-3.79	1.32	1.39
35	j3	303	PEE	C39-C38	3.79	1.53	1.31
35	A	501	PEE	C39-C38	3.79	1.53	1.31
35	m	301	PEE	C39-C38	3.79	1.53	1.31
35	a3	503	PEE	C39-C38	3.78	1.53	1.31
37	B2	1002	ADP	C5-C4	-3.78	1.32	1.39
35	L3	302	PEE	C18-C19	3.78	1.53	1.31
37	B4	1002	ADP	C5-C4	-3.77	1.32	1.39
35	L3	302	PEE	C39-C38	3.77	1.53	1.31
37	D4	501	ADP	C5-C4	-3.77	1.32	1.39
35	A	501	PEE	C18-C19	3.76	1.53	1.31
35	l3	302	PEE	C18-C19	3.76	1.53	1.31
35	J	303	PEE	C39-C38	3.76	1.53	1.31
35	l3	302	PEE	C39-C38	3.76	1.53	1.31
35	L	303	PEE	C39-C38	3.74	1.52	1.31
35	a3	503	PEE	C18-C19	3.74	1.52	1.31
35	L	303	PEE	C18-C19	3.74	1.52	1.31
37	D1	501	ADP	C5-C4	-3.71	1.32	1.39
37	B2	1002	ADP	O2'-C2'	3.69	1.52	1.43
37	D4	501	ADP	O2'-C2'	3.68	1.52	1.43
37	B4	1002	ADP	O2'-C2'	3.67	1.52	1.43
37	B1	1002	ADP	O2'-C2'	3.66	1.52	1.43
37	D5	501	ADP	O2'-C2'	3.66	1.52	1.43
37	D1	501	ADP	O2'-C2'	3.66	1.52	1.43
37	D2	501	ADP	O2'-C2'	3.65	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	B5	1002	ADP	O2'-C2'	3.65	1.52	1.43
36	E	900	NAD	O3B-C3B	3.06	1.50	1.43
36	e3	900	NAD	O3B-C3B	3.06	1.50	1.43
36	e	900	NAD	O3B-C3B	3.04	1.50	1.43
36	E3	900	NAD	O3B-C3B	3.03	1.50	1.43
29	I3	302	CDL	OA6-CA4	-3.02	1.39	1.46
36	E	900	NAD	C2N-N1N	2.98	1.38	1.35
33	g	301	ATP	C5-C4	-2.97	1.33	1.39
29	L	302	CDL	OA6-CA4	-2.96	1.39	1.46
33	G	301	ATP	C5-C4	-2.95	1.33	1.39
33	g3	301	ATP	C5-C4	-2.95	1.33	1.39
36	e	900	NAD	C2N-N1N	2.94	1.38	1.35
36	e3	900	NAD	C2N-N1N	2.93	1.38	1.35
29	l3	301	CDL	OA6-CA4	-2.93	1.39	1.46
29	A3	501	CDL	OA6-CA4	-2.93	1.39	1.46
36	E3	900	NAD	C2N-N1N	2.92	1.38	1.35
29	f3	304	CDL	OB6-CB4	-2.92	1.39	1.46
33	G3	301	ATP	C5-C4	-2.92	1.33	1.39
29	l	301	CDL	OA6-CA4	-2.91	1.39	1.46
29	A	502	CDL	OA6-CA4	-2.89	1.39	1.46
29	f	304	CDL	OB6-CB4	-2.88	1.39	1.46
29	a3	501	CDL	OA6-CA4	-2.88	1.39	1.46
29	a	501	CDL	OB6-CB4	-2.88	1.39	1.46
29	a	501	CDL	OA6-CA4	-2.87	1.39	1.46
29	b	401	CDL	OA6-CA4	-2.87	1.39	1.46
29	b3	401	CDL	OA6-CA4	-2.86	1.39	1.46
29	J	301	CDL	OA6-CA4	-2.85	1.39	1.46
29	g	305	CDL	OA6-CA4	-2.85	1.39	1.46
29	J3	301	CDL	OA6-CA4	-2.85	1.39	1.46
33	A2	601	ATP	C5-C4	-2.85	1.34	1.39
29	i3	302	CDL	OA6-CA4	-2.84	1.39	1.46
33	A1	601	ATP	C5-C4	-2.84	1.34	1.39
33	C5	601	ATP	C5-C4	-2.83	1.34	1.39
29	f3	302	CDL	OB6-CB4	-2.83	1.39	1.46
33	A4	601	ATP	C5-C4	-2.83	1.34	1.39
29	j	301	CDL	OA6-CA4	-2.83	1.39	1.46
33	C2	601	ATP	C5-C4	-2.82	1.34	1.39
29	j3	301	CDL	OA6-CA4	-2.82	1.40	1.46
33	B1	1003	ATP	C5-C4	-2.81	1.34	1.39
29	a3	501	CDL	OB6-CB4	-2.81	1.40	1.46
33	C1	601	ATP	C5-C4	-2.81	1.34	1.39
29	K	202	CDL	OA6-CA4	-2.80	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	l3	301	CDL	OB6-CB4	-2.80	1.40	1.46
33	C4	601	ATP	C5-C4	-2.80	1.34	1.39
29	I	302	CDL	OA6-CA4	-2.80	1.40	1.46
33	B4	1003	ATP	C5-C4	-2.80	1.34	1.39
33	B5	1003	ATP	C5-C4	-2.79	1.34	1.39
29	K3	202	CDL	OA6-CA4	-2.79	1.40	1.46
33	B2	1003	ATP	C5-C4	-2.79	1.34	1.39
29	f	302	CDL	OB6-CB4	-2.78	1.40	1.46
29	F	302	CDL	OB6-CB4	-2.78	1.40	1.46
29	I3	302	CDL	OB6-CB4	-2.78	1.40	1.46
29	I	301	CDL	OB6-CB4	-2.78	1.40	1.46
29	b3	401	CDL	OB6-CB4	-2.78	1.40	1.46
29	b	401	CDL	OB6-CB4	-2.78	1.40	1.46
29	i3	301	CDL	OB6-CB4	-2.77	1.40	1.46
29	B	402	CDL	OB6-CB4	-2.77	1.40	1.46
29	B	403	CDL	OB6-CB4	-2.77	1.40	1.46
29	A3	501	CDL	OB6-CB4	-2.77	1.40	1.46
29	l	301	CDL	OB6-CB4	-2.77	1.40	1.46
35	j3	303	PEE	O2-C2	-2.77	1.40	1.46
29	r	201	CDL	OB6-CB4	-2.77	1.40	1.46
29	B3	402	CDL	OA6-CA4	-2.76	1.40	1.46
30	g	304	PC1	O21-C2	-2.76	1.40	1.46
29	g3	305	CDL	OA6-CA4	-2.76	1.40	1.46
29	K	202	CDL	OB6-CB4	-2.76	1.40	1.46
29	J	302	CDL	OB6-CB4	-2.75	1.40	1.46
29	B	402	CDL	OA6-CA4	-2.75	1.40	1.46
29	A	502	CDL	OB6-CB4	-2.75	1.40	1.46
29	f	303	CDL	OB6-CB4	-2.74	1.40	1.46
33	A5	601	ATP	C5-C4	-2.74	1.34	1.39
29	a3	502	CDL	OB6-CB4	-2.74	1.40	1.46
29	L	302	CDL	OB6-CB4	-2.74	1.40	1.46
29	K3	202	CDL	OB6-CB4	-2.74	1.40	1.46
35	J	303	PEE	O2-C2	-2.73	1.40	1.46
29	B3	403	CDL	OB6-CB4	-2.73	1.40	1.46
30	g3	304	PC1	O21-C2	-2.73	1.40	1.46
29	f	304	CDL	OA6-CA4	-2.72	1.40	1.46
29	J	301	CDL	OB6-CB4	-2.72	1.40	1.46
29	P3	201	CDL	OA6-CA4	-2.72	1.40	1.46
29	B	401	CDL	OB6-CB4	-2.72	1.40	1.46
29	f3	303	CDL	OB6-CB4	-2.72	1.40	1.46
29	I3	303	CDL	OA6-CA4	-2.72	1.40	1.46
29	j3	301	CDL	OB6-CB4	-2.72	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	e	900	NAD	C2A-N1A	2.72	1.38	1.33
29	g	305	CDL	OB6-CB4	-2.71	1.40	1.46
29	J3	301	CDL	OB6-CB4	-2.71	1.40	1.46
29	J3	302	CDL	OB6-CB4	-2.69	1.40	1.46
29	B3	402	CDL	OB6-CB4	-2.69	1.40	1.46
37	B1	1002	ADP	C2'-C1'	2.69	1.62	1.53
29	i	301	CDL	OB6-CB4	-2.69	1.40	1.46
29	I3	301	CDL	OB6-CB4	-2.69	1.40	1.46
29	f3	304	CDL	OA6-CA4	-2.69	1.40	1.46
29	i	301	CDL	OA6-CA4	-2.69	1.40	1.46
29	g3	305	CDL	OB6-CB4	-2.69	1.40	1.46
37	B5	1002	ADP	C2'-C1'	2.69	1.61	1.53
36	E	900	NAD	C2A-N1A	2.68	1.38	1.33
29	P	201	CDL	OA6-CA4	-2.68	1.40	1.46
30	D	301	PC1	O21-C2	-2.68	1.40	1.46
29	j3	302	CDL	OB6-CB4	-2.68	1.40	1.46
30	g3	303	PC1	O21-C2	-2.68	1.40	1.46
35	m	301	PEE	O2-C2	-2.68	1.40	1.46
30	G3	303	PC1	O21-C2	-2.67	1.40	1.46
29	i3	301	CDL	OA6-CA4	-2.67	1.40	1.46
29	F3	302	CDL	OA6-CA4	-2.67	1.40	1.46
29	B3	401	CDL	OB6-CB4	-2.67	1.40	1.46
30	G	304	PC1	O21-C2	-2.67	1.40	1.46
29	j	301	CDL	OB6-CB4	-2.66	1.40	1.46
30	G	303	PC1	O21-C2	-2.66	1.40	1.46
29	k	201	CDL	OA6-CA4	-2.66	1.40	1.46
29	p	201	CDL	OA6-CA4	-2.66	1.40	1.46
29	k3	201	CDL	OA6-CA4	-2.66	1.40	1.46
36	e3	900	NAD	C2A-N1A	2.65	1.38	1.33
29	B	404	CDL	OB6-CB4	-2.65	1.40	1.46
37	B4	1002	ADP	C2'-C1'	2.64	1.61	1.53
35	L3	302	PEE	O2-C2	-2.64	1.40	1.46
36	e3	900	NAD	C5A-C4A	-2.64	1.34	1.39
29	k	201	CDL	OB6-CB4	-2.64	1.40	1.46
29	f3	303	CDL	OA6-CA4	-2.64	1.40	1.46
29	j	302	CDL	OB6-CB4	-2.64	1.40	1.46
29	i3	302	CDL	OB6-CB4	-2.64	1.40	1.46
29	p	201	CDL	OB6-CB4	-2.64	1.40	1.46
37	B2	1002	ADP	C2'-C1'	2.64	1.61	1.53
36	e	900	NAD	C5A-C4A	-2.64	1.34	1.39
29	K3	201	CDL	OA6-CA4	-2.63	1.40	1.46
35	a3	503	PEE	O2-C2	-2.63	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	K	201	CDL	OA6-CA4	-2.63	1.40	1.46
30	G3	304	PC1	O21-C2	-2.63	1.40	1.46
29	F	303	CDL	OA6-CA4	-2.63	1.40	1.46
36	e3	900	NAD	O2B-C2B	-2.63	1.36	1.43
29	L3	301	CDL	OB6-CB4	-2.63	1.40	1.46
30	D3	301	PC1	O21-C2	-2.63	1.40	1.46
29	p3	201	CDL	OB6-CB4	-2.62	1.40	1.46
29	B	404	CDL	OA6-CA4	-2.62	1.40	1.46
36	E3	900	NAD	C5A-C4A	-2.62	1.34	1.39
35	A	501	PEE	O2-C2	-2.62	1.40	1.46
29	k3	201	CDL	OB6-CB4	-2.62	1.40	1.46
29	I	301	CDL	OA6-CA4	-2.62	1.40	1.46
36	E3	900	NAD	C2A-N1A	2.62	1.38	1.33
35	l3	302	PEE	O2-C2	-2.62	1.40	1.46
29	P	201	CDL	OB6-CB4	-2.61	1.40	1.46
30	g	303	PC1	O21-C2	-2.61	1.40	1.46
29	I3	303	CDL	OB6-CB4	-2.60	1.40	1.46
29	p3	201	CDL	OA6-CA4	-2.60	1.40	1.46
29	f	303	CDL	OA6-CA4	-2.60	1.40	1.46
36	E	900	NAD	O2B-C2B	-2.60	1.36	1.43
29	r	201	CDL	OA6-CA4	-2.60	1.40	1.46
29	I	302	CDL	OB6-CB4	-2.60	1.40	1.46
29	f3	302	CDL	OA6-CA4	-2.59	1.40	1.46
30	d3	301	PC1	O21-C2	-2.59	1.40	1.46
29	L	301	CDL	OB6-CB4	-2.59	1.40	1.46
29	P	201	CDL	OB8-CB7	2.59	1.40	1.33
36	E3	900	NAD	C8A-N9A	-2.59	1.33	1.37
29	l	302	CDL	OB6-CB4	-2.58	1.40	1.46
29	B3	404	CDL	OB6-CB4	-2.58	1.40	1.46
29	P3	201	CDL	OB6-CB4	-2.58	1.40	1.46
29	P3	201	CDL	OB8-CB7	2.58	1.40	1.33
29	L3	301	CDL	OA6-CA4	-2.58	1.40	1.46
36	E	900	NAD	C5A-C4A	-2.58	1.34	1.39
36	E	900	NAD	C8A-N9A	-2.58	1.33	1.37
29	L	301	CDL	OB8-CB7	2.57	1.40	1.33
29	I	301	CDL	OA8-CA7	2.57	1.40	1.33
36	E3	900	NAD	O2B-C2B	-2.57	1.36	1.43
29	K3	201	CDL	OB6-CB4	-2.57	1.40	1.46
29	J3	301	CDL	OA8-CA7	2.57	1.40	1.33
29	K	201	CDL	OB6-CB4	-2.57	1.40	1.46
29	f	302	CDL	OA6-CA4	-2.57	1.40	1.46
29	B	403	CDL	OA6-CA4	-2.57	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B3	404	CDL	OA6-CA4	-2.57	1.40	1.46
29	l3	303	CDL	OB6-CB4	-2.56	1.40	1.46
29	L3	301	CDL	OB8-CB7	2.55	1.40	1.33
29	b3	401	CDL	OA8-CA7	2.55	1.40	1.33
35	L	303	PEE	O2-C2	-2.55	1.40	1.46
30	d	301	PC1	O21-C2	-2.55	1.40	1.46
29	K3	202	CDL	OA8-CA7	2.55	1.40	1.33
29	j	301	CDL	OA8-CA7	2.55	1.40	1.33
29	A	502	CDL	OA8-CA7	2.54	1.40	1.33
29	J	301	CDL	OB8-CB7	2.54	1.40	1.33
29	a3	501	CDL	OA8-CA7	2.54	1.40	1.33
36	e	900	NAD	O2B-C2B	-2.54	1.36	1.43
29	f	302	CDL	OA8-CA7	2.54	1.40	1.33
29	i	301	CDL	OA8-CA7	2.54	1.40	1.33
29	I3	301	CDL	OA8-CA7	2.54	1.40	1.33
29	l3	303	CDL	OA8-CA7	2.54	1.40	1.33
29	L	302	CDL	OA8-CA7	2.54	1.40	1.33
29	j	301	CDL	OB8-CB7	2.54	1.40	1.33
29	j3	301	CDL	OB8-CB7	2.54	1.40	1.33
29	F3	302	CDL	OB6-CB4	-2.54	1.40	1.46
29	A3	501	CDL	OA8-CA7	2.53	1.40	1.33
29	B3	403	CDL	OA6-CA4	-2.53	1.40	1.46
36	e3	900	NAD	C8A-N9A	-2.53	1.33	1.37
29	k	201	CDL	OB8-CB7	2.53	1.40	1.33
29	k3	201	CDL	OB8-CB7	2.53	1.40	1.33
29	L	301	CDL	OA6-CA4	-2.53	1.40	1.46
29	k	201	CDL	OA8-CA7	2.53	1.40	1.33
29	F3	302	CDL	OA8-CA7	2.53	1.40	1.33
29	I3	301	CDL	OA6-CA4	-2.52	1.40	1.46
29	b	401	CDL	OA8-CA7	2.52	1.40	1.33
29	K	201	CDL	OB8-CB7	2.52	1.40	1.33
29	l	302	CDL	OA8-CA7	2.52	1.40	1.33
29	J3	301	CDL	OB8-CB7	2.52	1.40	1.33
29	I	302	CDL	OA8-CA7	2.52	1.40	1.33
29	f3	302	CDL	OA8-CA7	2.52	1.40	1.33
29	g3	305	CDL	OA8-CA7	2.52	1.40	1.33
29	B	404	CDL	OB8-CB7	2.52	1.40	1.33
29	k3	201	CDL	OA8-CA7	2.52	1.40	1.33
29	B	402	CDL	OA8-CA7	2.52	1.40	1.33
29	I3	303	CDL	OA8-CA7	2.51	1.40	1.33
36	e	900	NAD	C8A-N9A	-2.51	1.33	1.37
29	l	302	CDL	OA6-CA4	-2.51	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	j	302	CDL	OA8-CA7	2.51	1.40	1.33
29	I3	302	CDL	OA8-CA7	2.51	1.40	1.33
29	L3	301	CDL	OA8-CA7	2.51	1.40	1.33
29	l3	303	CDL	OA6-CA4	-2.51	1.40	1.46
37	D5	501	ADP	C2'-C1'	2.51	1.61	1.53
29	i3	302	CDL	OA8-CA7	2.50	1.40	1.33
29	B	401	CDL	OA6-CA4	-2.50	1.40	1.46
29	g	305	CDL	OA8-CA7	2.50	1.40	1.33
29	F	303	CDL	OA8-CA7	2.50	1.40	1.33
29	B3	402	CDL	OA8-CA7	2.50	1.40	1.33
29	f3	303	CDL	OB8-CB7	2.50	1.40	1.33
29	g	305	CDL	OB8-CB7	2.50	1.40	1.33
29	p	201	CDL	OA8-CA7	2.49	1.40	1.33
29	a	501	CDL	OA8-CA7	2.49	1.40	1.33
29	B3	404	CDL	OB8-CB7	2.49	1.40	1.33
29	J3	302	CDL	OB8-CB7	2.49	1.40	1.33
37	D2	501	ADP	C2'-C1'	2.49	1.61	1.53
29	F	303	CDL	OB6-CB4	-2.49	1.40	1.46
29	g3	305	CDL	OB8-CB7	2.49	1.40	1.33
29	K3	201	CDL	OB8-CB7	2.48	1.40	1.33
29	f	304	CDL	OB8-CB7	2.48	1.40	1.33
29	B	401	CDL	OA8-CA7	2.48	1.40	1.33
29	B3	401	CDL	OA8-CA7	2.48	1.40	1.33
29	K	201	CDL	OA8-CA7	2.48	1.40	1.33
29	K	202	CDL	OA8-CA7	2.48	1.40	1.33
29	L	301	CDL	OA8-CA7	2.48	1.40	1.33
29	p3	201	CDL	OA8-CA7	2.47	1.40	1.33
29	j	302	CDL	OB8-CB7	2.47	1.40	1.33
29	F	303	CDL	OB8-CB7	2.47	1.40	1.33
29	J3	302	CDL	OA8-CA7	2.47	1.40	1.33
29	F3	302	CDL	OB8-CB7	2.47	1.40	1.33
29	f	303	CDL	OB8-CB7	2.47	1.40	1.33
30	g3	304	PC1	O31-C31	2.47	1.40	1.33
29	i	301	CDL	OB8-CB7	2.47	1.40	1.33
29	I3	301	CDL	OB8-CB7	2.47	1.40	1.33
29	B3	401	CDL	OA6-CA4	-2.47	1.40	1.46
29	f3	304	CDL	OB8-CB7	2.46	1.40	1.33
29	B	403	CDL	OB8-CB7	2.46	1.40	1.33
29	a3	502	CDL	OA6-CA4	-2.46	1.40	1.46
29	j3	302	CDL	OA8-CA7	2.45	1.40	1.33
29	K3	202	CDL	OB8-CB7	2.45	1.40	1.33
29	p	201	CDL	OB8-CB7	2.45	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	I3	302	CDL	OB8-CB7	2.45	1.40	1.33
29	J	302	CDL	OB8-CB7	2.45	1.40	1.33
29	J	302	CDL	OA8-CA7	2.45	1.40	1.33
29	J	301	CDL	OA8-CA7	2.45	1.40	1.33
37	D1	501	ADP	C2'-C1'	2.45	1.61	1.53
29	r	201	CDL	OB8-CB7	2.45	1.40	1.33
29	K	202	CDL	OB8-CB7	2.45	1.40	1.33
29	i3	301	CDL	OA8-CA7	2.45	1.40	1.33
29	B3	404	CDL	OA8-CA7	2.45	1.40	1.33
29	J	302	CDL	OA6-CA4	-2.45	1.40	1.46
29	p3	201	CDL	OB8-CB7	2.45	1.40	1.33
29	i3	302	CDL	OB8-CB7	2.44	1.40	1.33
30	G	304	PC1	O31-C31	2.44	1.40	1.33
29	P3	201	CDL	OA8-CA7	2.44	1.40	1.33
29	l	302	CDL	OB8-CB7	2.44	1.40	1.33
35	L3	302	PEE	O3-C30	2.44	1.40	1.33
29	P	201	CDL	OA8-CA7	2.44	1.40	1.33
29	I3	303	CDL	OB8-CB7	2.44	1.40	1.33
29	r	201	CDL	OA8-CA7	2.44	1.40	1.33
29	l	301	CDL	OA8-CA7	2.44	1.40	1.33
29	a3	502	CDL	OB8-CB7	2.43	1.40	1.33
29	b	401	CDL	OB8-CB7	2.43	1.40	1.33
37	D4	501	ADP	C2'-C1'	2.43	1.61	1.53
30	g	304	PC1	O31-C31	2.43	1.40	1.33
29	L	302	CDL	OB8-CB7	2.42	1.40	1.33
29	l3	301	CDL	OA8-CA7	2.42	1.40	1.33
29	l3	303	CDL	OB8-CB7	2.42	1.40	1.33
29	I	302	CDL	OB8-CB7	2.42	1.40	1.33
29	K3	201	CDL	OA8-CA7	2.42	1.40	1.33
29	B3	403	CDL	OB8-CB7	2.41	1.40	1.33
30	G3	303	PC1	O31-C31	2.41	1.40	1.33
29	I	301	CDL	OB8-CB7	2.41	1.40	1.33
29	b3	401	CDL	OB8-CB7	2.41	1.40	1.33
29	j3	301	CDL	OA8-CA7	2.41	1.40	1.33
30	G3	304	PC1	O31-C31	2.41	1.40	1.33
29	F	302	CDL	OA6-CA4	-2.41	1.40	1.46
35	J	303	PEE	O3-C30	2.40	1.40	1.33
30	g	303	PC1	O31-C31	2.40	1.40	1.33
29	f3	302	CDL	OB8-CB7	2.40	1.40	1.33
29	j3	302	CDL	OA6-CA4	-2.40	1.40	1.46
29	B3	403	CDL	OA8-CA7	2.40	1.40	1.33
29	J3	302	CDL	OA6-CA4	-2.40	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	f	302	CDL	OB8-CB7	2.40	1.40	1.33
29	j3	302	CDL	OB8-CB7	2.40	1.40	1.33
29	B	403	CDL	OA8-CA7	2.39	1.40	1.33
29	i3	301	CDL	OB8-CB7	2.39	1.40	1.33
29	f3	303	CDL	OA8-CA7	2.39	1.40	1.33
29	a3	501	CDL	OB8-CB7	2.39	1.40	1.33
36	E	900	NAD	O7N-C7N	-2.39	1.19	1.24
29	f	303	CDL	OA8-CA7	2.38	1.40	1.33
29	A3	501	CDL	OB8-CB6	-2.38	1.39	1.45
29	l3	301	CDL	OB8-CB7	2.38	1.40	1.33
36	e	900	NAD	O7N-C7N	-2.38	1.19	1.24
29	f3	304	CDL	OA8-CA7	2.38	1.40	1.33
32	I	303	UQ8	O3-C3M	-2.38	1.40	1.45
29	B	404	CDL	OA8-CA7	2.37	1.40	1.33
29	A	502	CDL	OB8-CB7	2.37	1.40	1.33
32	i3	303	UQ8	C6-C5	2.37	1.53	1.46
29	B3	402	CDL	OB8-CB7	2.36	1.40	1.33
29	a	501	CDL	OB8-CB7	2.36	1.40	1.33
32	i3	303	UQ8	O3-C3M	-2.36	1.40	1.45
29	j	302	CDL	OA6-CA4	-2.36	1.41	1.46
29	F	302	CDL	OB8-CB7	2.36	1.40	1.33
35	L	303	PEE	O3-C30	2.36	1.40	1.33
36	E3	900	NAD	O7N-C7N	-2.36	1.19	1.24
30	g3	303	PC1	O31-C31	2.36	1.40	1.33
32	I3	304	UQ8	C6-C5	2.36	1.53	1.46
36	e3	900	NAD	O7N-C7N	-2.35	1.19	1.24
29	l	301	CDL	OB8-CB7	2.35	1.40	1.33
29	A3	501	CDL	OB8-CB7	2.35	1.40	1.33
32	I	303	UQ8	C6-C5	2.35	1.53	1.46
35	m	301	PEE	O3-C30	2.35	1.40	1.33
29	a3	502	CDL	OA8-CA7	2.35	1.40	1.33
29	B	402	CDL	OB8-CB6	-2.35	1.39	1.45
30	d	301	PC1	O31-C31	2.35	1.40	1.33
29	B3	404	CDL	OA6-CA5	2.35	1.40	1.34
29	B3	401	CDL	OB8-CB7	2.34	1.40	1.33
29	B	401	CDL	OB8-CB7	2.34	1.40	1.33
30	G	303	PC1	O31-C31	2.34	1.40	1.33
30	D3	301	PC1	O31-C31	2.34	1.40	1.33
35	A	501	PEE	O3-C30	2.34	1.40	1.33
32	i	302	UQ8	C6-C5	2.34	1.53	1.46
29	F	302	CDL	OA8-CA6	-2.33	1.40	1.45
30	D	301	PC1	O31-C31	2.33	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	a3	503	PEE	O3-C30	2.33	1.40	1.33
32	I	303	UQ8	O4-C4M	-2.33	1.40	1.45
35	j3	303	PEE	O3-C30	2.33	1.40	1.33
33	G3	301	ATP	C8-N9	-2.33	1.33	1.37
29	B	402	CDL	OB8-CB7	2.33	1.40	1.33
32	I3	304	UQ8	O4-C4M	-2.33	1.40	1.45
35	l3	302	PEE	O3-C30	2.32	1.40	1.33
33	G	301	ATP	C8-N9	-2.32	1.33	1.37
33	g3	301	ATP	C8-N9	-2.32	1.33	1.37
29	B3	404	CDL	OB6-CB5	2.32	1.40	1.34
32	I3	304	UQ8	O3-C3M	-2.32	1.40	1.45
33	g	301	ATP	C8-N9	-2.32	1.33	1.37
29	A	502	CDL	OB8-CB6	-2.32	1.40	1.45
29	f	304	CDL	OA8-CA7	2.32	1.40	1.33
30	d3	301	PC1	O31-C31	2.32	1.40	1.33
32	i	302	UQ8	O4-C4M	-2.31	1.40	1.45
29	F	302	CDL	OA8-CA7	2.31	1.40	1.33
29	l3	301	CDL	OA8-CA6	-2.31	1.40	1.45
32	i	302	UQ8	O3-C3M	-2.30	1.40	1.45
29	f	304	CDL	OA8-CA6	-2.30	1.40	1.45
29	a3	502	CDL	OA8-CA6	-2.30	1.40	1.45
32	i3	303	UQ8	O4-C4M	-2.30	1.40	1.45
29	l3	303	CDL	OA6-CA5	2.29	1.40	1.34
29	B	404	CDL	OA6-CA5	2.29	1.40	1.34
29	f3	302	CDL	OB8-CB6	-2.28	1.40	1.45
29	B	404	CDL	OB6-CB5	2.28	1.40	1.34
29	F	302	CDL	OA6-CA5	2.28	1.40	1.34
29	F	302	CDL	OB8-CB6	-2.28	1.40	1.45
29	L3	301	CDL	OB6-CB5	2.28	1.40	1.34
29	I3	303	CDL	OB6-CB5	2.28	1.40	1.34
35	a3	503	PEE	O3-C3	-2.28	1.40	1.45
29	l	302	CDL	OA6-CA5	2.28	1.40	1.34
30	G3	303	PC1	O31-C3	-2.28	1.40	1.45
30	G	303	PC1	O31-C3	-2.27	1.40	1.45
29	I	302	CDL	OB6-CB5	2.27	1.40	1.34
30	d3	301	PC1	O21-C21	2.27	1.40	1.34
29	a3	502	CDL	OA6-CA5	2.26	1.40	1.34
35	A	501	PEE	O3-C3	-2.26	1.40	1.45
29	B	403	CDL	OA8-CA6	-2.26	1.40	1.45
29	j	302	CDL	OB6-CB5	2.26	1.40	1.34
29	K	201	CDL	OB6-CB5	2.26	1.40	1.34
29	L	301	CDL	OB6-CB5	2.26	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	301	PC1	O21-C21	2.26	1.40	1.34
29	f	303	CDL	OA6-CA5	2.26	1.40	1.34
29	F3	302	CDL	OB6-CB5	2.26	1.40	1.34
30	d3	301	PC1	O31-C3	-2.26	1.40	1.45
29	K3	201	CDL	OB6-CB5	2.26	1.40	1.34
33	G3	301	ATP	C5-N7	-2.25	1.35	1.39
29	B	403	CDL	OA6-CA5	2.25	1.40	1.34
33	G	301	ATP	C5-N7	-2.25	1.35	1.39
29	l	301	CDL	OB8-CB6	-2.25	1.40	1.45
29	B	401	CDL	OB8-CB6	-2.25	1.40	1.45
30	g3	303	PC1	O31-C3	-2.25	1.40	1.45
29	B3	401	CDL	OA6-CA5	2.25	1.40	1.34
35	L	303	PEE	O2-C10	2.25	1.40	1.34
29	k3	201	CDL	OA6-CA5	2.24	1.40	1.34
29	K	201	CDL	OA6-CA5	2.24	1.40	1.34
29	l	302	CDL	OB6-CB5	2.24	1.40	1.34
30	D3	301	PC1	O31-C3	-2.24	1.40	1.45
29	F3	302	CDL	OA6-CA5	2.24	1.40	1.34
30	D	301	PC1	O31-C3	-2.24	1.40	1.45
29	k	201	CDL	OB6-CB5	2.24	1.40	1.34
37	D4	501	ADP	C8-N9	-2.24	1.33	1.37
29	B3	403	CDL	OA6-CA5	2.24	1.40	1.34
29	f3	303	CDL	OA6-CA5	2.24	1.40	1.34
29	B3	403	CDL	OB8-CB6	-2.24	1.40	1.45
29	B3	401	CDL	OB8-CB6	-2.23	1.40	1.45
29	f3	304	CDL	OA6-CA5	2.23	1.40	1.34
29	F	303	CDL	OA6-CA5	2.23	1.40	1.34
35	a3	503	PEE	O2-C10	2.23	1.40	1.34
33	g	301	ATP	C5-N7	-2.23	1.35	1.39
33	g3	301	ATP	C5-N7	-2.23	1.35	1.39
29	L	301	CDL	OA6-CA5	2.23	1.40	1.34
29	F	303	CDL	OB6-CB5	2.23	1.40	1.34
29	f	302	CDL	OB8-CB6	-2.23	1.40	1.45
33	B4	1003	ATP	C5-N7	-2.22	1.35	1.39
29	i3	302	CDL	OB6-CB5	2.22	1.40	1.34
29	B	404	CDL	OA8-CA6	-2.22	1.40	1.45
30	G	304	PC1	O21-C21	2.22	1.40	1.34
29	p3	201	CDL	OB6-CB5	2.22	1.40	1.34
29	k	201	CDL	OA6-CA5	2.22	1.40	1.34
30	G3	304	PC1	O21-C21	2.22	1.40	1.34
35	l3	302	PEE	O2-C10	2.22	1.40	1.34
29	a3	502	CDL	OB8-CB6	-2.22	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	g	303	PC1	O31-C3	-2.22	1.40	1.45
29	j3	302	CDL	OB6-CB5	2.22	1.40	1.34
29	B	403	CDL	OB8-CB6	-2.22	1.40	1.45
35	j3	303	PEE	O3-C3	-2.22	1.40	1.45
29	g	305	CDL	OB6-CB5	2.22	1.40	1.34
29	p	201	CDL	OA6-CA5	2.22	1.40	1.34
35	L	303	PEE	O3-C3	-2.22	1.40	1.45
33	C5	601	ATP	C5-N7	-2.22	1.35	1.39
35	A	501	PEE	O2-C10	2.22	1.40	1.34
29	B	401	CDL	OB6-CB5	2.21	1.40	1.34
29	P3	201	CDL	OB6-CB5	2.21	1.40	1.34
29	f	302	CDL	OA6-CA5	2.21	1.40	1.34
29	B3	402	CDL	OB8-CB6	-2.21	1.40	1.45
29	l3	303	CDL	OB6-CB5	2.21	1.40	1.34
29	b3	401	CDL	OB8-CB6	-2.21	1.40	1.45
33	C4	601	ATP	C5-N7	-2.21	1.35	1.39
29	J3	302	CDL	OA6-CA5	2.21	1.40	1.34
37	D1	501	ADP	C8-N9	-2.21	1.33	1.37
29	a	501	CDL	OB8-CB6	-2.21	1.40	1.45
29	A3	501	CDL	OA8-CA6	-2.21	1.40	1.45
35	l3	302	PEE	O3-C3	-2.21	1.40	1.45
29	I3	301	CDL	OB6-CB5	2.21	1.40	1.34
33	C2	601	ATP	C5-N7	-2.21	1.35	1.39
29	K3	201	CDL	OA6-CA5	2.21	1.40	1.34
33	C1	601	ATP	C5'-C4'	2.20	1.58	1.51
33	C5	601	ATP	C8-N9	-2.20	1.33	1.37
29	f3	304	CDL	OA8-CA6	-2.20	1.40	1.45
29	f	304	CDL	OA6-CA5	2.20	1.40	1.34
29	k3	201	CDL	OB6-CB5	2.20	1.40	1.34
29	p	201	CDL	OB6-CB5	2.20	1.40	1.34
33	B1	1003	ATP	C5-N7	-2.20	1.35	1.39
29	f	303	CDL	OB6-CB5	2.20	1.40	1.34
29	J	302	CDL	OA6-CA5	2.20	1.40	1.34
33	C1	601	ATP	C5-N7	-2.20	1.35	1.39
29	j	302	CDL	OA6-CA5	2.20	1.40	1.34
33	A5	601	ATP	C5-N7	-2.20	1.35	1.39
29	l	302	CDL	OB8-CB6	-2.19	1.40	1.45
29	B	401	CDL	OA6-CA5	2.19	1.40	1.34
29	f3	302	CDL	OA6-CA5	2.19	1.40	1.34
29	A3	501	CDL	OB6-CB5	2.19	1.40	1.34
29	j3	301	CDL	OB6-CB5	2.19	1.40	1.34
29	B3	401	CDL	OB6-CB5	2.19	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	l3	303	CDL	OB8-CB6	-2.19	1.40	1.45
33	B2	1003	ATP	C5-N7	-2.19	1.35	1.39
29	B3	403	CDL	OA8-CA6	-2.19	1.40	1.45
29	j3	302	CDL	OA6-CA5	2.19	1.40	1.34
29	I	301	CDL	OB6-CB5	2.19	1.40	1.34
33	A2	601	ATP	C8-N9	-2.19	1.33	1.37
29	P	201	CDL	OB6-CB5	2.19	1.40	1.34
29	j3	302	CDL	OB8-CB6	-2.18	1.40	1.45
33	A2	601	ATP	C5-N7	-2.18	1.35	1.39
29	p3	201	CDL	OA6-CA5	2.18	1.40	1.34
29	J	301	CDL	OB6-CB5	2.18	1.40	1.34
33	C4	601	ATP	C5'-C4'	2.18	1.58	1.51
29	F	302	CDL	OB6-CB5	2.18	1.40	1.34
29	a3	501	CDL	OB8-CB6	-2.18	1.40	1.45
29	I	302	CDL	OB8-CB6	-2.18	1.40	1.45
29	B3	404	CDL	OA8-CA6	-2.18	1.40	1.45
33	B5	1003	ATP	C5-N7	-2.18	1.35	1.39
29	i	301	CDL	OB6-CB5	2.18	1.40	1.34
29	l3	301	CDL	OB8-CB6	-2.18	1.40	1.45
30	D	301	PC1	O21-C21	2.18	1.40	1.34
29	B3	402	CDL	OB6-CB5	2.18	1.40	1.34
29	B3	404	CDL	OB8-CB6	-2.18	1.40	1.45
29	L3	301	CDL	OA6-CA5	2.18	1.40	1.34
36	E3	900	NAD	PA-O5B	2.18	1.67	1.59
33	A5	601	ATP	C8-N9	-2.18	1.33	1.37
29	I3	303	CDL	OB8-CB6	-2.17	1.40	1.45
29	l	302	CDL	OA8-CA6	-2.17	1.40	1.45
35	J	303	PEE	O3-C3	-2.17	1.40	1.45
29	J3	302	CDL	OB6-CB5	2.17	1.40	1.34
29	f	303	CDL	OA8-CA6	-2.17	1.40	1.45
33	B2	1003	ATP	C5'-C4'	2.17	1.58	1.51
33	A4	601	ATP	C5-N7	-2.17	1.35	1.39
29	g3	305	CDL	OB6-CB5	2.17	1.40	1.34
29	A	502	CDL	OB6-CB5	2.17	1.40	1.34
29	I3	303	CDL	OA6-CA5	2.17	1.40	1.34
29	J	302	CDL	OA8-CA6	-2.17	1.40	1.45
30	d	301	PC1	O31-C3	-2.17	1.40	1.45
33	A1	601	ATP	C8-N9	-2.17	1.33	1.37
29	f3	303	CDL	OA8-CA6	-2.17	1.40	1.45
29	j	302	CDL	OB8-CB6	-2.17	1.40	1.45
29	I3	302	CDL	OB8-CB6	-2.17	1.40	1.45
29	K3	202	CDL	OB6-CB5	2.17	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	J3	301	CDL	OB6-CB5	2.17	1.40	1.34
29	a3	502	CDL	OB6-CB5	2.16	1.40	1.34
33	G3	301	ATP	C5'-C4'	2.16	1.58	1.51
33	A4	601	ATP	C8-N9	-2.16	1.33	1.37
33	C2	601	ATP	C8-N9	-2.16	1.33	1.37
36	e	900	NAD	PA-O5B	2.16	1.67	1.59
33	B4	1003	ATP	C5'-C4'	2.16	1.58	1.51
33	B4	1003	ATP	C8-N9	-2.16	1.33	1.37
29	I	302	CDL	OA6-CA5	2.16	1.40	1.34
30	g3	303	PC1	O21-C21	2.16	1.40	1.34
29	j	301	CDL	OB6-CB5	2.16	1.40	1.34
29	B3	402	CDL	OA6-CA5	2.16	1.40	1.34
30	g	303	PC1	O21-C21	2.16	1.40	1.34
33	B2	1003	ATP	C8-N9	-2.16	1.33	1.37
30	D3	301	PC1	O21-C21	2.15	1.40	1.34
35	m	301	PEE	O2-C10	2.15	1.40	1.34
29	i3	301	CDL	OB8-CB6	-2.15	1.40	1.45
35	L3	302	PEE	O2-C10	2.15	1.40	1.34
33	B1	1003	ATP	C8-N9	-2.15	1.33	1.37
29	j	301	CDL	OA6-CA5	2.15	1.40	1.34
33	A2	601	ATP	C5'-C4'	2.15	1.58	1.51
33	A4	601	ATP	C5'-C4'	2.15	1.58	1.51
29	K3	201	CDL	OA8-CA6	-2.15	1.40	1.45
33	B5	1003	ATP	C8-N9	-2.15	1.33	1.37
29	B	402	CDL	OA6-CA5	2.15	1.40	1.34
33	A1	601	ATP	C5-N7	-2.14	1.35	1.39
29	f	303	CDL	OB8-CB6	-2.14	1.40	1.45
30	G3	304	PC1	O31-C3	-2.14	1.40	1.45
29	B	401	CDL	OA8-CA6	-2.14	1.40	1.45
29	K3	202	CDL	OA8-CA6	-2.14	1.40	1.45
33	C4	601	ATP	C8-N9	-2.14	1.33	1.37
35	m	301	PEE	O3-C3	-2.14	1.40	1.45
29	r	201	CDL	OB6-CB5	2.14	1.40	1.34
30	G	303	PC1	O21-C21	2.14	1.40	1.34
33	B1	1003	ATP	C5'-C4'	2.14	1.58	1.51
29	B	403	CDL	OB6-CB5	2.14	1.40	1.34
29	i3	301	CDL	OA8-CA6	-2.14	1.40	1.45
29	r	201	CDL	OA8-CA6	-2.14	1.40	1.45
29	K	202	CDL	OB6-CB5	2.14	1.40	1.34
33	C1	601	ATP	C8-N9	-2.14	1.33	1.37
29	l	301	CDL	OA8-CA6	-2.14	1.40	1.45
29	A3	501	CDL	OA6-CA5	2.14	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a3	501	CDL	OA8-CA6	-2.13	1.40	1.45
29	P3	201	CDL	OA6-CA5	2.13	1.40	1.34
33	B5	1003	ATP	C5'-C4'	2.13	1.58	1.51
33	A5	601	ATP	C5'-C4'	2.13	1.58	1.51
29	f	304	CDL	OB8-CB6	-2.13	1.40	1.45
36	e3	900	NAD	C8A-N7A	2.13	1.35	1.31
36	E3	900	NAD	C8A-N7A	2.13	1.35	1.31
29	g	305	CDL	OA8-CA6	-2.13	1.40	1.45
29	B3	401	CDL	OA8-CA6	-2.13	1.40	1.45
29	K	202	CDL	OA8-CA6	-2.13	1.40	1.45
29	J3	302	CDL	OA8-CA6	-2.13	1.40	1.45
29	I3	302	CDL	OB6-CB5	2.13	1.40	1.34
29	J	302	CDL	OB6-CB5	2.13	1.40	1.34
29	f3	303	CDL	OB6-CB5	2.13	1.40	1.34
35	L3	302	PEE	O3-C3	-2.13	1.40	1.45
29	K3	202	CDL	OB8-CB6	-2.13	1.40	1.45
36	e3	900	NAD	PA-O5B	2.13	1.67	1.59
29	L	302	CDL	OA8-CA6	-2.13	1.40	1.45
35	J	303	PEE	O2-C10	2.13	1.40	1.34
29	f3	304	CDL	OB8-CB6	-2.13	1.40	1.45
29	i	301	CDL	OA6-CA5	2.13	1.40	1.34
29	a3	501	CDL	OA6-CA5	2.12	1.40	1.34
29	L	302	CDL	OB8-CB6	-2.12	1.40	1.45
29	L3	301	CDL	OB8-CB6	-2.12	1.40	1.45
29	i3	301	CDL	OB6-CB5	2.12	1.40	1.34
33	C2	601	ATP	C5'-C4'	2.12	1.57	1.51
29	b	401	CDL	OB6-CB5	2.12	1.40	1.34
29	B	402	CDL	OB6-CB5	2.12	1.40	1.34
29	j3	301	CDL	OA6-CA5	2.12	1.40	1.34
29	r	201	CDL	OA6-CA5	2.12	1.40	1.34
36	e	900	NAD	C8A-N7A	2.12	1.35	1.31
29	P	201	CDL	OA8-CA6	-2.12	1.40	1.45
29	A	502	CDL	OA6-CA5	2.12	1.40	1.34
29	K3	201	CDL	OB8-CB6	-2.12	1.40	1.45
36	E	900	NAD	C8A-N7A	2.12	1.35	1.31
33	C5	601	ATP	C5'-C4'	2.11	1.57	1.51
29	l	301	CDL	OB6-CB5	2.11	1.40	1.34
29	B3	403	CDL	OB6-CB5	2.11	1.40	1.34
29	f3	304	CDL	OB6-CB5	2.11	1.40	1.34
29	f	304	CDL	OB6-CB5	2.11	1.40	1.34
29	i3	302	CDL	OA6-CA5	2.11	1.40	1.34
29	j3	301	CDL	OA8-CA6	-2.11	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	G3	303	PC1	O21-C21	2.11	1.40	1.34
33	A1	601	ATP	C5'-C4'	2.11	1.57	1.51
29	j3	302	CDL	OA8-CA6	-2.11	1.40	1.45
36	E	900	NAD	PA-O5B	2.11	1.67	1.59
29	l3	303	CDL	OA8-CA6	-2.11	1.40	1.45
29	L	302	CDL	OB6-CB5	2.11	1.40	1.34
29	J3	302	CDL	OB8-CB6	-2.11	1.40	1.45
29	a	501	CDL	OB6-CB5	2.11	1.40	1.34
29	a	501	CDL	OA6-CA5	2.11	1.40	1.34
29	P	201	CDL	OA6-CA5	2.11	1.40	1.34
29	g	305	CDL	OB8-CB6	-2.11	1.40	1.45
29	b3	401	CDL	OB6-CB5	2.10	1.40	1.34
29	a3	501	CDL	OB6-CB5	2.10	1.40	1.34
29	g3	305	CDL	OA8-CA6	-2.10	1.40	1.45
29	K	201	CDL	OB8-CB6	-2.10	1.40	1.45
29	I3	301	CDL	OA6-CA5	2.10	1.40	1.34
29	K	202	CDL	OA6-CA5	2.10	1.40	1.34
29	g	305	CDL	OA6-CA5	2.09	1.40	1.34
30	g	304	PC1	O21-C21	2.09	1.40	1.34
29	g3	305	CDL	OB8-CB6	-2.09	1.40	1.45
29	p3	201	CDL	OB8-CB6	-2.09	1.40	1.45
29	I	301	CDL	OA6-CA5	2.09	1.40	1.34
29	A	502	CDL	OA8-CA6	-2.09	1.40	1.45
33	g	301	ATP	C5'-C4'	2.09	1.57	1.51
29	g3	305	CDL	OA6-CA5	2.09	1.40	1.34
29	i	301	CDL	OB8-CB6	-2.09	1.40	1.45
30	g3	304	PC1	O31-C3	-2.09	1.40	1.45
29	r	201	CDL	OB8-CB6	-2.09	1.40	1.45
30	g	304	PC1	O31-C3	-2.09	1.40	1.45
29	f	302	CDL	OA8-CA6	-2.09	1.40	1.45
29	k	201	CDL	OA8-CA6	-2.09	1.40	1.45
29	b	401	CDL	OB8-CB6	-2.09	1.40	1.45
29	p3	201	CDL	OA8-CA6	-2.09	1.40	1.45
29	b	401	CDL	OA6-CA5	2.09	1.40	1.34
29	b3	401	CDL	OA6-CA5	2.09	1.40	1.34
29	B	404	CDL	OB8-CB6	-2.09	1.40	1.45
29	i3	302	CDL	OB8-CB6	-2.09	1.40	1.45
33	G	301	ATP	C5'-C4'	2.09	1.57	1.51
29	P3	201	CDL	OA8-CA6	-2.09	1.40	1.45
30	g3	304	PC1	O21-C21	2.08	1.40	1.34
29	K3	202	CDL	OA6-CA5	2.08	1.40	1.34
29	a	501	CDL	OA8-CA6	-2.08	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	f3	303	CDL	OB8-CB6	-2.08	1.40	1.45
29	j	302	CDL	OA8-CA6	-2.08	1.40	1.45
29	K	201	CDL	OA8-CA6	-2.08	1.40	1.45
29	p	201	CDL	OA8-CA6	-2.08	1.40	1.45
30	G	304	PC1	O31-C3	-2.08	1.40	1.45
35	j3	303	PEE	O2-C10	2.08	1.40	1.34
29	J3	301	CDL	OB8-CB6	-2.08	1.40	1.45
29	f3	302	CDL	OB6-CB5	2.08	1.40	1.34
29	J	301	CDL	OA8-CA6	-2.08	1.40	1.45
29	L3	301	CDL	OA8-CA6	-2.08	1.40	1.45
29	J3	301	CDL	OA6-CA5	2.07	1.40	1.34
29	K	202	CDL	OB8-CB6	-2.07	1.40	1.45
29	L	301	CDL	OA8-CA6	-2.07	1.40	1.45
29	I	301	CDL	OB8-CB6	-2.07	1.40	1.45
29	J	301	CDL	OA6-CA5	2.07	1.40	1.34
29	I3	301	CDL	OB8-CB6	-2.07	1.40	1.45
29	L	301	CDL	OB8-CB6	-2.07	1.40	1.45
29	B	402	CDL	OA8-CA6	-2.07	1.40	1.45
32	i	302	UQ8	O5-C5	-2.07	1.18	1.23
32	I3	304	UQ8	O5-C5	-2.06	1.18	1.23
29	J	302	CDL	OB8-CB6	-2.06	1.40	1.45
29	f3	302	CDL	OA8-CA6	-2.06	1.40	1.45
29	p	201	CDL	OB8-CB6	-2.06	1.40	1.45
32	I3	304	UQ8	O2-C2	-2.06	1.18	1.23
29	I3	301	CDL	OA8-CA6	-2.06	1.40	1.45
29	I	301	CDL	OA8-CA6	-2.05	1.40	1.45
32	i	302	UQ8	O2-C2	-2.05	1.18	1.23
29	k	201	CDL	OB8-CB6	-2.05	1.40	1.45
29	f	302	CDL	OB6-CB5	2.05	1.40	1.34
32	i3	303	UQ8	O2-C2	-2.05	1.18	1.23
32	I	303	UQ8	O2-C2	-2.05	1.18	1.23
29	l3	301	CDL	OA6-CA5	2.05	1.40	1.34
32	i3	303	UQ8	O5-C5	-2.05	1.18	1.23
29	i3	301	CDL	OA6-CA5	2.05	1.40	1.34
32	I	303	UQ8	O5-C5	-2.04	1.18	1.23
29	F	303	CDL	OA8-CA6	-2.04	1.40	1.45
29	i3	302	CDL	OA8-CA6	-2.04	1.40	1.45
29	j	301	CDL	OA8-CA6	-2.03	1.40	1.45
29	b3	401	CDL	OA8-CA6	-2.03	1.40	1.45
29	F3	302	CDL	OB8-CB6	-2.03	1.40	1.45
29	j3	301	CDL	OB8-CB6	-2.03	1.40	1.45
29	l3	301	CDL	OB6-CB5	2.03	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B3	402	CDL	OA8-CA6	-2.03	1.40	1.45
29	k3	201	CDL	OA8-CA6	-2.03	1.40	1.45
33	g3	301	ATP	C5'-C4'	2.02	1.57	1.51
29	F	303	CDL	OB8-CB6	-2.02	1.40	1.45
29	k3	201	CDL	OB8-CB6	-2.02	1.40	1.45
29	I3	303	CDL	OA8-CA6	-2.02	1.40	1.45
29	I3	302	CDL	OA8-CA6	-2.02	1.40	1.45
29	F3	302	CDL	OA8-CA6	-2.01	1.40	1.45
29	l	301	CDL	OA6-CA5	2.01	1.40	1.34
29	j	301	CDL	OB8-CB6	-2.01	1.40	1.45
29	L	302	CDL	OA6-CA5	2.00	1.39	1.34
29	J3	301	CDL	OA8-CA6	-2.00	1.40	1.45
29	I3	302	CDL	OA6-CA5	2.00	1.39	1.34

All (772) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D4	501	ADP	C1'-N9-C8	-13.42	97.31	127.09
37	D1	501	ADP	C1'-N9-C8	-13.38	97.40	127.09
37	B5	1002	ADP	C1'-N9-C8	-12.29	99.81	127.09
37	B1	1002	ADP	C1'-N9-C8	-12.27	99.87	127.09
37	B4	1002	ADP	C1'-N9-C8	-12.25	99.91	127.09
37	B2	1002	ADP	C1'-N9-C8	-12.24	99.94	127.09
37	D5	501	ADP	C1'-N9-C8	-12.06	100.33	127.09
37	D2	501	ADP	C1'-N9-C8	-12.03	100.39	127.09
37	D4	501	ADP	C4-N9-C1'	12.02	154.74	126.63
37	D1	501	ADP	C4-N9-C1'	12.00	154.69	126.63
37	B5	1002	ADP	C4-N9-C1'	11.21	152.85	126.63
37	B1	1002	ADP	C4-N9-C1'	11.21	152.84	126.63
37	B2	1002	ADP	C4-N9-C1'	11.18	152.77	126.63
37	B4	1002	ADP	C4-N9-C1'	11.17	152.75	126.63
37	D5	501	ADP	C4-N9-C1'	11.03	152.43	126.63
37	D2	501	ADP	C4-N9-C1'	11.00	152.35	126.63
36	e	900	NAD	C4A-N9A-C1B	-6.57	111.28	126.63
36	e3	900	NAD	C4A-N9A-C1B	-6.51	111.41	126.63
36	E3	900	NAD	C4A-N9A-C1B	-6.39	111.70	126.63
36	E	900	NAD	C4A-N9A-C1B	-6.33	111.83	126.63
33	g	301	ATP	C1'-N9-C8	-5.84	114.14	127.09
33	G3	301	ATP	C1'-N9-C8	-5.82	114.17	127.09
33	g3	301	ATP	C1'-N9-C8	-5.74	114.35	127.09
33	A2	601	ATP	C1'-N9-C8	-5.71	114.43	127.09
33	G	301	ATP	C1'-N9-C8	-5.70	114.45	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	A5	601	ATP	C1'-N9-C8	-5.68	114.48	127.09
33	A4	601	ATP	C1'-N9-C8	-5.68	114.48	127.09
37	B5	1002	ADP	N3-C2-N1	-5.67	120.00	128.58
33	C2	601	ATP	C1'-N9-C8	-5.66	114.52	127.09
37	B2	1002	ADP	N3-C2-N1	-5.66	120.01	128.58
37	D1	501	ADP	N3-C2-N1	-5.66	120.01	128.58
37	B4	1002	ADP	N3-C2-N1	-5.65	120.02	128.58
33	C5	601	ATP	C1'-N9-C8	-5.65	114.56	127.09
37	D5	501	ADP	N3-C2-N1	-5.64	120.04	128.58
33	A1	601	ATP	C1'-N9-C8	-5.64	114.57	127.09
33	C4	601	ATP	C1'-N9-C8	-5.63	114.59	127.09
33	B5	1003	ATP	C1'-N9-C8	-5.63	114.60	127.09
37	D2	501	ADP	N3-C2-N1	-5.63	120.06	128.58
33	B5	1003	ATP	N3-C2-N1	-5.63	120.07	128.58
37	B1	1002	ADP	N3-C2-N1	-5.62	120.07	128.58
33	C1	601	ATP	C1'-N9-C8	-5.62	114.62	127.09
37	D4	501	ADP	N3-C2-N1	-5.62	120.07	128.58
33	B2	1003	ATP	C1'-N9-C8	-5.62	114.62	127.09
33	C4	601	ATP	N3-C2-N1	-5.62	120.07	128.58
33	G	301	ATP	N3-C2-N1	-5.62	120.08	128.58
33	g	301	ATP	N3-C2-N1	-5.61	120.08	128.58
33	B1	1003	ATP	N3-C2-N1	-5.61	120.09	128.58
33	A5	601	ATP	N3-C2-N1	-5.61	120.09	128.58
33	C2	601	ATP	N3-C2-N1	-5.61	120.09	128.58
33	C5	601	ATP	N3-C2-N1	-5.60	120.11	128.58
33	g3	301	ATP	N3-C2-N1	-5.60	120.11	128.58
33	A4	601	ATP	N3-C2-N1	-5.60	120.11	128.58
33	B4	1003	ATP	N3-C2-N1	-5.60	120.11	128.58
33	G3	301	ATP	N3-C2-N1	-5.60	120.11	128.58
33	B4	1003	ATP	C1'-N9-C8	-5.60	114.67	127.09
33	A1	601	ATP	N3-C2-N1	-5.59	120.11	128.58
33	B2	1003	ATP	N3-C2-N1	-5.58	120.13	128.58
33	C1	601	ATP	N3-C2-N1	-5.58	120.13	128.58
33	A2	601	ATP	N3-C2-N1	-5.57	120.14	128.58
33	B1	1003	ATP	C1'-N9-C8	-5.55	114.78	127.09
36	e	900	NAD	N3A-C2A-N1A	-5.53	120.22	128.58
36	e3	900	NAD	N3A-C2A-N1A	-5.51	120.24	128.58
36	E3	900	NAD	N3A-C2A-N1A	-5.51	120.24	128.58
36	E	900	NAD	N3A-C2A-N1A	-5.50	120.26	128.58
36	e	900	NAD	C1B-N9A-C8A	5.31	138.88	127.09
36	e3	900	NAD	C1B-N9A-C8A	5.23	138.69	127.09
36	E3	900	NAD	C1B-N9A-C8A	5.14	138.50	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D5	501	ADP	C5-C4-N3	-5.08	119.72	126.72
36	E	900	NAD	C1B-N9A-C8A	5.07	138.34	127.09
37	D2	501	ADP	C5-C4-N3	-5.07	119.74	126.72
37	B4	1002	ADP	C5-C4-N3	-5.07	119.74	126.72
37	B5	1002	ADP	C5-C4-N3	-5.05	119.76	126.72
37	B2	1002	ADP	C5-C4-N3	-5.04	119.78	126.72
36	e3	900	NAD	N9A-C8A-N7A	-5.02	106.82	113.94
37	B1	1002	ADP	C5-C4-N3	-5.01	119.82	126.72
36	e	900	NAD	N9A-C8A-N7A	-4.99	106.86	113.94
37	D1	501	ADP	C5-C4-N3	-4.97	119.88	126.72
29	l	302	CDL	OB6-CB5-C51	4.96	122.21	111.48
37	D4	501	ADP	C5-C4-N3	-4.95	119.90	126.72
36	E	900	NAD	N9A-C8A-N7A	-4.94	106.92	113.94
29	l3	303	CDL	OB6-CB5-C51	4.94	122.16	111.48
36	E3	900	NAD	N9A-C8A-N7A	-4.93	106.94	113.94
36	E	900	NAD	N6A-C6A-N1A	-4.92	107.41	118.38
36	E3	900	NAD	N6A-C6A-N1A	-4.91	107.44	118.38
29	B3	402	CDL	OB6-CB5-C51	4.91	122.10	111.48
36	e3	900	NAD	N6A-C6A-N1A	-4.88	107.50	118.38
36	E3	900	NAD	C5A-C4A-N3A	-4.87	120.00	126.72
29	B	402	CDL	OB6-CB5-C51	4.86	122.00	111.48
36	e	900	NAD	N6A-C6A-N1A	-4.86	107.56	118.38
36	E	900	NAD	C5A-C4A-N3A	-4.85	120.03	126.72
33	A1	601	ATP	C5-C4-N3	-4.80	120.10	126.72
33	B2	1003	ATP	C5-C4-N3	-4.80	120.11	126.72
33	A5	601	ATP	C5-C4-N3	-4.78	120.14	126.72
33	C4	601	ATP	C5-C4-N3	-4.77	120.15	126.72
33	A4	601	ATP	C5-C4-N3	-4.77	120.15	126.72
33	A2	601	ATP	C5-C4-N3	-4.76	120.16	126.72
33	B5	1003	ATP	C5-C4-N3	-4.75	120.17	126.72
33	C1	601	ATP	C5-C4-N3	-4.75	120.18	126.72
36	e	900	NAD	C5A-C4A-N3A	-4.75	120.18	126.72
33	C5	601	ATP	C5-C4-N3	-4.74	120.19	126.72
33	B1	1003	ATP	C5-C4-N3	-4.73	120.20	126.72
33	B4	1003	ATP	C5-C4-N3	-4.71	120.24	126.72
33	C2	601	ATP	C5-C4-N3	-4.70	120.25	126.72
36	e3	900	NAD	C5A-C4A-N3A	-4.69	120.26	126.72
33	g	301	ATP	N9-C8-N7	-4.67	107.31	113.94
33	G3	301	ATP	N9-C8-N7	-4.66	107.33	113.94
33	G	301	ATP	N9-C8-N7	-4.65	107.33	113.94
33	G	301	ATP	N6-C6-N1	-4.65	108.02	118.38
33	g3	301	ATP	C5-C4-N3	-4.65	120.32	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	A2	601	ATP	N9-C8-N7	-4.64	107.36	113.94
33	A5	601	ATP	N9-C8-N7	-4.64	107.36	113.94
33	A1	601	ATP	N9-C8-N7	-4.64	107.36	113.94
33	g3	301	ATP	N9-C8-N7	-4.63	107.36	113.94
33	B5	1003	ATP	N9-C8-N7	-4.63	107.36	113.94
33	C5	601	ATP	N9-C8-N7	-4.63	107.36	113.94
33	G	301	ATP	C5-C4-N3	-4.62	120.35	126.72
33	A1	601	ATP	N6-C6-N1	-4.62	108.10	118.38
33	A4	601	ATP	N9-C8-N7	-4.61	107.39	113.94
37	D1	501	ADP	N6-C6-N1	-4.61	108.11	118.38
33	B2	1003	ATP	N9-C8-N7	-4.61	107.40	113.94
33	g3	301	ATP	N6-C6-N1	-4.61	108.12	118.38
33	B1	1003	ATP	N6-C6-N1	-4.60	108.13	118.38
33	B4	1003	ATP	N9-C8-N7	-4.60	107.41	113.94
33	C4	601	ATP	N9-C8-N7	-4.60	107.41	113.94
33	B4	1003	ATP	N6-C6-N1	-4.59	108.15	118.38
33	C1	601	ATP	N9-C8-N7	-4.59	107.42	113.94
37	D4	501	ADP	N6-C6-N1	-4.59	108.16	118.38
33	C2	601	ATP	N9-C8-N7	-4.59	107.43	113.94
37	B2	1002	ADP	N6-C6-N1	-4.58	108.18	118.38
33	B2	1003	ATP	N6-C6-N1	-4.57	108.19	118.38
33	A4	601	ATP	N6-C6-N1	-4.57	108.20	118.38
33	A5	601	ATP	N6-C6-N1	-4.57	108.20	118.38
33	C5	601	ATP	N6-C6-N1	-4.57	108.20	118.38
33	A2	601	ATP	N6-C6-N1	-4.57	108.20	118.38
33	G3	301	ATP	N6-C6-N1	-4.57	108.20	118.38
37	B5	1002	ADP	N6-C6-N1	-4.57	108.20	118.38
37	B4	1002	ADP	N6-C6-N1	-4.57	108.21	118.38
33	B1	1003	ATP	N9-C8-N7	-4.56	107.46	113.94
37	B1	1002	ADP	N6-C6-N1	-4.56	108.21	118.38
33	g	301	ATP	N6-C6-N1	-4.56	108.22	118.38
33	B5	1003	ATP	N6-C6-N1	-4.56	108.23	118.38
37	D2	501	ADP	N6-C6-N1	-4.55	108.23	118.38
29	F3	302	CDL	OB6-CB5-C51	4.55	121.32	111.48
30	d3	301	PC1	O21-C21-C22	4.55	121.32	111.48
33	G3	301	ATP	C5-C4-N3	-4.55	120.46	126.72
33	C4	601	ATP	N6-C6-N1	-4.54	108.26	118.38
33	C2	601	ATP	N6-C6-N1	-4.54	108.26	118.38
37	D5	501	ADP	N6-C6-N1	-4.54	108.27	118.38
33	C1	601	ATP	N6-C6-N1	-4.52	108.30	118.38
30	d	301	PC1	O21-C21-C22	4.51	121.24	111.48
29	f3	304	CDL	OA6-CA5-C11	4.50	121.21	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	g	301	ATP	C5-C4-N3	-4.50	120.52	126.72
32	I3	304	UQ8	C25-C24-C26	4.43	122.92	115.23
29	B3	401	CDL	OA6-CA5-C11	4.41	121.02	111.48
29	B	401	CDL	OA6-CA5-C11	4.39	120.97	111.48
29	F	303	CDL	OB6-CB5-C51	4.37	120.93	111.48
29	f	304	CDL	OA6-CA5-C11	4.33	120.86	111.48
32	I	303	UQ8	C25-C24-C26	4.33	122.75	115.23
29	K3	201	CDL	OA6-CA5-C11	4.31	120.80	111.48
29	A	502	CDL	OB6-CB5-C51	4.30	120.78	111.48
29	k	201	CDL	OA6-CA5-C11	4.29	120.77	111.48
33	g	301	ATP	C4-N9-C1'	4.29	136.67	126.63
33	G3	301	ATP	C4-N9-C1'	4.28	136.64	126.63
33	A2	601	ATP	C4-N9-C1'	4.27	136.62	126.63
35	A	501	PEE	O2-C10-C11	4.26	120.70	111.48
33	g3	301	ATP	C4-N9-C1'	4.26	136.59	126.63
33	A4	601	ATP	C4-N9-C1'	4.26	136.59	126.63
33	A5	601	ATP	C4-N9-C1'	4.24	136.56	126.63
33	C2	601	ATP	C4-N9-C1'	4.24	136.55	126.63
36	e	900	NAD	C4D-O4D-C1D	-4.23	106.05	109.92
33	A1	601	ATP	C4-N9-C1'	4.23	136.51	126.63
29	a	501	CDL	OB6-CB5-C51	4.22	120.62	111.48
33	C4	601	ATP	C4-N9-C1'	4.22	136.49	126.63
33	G	301	ATP	C4-N9-C1'	4.21	136.47	126.63
33	C5	601	ATP	C4-N9-C1'	4.21	136.47	126.63
37	D4	501	ADP	N9-C8-N7	-4.20	107.97	113.94
33	B2	1003	ATP	C4-N9-C1'	4.20	136.46	126.63
30	G3	304	PC1	O21-C21-C22	4.20	120.57	111.48
33	C1	601	ATP	C4-N9-C1'	4.20	136.46	126.63
33	B5	1003	ATP	C4-N9-C1'	4.20	136.44	126.63
37	D1	501	ADP	N9-C8-N7	-4.19	107.98	113.94
33	B4	1003	ATP	C4-N9-C1'	4.19	136.43	126.63
29	K3	202	CDL	OA6-CA5-C11	4.18	120.53	111.48
36	E3	900	NAD	C4D-O4D-C1D	-4.18	106.10	109.92
29	k3	201	CDL	OA6-CA5-C11	4.18	120.52	111.48
35	a3	503	PEE	O2-C10-C11	4.17	120.51	111.48
35	l3	302	PEE	O2-C10-C11	4.17	120.50	111.48
33	B1	1003	ATP	C4-N9-C1'	4.16	136.36	126.63
29	f	303	CDL	OA6-CA5-C11	4.14	120.44	111.48
29	K	201	CDL	OA6-CA5-C11	4.13	120.42	111.48
29	a3	501	CDL	OB6-CB5-C51	4.11	120.37	111.48
29	F	303	CDL	OA6-CA5-C11	4.10	120.36	111.48
30	D3	301	PC1	O21-C21-C22	4.10	120.36	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	p3	201	CDL	OB6-CB5-C51	4.10	120.35	111.48
29	I	302	CDL	OA6-CA5-C11	4.10	120.34	111.48
29	P	201	CDL	OA6-CA5-C11	4.09	120.32	111.48
29	B3	404	CDL	OB6-CB5-C51	4.07	120.29	111.48
29	A3	501	CDL	OB6-CB5-C51	4.07	120.29	111.48
29	J	301	CDL	OB6-CB5-C51	4.07	120.29	111.48
29	P3	201	CDL	OA6-CA5-C11	4.07	120.29	111.48
29	j	301	CDL	OB6-CB5-C51	4.06	120.27	111.48
37	D2	501	ADP	N9-C8-N7	-4.06	108.17	113.94
30	G	304	PC1	O21-C21-C22	4.06	120.27	111.48
29	f3	303	CDL	OA6-CA5-C11	4.06	120.26	111.48
29	i	301	CDL	OA6-CA5-C11	4.05	120.25	111.48
35	L	303	PEE	O2-C10-C11	4.05	120.24	111.48
37	B2	1002	ADP	N9-C8-N7	-4.03	108.22	113.94
29	I3	303	CDL	OA6-CA5-C11	4.03	120.20	111.48
37	D5	501	ADP	N9-C8-N7	-4.03	108.22	113.94
37	B4	1002	ADP	N9-C8-N7	-4.02	108.23	113.94
37	B5	1002	ADP	N9-C8-N7	-4.02	108.24	113.94
30	D	301	PC1	O21-C21-C22	4.01	120.17	111.48
37	B1	1002	ADP	N9-C8-N7	-4.01	108.24	113.94
29	p	201	CDL	OB6-CB5-C51	4.01	120.16	111.48
29	F3	302	CDL	OA6-CA5-C11	4.01	120.16	111.48
29	f	302	CDL	OA6-CA5-C11	4.00	120.14	111.48
29	L	302	CDL	OB6-CB5-C51	4.00	120.13	111.48
29	B	404	CDL	OA6-CA5-C11	4.00	120.13	111.48
29	b	401	CDL	OB6-CB5-C51	3.98	120.09	111.48
29	b3	401	CDL	OA6-CA5-C11	3.98	120.09	111.48
29	f	304	CDL	OB6-CB5-C51	3.98	120.08	111.48
29	j3	301	CDL	OA6-CA5-C11	3.97	120.07	111.48
30	G	303	PC1	O21-C21-C22	3.97	120.07	111.48
29	K	202	CDL	OA6-CA5-C11	3.97	120.07	111.48
29	f3	302	CDL	OB6-CB5-C51	3.97	120.06	111.48
29	b3	401	CDL	OB6-CB5-C51	3.97	120.06	111.48
29	j3	301	CDL	OB6-CB5-C51	3.96	120.05	111.48
29	J3	301	CDL	OA6-CA5-C11	3.96	120.04	111.48
29	f3	304	CDL	OB6-CB5-C51	3.96	120.04	111.48
29	g3	305	CDL	OB6-CB5-C51	3.96	120.04	111.48
36	e3	900	NAD	C4A-N9A-C8A	3.96	109.89	105.74
30	g3	303	PC1	O21-C21-C22	3.96	120.04	111.48
29	P3	201	CDL	OB6-CB5-C51	3.95	120.03	111.48
29	g3	305	CDL	OA6-CA5-C11	3.93	119.98	111.48
29	b	401	CDL	OA6-CA5-C11	3.92	119.97	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	f	302	CDL	OB6-CB5-C51	3.92	119.97	111.48
30	g	303	PC1	O21-C21-C22	3.92	119.97	111.48
29	j	301	CDL	OA6-CA5-C11	3.92	119.97	111.48
36	e	900	NAD	C4A-N9A-C8A	3.92	109.85	105.74
29	I3	303	CDL	OB6-CB5-C51	3.91	119.95	111.48
29	B	404	CDL	OB6-CB5-C51	3.91	119.93	111.48
30	G3	303	PC1	O21-C21-C22	3.91	119.93	111.48
29	f3	302	CDL	OA6-CA5-C11	3.91	119.93	111.48
29	I	302	CDL	OB6-CB5-C51	3.90	119.93	111.48
29	f3	303	CDL	OB6-CB5-C51	3.90	119.93	111.48
36	E	900	NAD	C4A-N9A-C8A	3.89	109.83	105.74
29	F	302	CDL	OA6-CA5-C11	3.89	119.90	111.48
29	J	301	CDL	OA6-CA5-C11	3.87	119.85	111.48
36	E3	900	NAD	C4A-N9A-C8A	3.87	109.80	105.74
32	I3	304	UQ8	C40-C39-C41	3.87	121.94	115.23
29	i3	302	CDL	OB6-CB5-C51	3.86	119.83	111.48
29	I3	302	CDL	OB6-CB5-C51	3.85	119.81	111.48
29	a	501	CDL	OA6-CA5-C11	3.84	119.80	111.48
29	a3	502	CDL	OA6-CA5-C11	3.84	119.79	111.48
35	L3	302	PEE	O2-C10-C11	3.84	119.79	111.48
29	B	403	CDL	OB6-CB5-C51	3.84	119.79	111.48
29	g	305	CDL	OA6-CA5-C11	3.84	119.78	111.48
29	I3	301	CDL	OB6-CB5-C51	3.83	119.78	111.48
29	B3	402	CDL	OA6-CA5-C11	3.81	119.73	111.48
29	a3	501	CDL	OA6-CA5-C11	3.81	119.73	111.48
29	l	301	CDL	OB6-CB5-C51	3.81	119.72	111.48
29	i	301	CDL	OB6-CB5-C51	3.80	119.71	111.48
29	i3	302	CDL	OA6-CA5-C11	3.80	119.69	111.48
29	L	301	CDL	OB6-CB5-C51	3.79	119.69	111.48
29	L	302	CDL	OA6-CA5-C11	3.79	119.68	111.48
29	p3	201	CDL	OA6-CA5-C11	3.79	119.68	111.48
29	f	303	CDL	OB6-CB5-C51	3.79	119.67	111.48
29	P	201	CDL	OB6-CB5-C51	3.79	119.67	111.48
29	g	305	CDL	OB6-CB5-C51	3.78	119.67	111.48
29	J3	302	CDL	OA6-CA5-C11	3.78	119.66	111.48
29	B3	404	CDL	OA6-CA5-C11	3.77	119.64	111.48
29	L	301	CDL	OA6-CA5-C11	3.77	119.64	111.48
29	J3	301	CDL	OB6-CB5-C51	3.76	119.62	111.48
29	p	201	CDL	OA6-CA5-C11	3.76	119.61	111.48
32	I	303	UQ8	C40-C39-C41	3.75	121.74	115.23
29	K3	201	CDL	OB6-CB5-C51	3.75	119.59	111.48
36	e3	900	NAD	C5A-C6A-N6A	3.74	132.54	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	l	301	CDL	OA6-CA5-C11	3.73	119.55	111.48
36	E	900	NAD	C5A-C6A-N6A	3.72	132.50	123.29
29	K	201	CDL	OB6-CB5-C51	3.72	119.53	111.48
29	k3	201	CDL	OB6-CB5-C51	3.72	119.53	111.48
29	B3	403	CDL	OA6-CA5-C11	3.72	119.53	111.48
29	l3	301	CDL	OA6-CA5-C11	3.71	119.52	111.48
29	B3	403	CDL	OB6-CB5-C51	3.71	119.51	111.48
29	I	301	CDL	OA6-CA5-C11	3.71	119.50	111.48
29	B	402	CDL	OA6-CA5-C11	3.70	119.49	111.48
29	J3	302	CDL	OB6-CB5-C51	3.70	119.48	111.48
36	E3	900	NAD	N3A-C4A-N9A	3.69	133.45	127.17
36	E3	900	NAD	C5A-C6A-N6A	3.69	132.42	123.29
29	I3	301	CDL	OA6-CA5-C11	3.67	119.42	111.48
29	J	302	CDL	OA6-CA5-C11	3.66	119.40	111.48
36	E	900	NAD	N3A-C4A-N9A	3.66	133.39	127.17
29	j	302	CDL	OA6-CA5-C11	3.66	119.39	111.48
29	j	302	CDL	OB6-CB5-C51	3.65	119.39	111.48
29	B	403	CDL	OA6-CA5-C11	3.65	119.38	111.48
36	E	900	NAD	C4D-O4D-C1D	-3.65	106.58	109.92
36	e3	900	NAD	C4D-O4D-C1D	-3.65	106.58	109.92
35	J	303	PEE	O2-C10-C11	3.64	119.37	111.48
36	e	900	NAD	C5A-C6A-N6A	3.63	132.28	123.29
29	A	502	CDL	OA6-CA5-C11	3.63	119.34	111.48
29	J	302	CDL	OB6-CB5-C51	3.62	119.31	111.48
29	i3	301	CDL	OA6-CA5-C11	3.61	119.29	111.48
29	a3	502	CDL	OB6-CB5-C51	3.59	119.25	111.48
29	L3	301	CDL	OA6-CA5-C11	3.58	119.22	111.48
29	K	202	CDL	OB6-CB5-C51	3.58	119.22	111.48
36	e	900	NAD	N3A-C4A-N9A	3.57	133.24	127.17
29	I3	302	CDL	OA6-CA5-C11	3.57	119.20	111.48
29	L3	301	CDL	OB6-CB5-C51	3.56	119.18	111.48
29	j3	302	CDL	OB6-CB5-C51	3.56	119.17	111.48
29	l3	301	CDL	OB6-CB5-C51	3.55	119.17	111.48
29	k	201	CDL	OB6-CB5-C51	3.54	119.14	111.48
29	I	301	CDL	OB6-CB5-C51	3.54	119.14	111.48
29	A3	501	CDL	OA6-CA5-C11	3.53	119.13	111.48
36	e3	900	NAD	N3A-C4A-N9A	3.53	133.17	127.17
29	r	201	CDL	OA6-CA5-C11	3.51	119.08	111.48
33	A1	601	ATP	C5-C6-N6	3.50	131.96	123.29
29	B3	401	CDL	OB6-CB5-C51	3.50	119.05	111.48
33	G	301	ATP	C5-C6-N6	3.50	131.94	123.29
29	r	201	CDL	OB6-CB5-C51	3.49	119.04	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D1	501	ADP	C5-C6-N6	3.49	131.92	123.29
33	B1	1003	ATP	C5-C6-N6	3.49	131.92	123.29
30	g	304	PC1	O21-C21-C22	3.49	119.02	111.48
29	j3	302	CDL	OA6-CA5-C11	3.48	119.01	111.48
33	g3	301	ATP	C5-C6-N6	3.48	131.90	123.29
33	B2	1003	ATP	C5-C6-N6	3.46	131.86	123.29
33	B4	1003	ATP	C5-C6-N6	3.46	131.86	123.29
33	A5	601	ATP	C5-C6-N6	3.46	131.86	123.29
33	C5	601	ATP	C5-C6-N6	3.45	131.84	123.29
33	A4	601	ATP	C5-C6-N6	3.45	131.82	123.29
33	A2	601	ATP	C5-C6-N6	3.44	131.81	123.29
33	G3	301	ATP	C5-C6-N6	3.44	131.80	123.29
37	B5	1002	ADP	C5-C6-N6	3.44	131.80	123.29
33	B5	1003	ATP	C5-C6-N6	3.44	131.80	123.29
37	B1	1002	ADP	C5-C6-N6	3.44	131.80	123.29
33	C4	601	ATP	C5-C6-N6	3.44	131.79	123.29
29	K3	202	CDL	OB6-CB5-C51	3.43	118.91	111.48
32	i3	303	UQ8	C17-C18-C19	-3.43	119.77	127.62
37	B4	1002	ADP	C5-C6-N6	3.43	131.78	123.29
33	C2	601	ATP	C5-C6-N6	3.43	131.77	123.29
37	B2	1002	ADP	C5-C6-N6	3.42	131.76	123.29
37	D4	501	ADP	C5-C6-N6	3.42	131.76	123.29
37	D5	501	ADP	C2-N3-C4	3.42	120.19	111.83
37	B5	1002	ADP	C2-N3-C4	3.42	120.19	111.83
33	g	301	ATP	C5-C6-N6	3.42	131.75	123.29
33	C1	601	ATP	C5-C6-N6	3.41	131.74	123.29
32	i	302	UQ8	C30-C29-C31	3.41	121.15	115.23
32	i3	303	UQ8	C25-C24-C26	3.41	121.15	115.23
37	D2	501	ADP	C2-N3-C4	3.41	120.15	111.83
37	B2	1002	ADP	C2-N3-C4	3.41	120.15	111.83
37	B4	1002	ADP	C2-N3-C4	3.41	120.15	111.83
32	I	303	UQ8	C17-C18-C19	-3.41	119.83	127.62
35	m	301	PEE	O2-C10-C11	3.40	118.84	111.48
37	D2	501	ADP	C5-C6-N6	3.40	131.70	123.29
37	D5	501	ADP	C5-C6-N6	3.40	131.69	123.29
37	D1	501	ADP	C2-N3-C4	3.39	120.10	111.83
37	B1	1002	ADP	C2-N3-C4	3.38	120.09	111.83
30	g3	304	PC1	O21-C21-C22	3.37	118.76	111.48
37	D4	501	ADP	C2-N3-C4	3.36	120.04	111.83
32	I3	304	UQ8	C17-C18-C19	-3.36	119.94	127.62
32	i	302	UQ8	C17-C18-C19	-3.35	119.97	127.62
33	A5	601	ATP	C2-N3-C4	3.34	120.00	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	B1	1003	ATP	C2-N3-C4	3.34	119.99	111.83
33	A1	601	ATP	C2-N3-C4	3.34	119.99	111.83
33	C4	601	ATP	C2-N3-C4	3.34	119.99	111.83
33	B5	1003	ATP	C2-N3-C4	3.34	119.99	111.83
33	C1	601	ATP	C2-N3-C4	3.34	119.98	111.83
29	B	401	CDL	OB6-CB5-C51	3.33	118.69	111.48
33	B2	1003	ATP	C2-N3-C4	3.33	119.97	111.83
33	A4	601	ATP	C2-N3-C4	3.33	119.97	111.83
35	j3	303	PEE	O2-C10-C11	3.33	118.69	111.48
33	C5	601	ATP	C2-N3-C4	3.33	119.95	111.83
33	B4	1003	ATP	C2-N3-C4	3.32	119.93	111.83
33	C2	601	ATP	C2-N3-C4	3.32	119.93	111.83
33	A2	601	ATP	C2-N3-C4	3.31	119.93	111.83
29	F	302	CDL	OB6-CB5-C51	3.31	118.65	111.48
29	i3	301	CDL	OB6-CB5-C51	3.30	118.63	111.48
36	E3	900	NAD	C2A-N3A-C4A	3.29	119.86	111.83
33	g	301	ATP	C4-N9-C8	3.29	109.19	105.74
33	g3	301	ATP	C2-N3-C4	3.29	119.86	111.83
33	G	301	ATP	C2-N3-C4	3.28	119.85	111.83
33	G3	301	ATP	C4-N9-C8	3.28	109.19	105.74
32	i3	303	UQ8	C30-C29-C31	3.28	120.92	115.23
32	i	302	UQ8	C25-C24-C26	3.28	120.92	115.23
29	l3	303	CDL	OA6-CA5-C11	3.28	118.57	111.48
36	E	900	NAD	C2A-N3A-C4A	3.27	119.82	111.83
29	l	302	CDL	OA6-CA5-C11	3.26	118.54	111.48
33	G3	301	ATP	C2-N3-C4	3.26	119.80	111.83
33	g	301	ATP	C2-N3-C4	3.26	119.79	111.83
36	e	900	NAD	C2A-N3A-C4A	3.25	119.77	111.83
36	e3	900	NAD	C2A-N3A-C4A	3.21	119.67	111.83
32	I	303	UQ8	C20-C19-C21	3.20	120.78	115.23
29	i3	302	CDL	OB8-CB7-C71	3.19	121.57	111.83
33	G	301	ATP	C4-N9-C8	3.18	109.07	105.74
32	i3	303	UQ8	C22-C23-C24	-3.18	120.36	127.62
32	I	303	UQ8	C12-C13-C14	-3.17	120.36	127.62
33	g3	301	ATP	C4-N9-C8	3.15	109.05	105.74
29	b3	401	CDL	OA8-CA7-C31	3.14	121.41	111.83
29	i	301	CDL	OB8-CB7-C71	3.13	121.38	111.83
32	i3	303	UQ8	C20-C19-C21	3.12	120.64	115.23
33	C1	601	ATP	N3-C4-N9	3.11	132.46	127.17
33	C4	601	ATP	N3-C4-N9	3.11	132.46	127.17
33	A5	601	ATP	N3-C4-N9	3.11	132.46	127.17
33	B2	1003	ATP	N3-C4-N9	3.11	132.45	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	A2	601	ATP	N3-C4-N9	3.11	132.45	127.17
36	E	900	NAD	C5A-N7A-C8A	3.10	108.33	103.45
33	A4	601	ATP	N3-C4-N9	3.10	132.44	127.17
33	C5	601	ATP	N3-C4-N9	3.10	132.44	127.17
36	e3	900	NAD	C5A-N7A-C8A	3.10	108.32	103.45
33	B5	1003	ATP	N3-C4-N9	3.09	132.42	127.17
36	e	900	NAD	C5A-N7A-C8A	3.09	108.31	103.45
33	C2	601	ATP	N3-C4-N9	3.08	132.41	127.17
29	b	401	CDL	OA8-CA7-C31	3.08	121.23	111.83
33	G	301	ATP	C3'-C2'-C1'	3.08	107.29	101.46
32	I3	304	UQ8	C7-C8-C9	-3.08	121.53	126.83
33	C5	601	ATP	C4-N9-C8	3.08	108.97	105.74
33	A5	601	ATP	C4-N9-C8	3.07	108.97	105.74
36	E3	900	NAD	C5A-N7A-C8A	3.07	108.28	103.45
33	A1	601	ATP	N3-C4-N9	3.07	132.39	127.17
32	i	302	UQ8	C22-C23-C24	-3.07	120.60	127.62
33	B5	1003	ATP	C4-N9-C8	3.06	108.95	105.74
33	A2	601	ATP	C4-N9-C8	3.06	108.95	105.74
35	L3	302	PEE	O3-C30-C31	3.06	121.15	111.83
33	B1	1003	ATP	N3-C4-N9	3.06	132.37	127.17
37	D4	501	ADP	C2'-C3'-C4'	3.05	108.50	102.61
33	G3	301	ATP	C3'-C2'-C1'	3.04	107.22	101.46
33	B4	1003	ATP	N3-C4-N9	3.04	132.34	127.17
33	A4	601	ATP	C4-N9-C8	3.04	108.93	105.74
33	C2	601	ATP	C4-N9-C8	3.04	108.93	105.74
33	C1	601	ATP	C4-N9-C8	3.04	108.92	105.74
33	B2	1003	ATP	C4-N9-C8	3.03	108.92	105.74
33	A1	601	ATP	C4-N9-C8	3.03	108.92	105.74
33	A5	601	ATP	C5-N7-C8	3.02	108.20	103.45
33	C4	601	ATP	C4-N9-C8	3.02	108.91	105.74
33	G3	301	ATP	N3-C4-N9	3.02	132.31	127.17
33	G	301	ATP	N3-C4-N9	3.02	132.30	127.17
33	g3	301	ATP	N3-C4-N9	3.02	132.30	127.17
33	B5	1003	ATP	C5-N7-C8	3.01	108.18	103.45
37	D2	501	ADP	C5-N7-C8	3.01	108.18	103.45
33	B4	1003	ATP	C4-N9-C8	3.01	108.90	105.74
33	A1	601	ATP	C5-N7-C8	3.00	108.17	103.45
33	A2	601	ATP	C5-N7-C8	3.00	108.17	103.45
35	J	303	PEE	O3-C30-C31	3.00	120.99	111.83
33	A4	601	ATP	C5-N7-C8	3.00	108.17	103.45
37	B2	1002	ADP	C5-N7-C8	2.99	108.16	103.45
33	B2	1003	ATP	C5-N7-C8	2.99	108.15	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	B4	1003	ATP	C5-N7-C8	2.99	108.15	103.45
33	C5	601	ATP	C5-N7-C8	2.99	108.15	103.45
37	D5	501	ADP	C5-N7-C8	2.99	108.14	103.45
32	I	303	UQ8	C22-C23-C24	-2.98	120.79	127.62
33	g	301	ATP	N3-C4-N9	2.98	132.24	127.17
29	i3	301	CDL	OA8-CA7-C31	2.98	120.91	111.83
33	C4	601	ATP	C5-N7-C8	2.98	108.13	103.45
37	D1	501	ADP	C5-N7-C8	2.98	108.13	103.45
33	B1	1003	ATP	C4-N9-C8	2.97	108.86	105.74
29	B3	402	CDL	OA8-CA7-C31	2.97	120.90	111.83
37	B1	1002	ADP	C5-N7-C8	2.97	108.11	103.45
33	C2	601	ATP	C5-N7-C8	2.97	108.11	103.45
37	D4	501	ADP	C5-N7-C8	2.97	108.11	103.45
32	i	302	UQ8	C20-C19-C21	2.96	120.37	115.23
32	I3	304	UQ8	C12-C13-C14	-2.96	120.86	127.62
29	r	201	CDL	OB8-CB7-C71	2.96	120.85	111.83
37	B4	1002	ADP	C5-N7-C8	2.95	108.09	103.45
29	K3	201	CDL	OB8-CB7-C71	2.95	120.83	111.83
33	G	301	ATP	C5-N7-C8	2.95	108.08	103.45
33	B1	1003	ATP	C5-N7-C8	2.95	108.08	103.45
33	C1	601	ATP	C5-N7-C8	2.94	108.08	103.45
29	l3	301	CDL	OB8-CB7-C71	2.94	120.79	111.83
32	I	303	UQ8	C7-C8-C9	-2.94	121.77	126.83
37	B5	1002	ADP	C5-N7-C8	2.93	108.06	103.45
29	B3	404	CDL	OB8-CB7-C71	2.92	120.75	111.83
32	I3	304	UQ8	C20-C19-C21	2.92	120.30	115.23
33	g3	301	ATP	C5-N7-C8	2.92	108.04	103.45
32	i	302	UQ8	C32-C33-C34	-2.91	120.96	127.62
29	I	302	CDL	OA8-CA7-C31	2.91	120.71	111.83
37	D1	501	ADP	N3-C4-N9	2.89	132.09	127.17
29	l	301	CDL	OA8-CA7-C31	2.89	120.65	111.83
37	D4	501	ADP	N3-C4-N9	2.89	132.09	127.17
29	F	303	CDL	OB8-CB7-C71	2.89	120.65	111.83
35	m	301	PEE	O3-C30-C31	2.89	120.65	111.83
29	K	202	CDL	OA8-CA7-C31	2.89	120.64	111.83
32	i3	303	UQ8	C32-C33-C34	-2.89	121.02	127.62
37	D4	501	ADP	C3'-C2'-C1'	2.88	106.92	101.46
33	g3	301	ATP	C3'-C2'-C1'	2.88	106.91	101.46
33	G3	301	ATP	C5-N7-C8	2.87	107.97	103.45
29	f	303	CDL	OB8-CB7-C71	2.87	120.59	111.83
29	B	402	CDL	OA8-CA7-C31	2.87	120.59	111.83
33	g	301	ATP	C5-N7-C8	2.87	107.96	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	301	PC1	O31-C31-C32	2.87	120.58	111.83
37	D1	501	ADP	C2'-C3'-C4'	2.87	108.15	102.61
29	K	201	CDL	OB8-CB7-C71	2.86	120.55	111.83
33	g	301	ATP	C3'-C2'-C1'	2.85	106.85	101.46
37	D1	501	ADP	C3'-C2'-C1'	2.84	106.84	101.46
29	A	502	CDL	OA8-CA7-C31	2.84	120.50	111.83
32	i	302	UQ8	C7-C8-C9	-2.84	121.94	126.83
30	D3	301	PC1	O31-C31-C32	2.84	120.49	111.83
29	i3	301	CDL	OB8-CB7-C71	2.83	120.48	111.83
32	I	303	UQ8	C1M-C1-C6	-2.83	119.79	124.45
29	B3	404	CDL	OA8-CA7-C31	2.83	120.47	111.83
29	p3	201	CDL	OB8-CB7-C71	2.83	120.46	111.83
32	i3	303	UQ8	C40-C39-C38	-2.83	116.37	123.63
32	i	302	UQ8	C40-C39-C41	2.83	120.13	115.23
29	B3	403	CDL	OB8-CB7-C71	2.82	120.45	111.83
29	p	201	CDL	OB8-CB7-C71	2.82	120.44	111.83
32	I3	304	UQ8	C22-C23-C24	-2.82	121.17	127.62
29	l3	301	CDL	OA8-CA7-C31	2.82	120.43	111.83
29	F3	302	CDL	OA8-CA7-C31	2.81	120.41	111.83
30	g3	304	PC1	O31-C31-C32	2.81	120.40	111.83
29	k	201	CDL	OB8-CB7-C71	2.81	120.39	111.83
29	r	201	CDL	OA8-CA7-C31	2.81	120.39	111.83
29	f3	303	CDL	OB8-CB7-C71	2.79	120.35	111.83
29	B	404	CDL	OA8-CA7-C31	2.79	120.35	111.83
29	J	301	CDL	OB8-CB7-C71	2.79	120.34	111.83
29	B	404	CDL	OB8-CB7-C71	2.79	120.33	111.83
29	J	301	CDL	OA8-CA7-C31	2.78	120.32	111.83
29	b3	401	CDL	OB8-CB7-C71	2.78	120.30	111.83
29	k3	201	CDL	OA8-CA7-C31	2.77	120.30	111.83
29	j3	302	CDL	OB8-CB7-C71	2.77	120.29	111.83
32	i3	303	UQ8	C40-C39-C41	2.77	120.04	115.23
29	A3	501	CDL	OA8-CA7-C31	2.77	120.28	111.83
29	i3	302	CDL	OA8-CA7-C31	2.77	120.28	111.83
30	G	303	PC1	O31-C31-C32	2.76	120.26	111.83
29	g3	305	CDL	OA8-CA7-C31	2.76	120.24	111.83
29	b	401	CDL	OB8-CB7-C71	2.75	120.23	111.83
32	i	302	UQ8	C40-C39-C38	-2.75	116.56	123.63
35	j3	303	PEE	O3-C30-C31	2.75	120.22	111.83
35	l3	302	PEE	O3-C30-C31	2.75	120.22	111.83
29	J3	301	CDL	OA8-CA7-C31	2.75	120.22	111.83
29	g	305	CDL	OA8-CA7-C31	2.75	120.21	111.83
29	K	201	CDL	OA8-CA7-C31	2.74	120.19	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	l	301	CDL	OB8-CB7-C71	2.74	120.18	111.83
29	L	301	CDL	OB8-CB7-C71	2.74	120.18	111.83
29	B	403	CDL	OB8-CB7-C71	2.74	120.18	111.83
29	F	303	CDL	OA8-CA7-C31	2.73	120.17	111.83
29	J	302	CDL	OB8-CB7-C71	2.73	120.17	111.83
37	D2	501	ADP	O4'-C1'-N9	2.73	113.34	108.09
37	B5	1002	ADP	N3-C4-N9	2.73	131.81	127.17
29	j	302	CDL	OB8-CB7-C71	2.73	120.16	111.83
29	I3	303	CDL	OA8-CA7-C31	2.73	120.15	111.83
37	B4	1002	ADP	N3-C4-N9	2.72	131.80	127.17
29	I3	301	CDL	OA8-CA7-C31	2.72	120.14	111.83
30	d	301	PC1	O31-C31-C32	2.72	120.13	111.83
29	a3	501	CDL	OB8-CB7-C71	2.72	120.12	111.83
30	g	304	PC1	O31-C31-C32	2.72	120.12	111.83
29	F3	302	CDL	OB8-CB7-C71	2.71	120.11	111.83
29	g	305	CDL	OB8-CB7-C71	2.71	120.10	111.83
29	j	301	CDL	OA8-CA7-C31	2.71	120.08	111.83
29	B3	402	CDL	OB8-CB7-C71	2.70	120.08	111.83
37	B1	1002	ADP	N3-C4-N9	2.70	131.75	127.17
37	D5	501	ADP	C2'-C3'-C4'	2.70	107.82	102.61
37	D5	501	ADP	N3-C4-N9	2.70	131.75	127.17
29	j3	302	CDL	OA8-CA7-C31	2.69	120.05	111.83
29	j3	301	CDL	OA8-CA7-C31	2.69	120.03	111.83
37	D2	501	ADP	N3-C4-N9	2.68	131.73	127.17
30	d3	301	PC1	O31-C31-C32	2.68	120.01	111.83
37	D2	501	ADP	C2'-C3'-C4'	2.68	107.78	102.61
29	L3	301	CDL	OB8-CB7-C71	2.68	120.00	111.83
37	B2	1002	ADP	N3-C4-N9	2.68	131.72	127.17
29	L3	301	CDL	OA8-CA7-C31	2.67	119.98	111.83
37	D5	501	ADP	O4'-C1'-N9	2.67	113.21	108.09
29	f3	303	CDL	OA8-CA7-C31	2.66	119.96	111.83
29	I3	301	CDL	OB8-CB7-C71	2.66	119.95	111.83
29	J	302	CDL	OA8-CA7-C31	2.66	119.94	111.83
29	J3	302	CDL	OB8-CB7-C71	2.66	119.93	111.83
30	G	304	PC1	O31-C31-C32	2.65	119.93	111.83
29	a	501	CDL	OB8-CB7-C71	2.65	119.92	111.83
29	f3	302	CDL	OA8-CA7-C31	2.65	119.92	111.83
29	I3	303	CDL	OB8-CB7-C71	2.65	119.91	111.83
30	g3	303	PC1	O31-C31-C32	2.65	119.91	111.83
29	L	301	CDL	OA8-CA7-C31	2.64	119.88	111.83
32	i3	303	UQ8	C27-C28-C29	-2.64	121.59	127.62
29	K3	202	CDL	OA8-CA7-C31	2.63	119.86	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	K	202	CDL	OB8-CB7-C71	2.63	119.86	111.83
29	I3	302	CDL	OA8-CA7-C31	2.63	119.85	111.83
32	I	303	UQ8	C37-C38-C39	-2.63	121.61	127.62
29	g3	305	CDL	OB8-CB7-C71	2.63	119.84	111.83
32	I3	304	UQ8	C1M-C1-C6	-2.62	120.14	124.45
29	A	502	CDL	OB8-CB7-C71	2.62	119.83	111.83
29	f	302	CDL	OA8-CA7-C31	2.61	119.81	111.83
29	J3	301	CDL	OB8-CB7-C71	2.61	119.80	111.83
37	B4	1002	ADP	C3'-C2'-C1'	2.61	106.39	101.46
32	I	303	UQ8	C7-C6-C1	-2.60	120.43	124.89
32	I	303	UQ8	C27-C28-C29	-2.60	121.67	127.62
30	G3	304	PC1	O31-C31-C32	2.59	119.74	111.83
29	k3	201	CDL	OB8-CB7-C71	2.59	119.74	111.83
35	A	501	PEE	O3-C30-C31	2.59	119.74	111.83
29	i	301	CDL	OA8-CA7-C31	2.59	119.73	111.83
29	f	303	CDL	OA8-CA7-C31	2.59	119.72	111.83
37	B1	1002	ADP	C3'-C2'-C1'	2.59	106.36	101.46
29	K3	202	CDL	OB8-CB7-C71	2.58	119.70	111.83
32	i3	303	UQ8	C7-C8-C9	-2.58	122.39	126.83
29	l3	303	CDL	OA8-CA7-C31	2.58	119.69	111.83
37	B2	1002	ADP	C3'-C2'-C1'	2.56	106.31	101.46
29	a	501	CDL	OA8-CA7-C31	2.56	119.64	111.83
37	B5	1002	ADP	C3'-C2'-C1'	2.56	106.30	101.46
37	B2	1002	ADP	C4'-O4'-C1'	-2.56	103.82	109.47
32	I3	304	UQ8	C27-C28-C29	-2.56	121.77	127.62
29	I	302	CDL	OB8-CB7-C71	2.56	119.63	111.83
32	i	302	UQ8	C35-C34-C36	2.55	119.66	115.23
29	l	302	CDL	OA8-CA7-C31	2.55	119.60	111.83
29	P3	201	CDL	OB8-CB7-C71	2.54	119.59	111.83
29	P3	201	CDL	OA8-CA7-C31	2.54	119.57	111.83
32	i3	303	UQ8	C1M-C1-C6	-2.53	120.29	124.45
30	g	303	PC1	O31-C31-C32	2.53	119.56	111.83
32	i	302	UQ8	C27-C28-C29	-2.53	121.83	127.62
29	B	402	CDL	OB8-CB7-C71	2.53	119.55	111.83
33	B5	1003	ATP	C3'-C2'-C1'	2.52	106.23	101.46
29	f3	304	CDL	OB8-CB7-C71	2.52	119.52	111.83
29	K3	201	CDL	OA8-CA7-C31	2.51	119.48	111.83
32	i	302	UQ8	C1M-C1-C6	-2.51	120.33	124.45
29	j	301	CDL	OB8-CB7-C71	2.50	119.47	111.83
29	B3	403	CDL	OA8-CA7-C31	2.50	119.47	111.83
29	a3	502	CDL	OB8-CB7-C71	2.50	119.47	111.83
29	p	201	CDL	OA8-CA7-C31	2.50	119.46	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	P	201	CDL	OB8-CB7-C71	2.50	119.46	111.83
29	j3	301	CDL	OB8-CB7-C71	2.50	119.45	111.83
37	D2	501	ADP	C5-C4-N9	2.49	108.53	105.81
29	k	201	CDL	OA8-CA7-C31	2.49	119.44	111.83
37	D5	501	ADP	C5-C4-N9	2.49	108.53	105.81
29	P	201	CDL	OA8-CA7-C31	2.49	119.43	111.83
29	p3	201	CDL	OA8-CA7-C31	2.49	119.42	111.83
29	F	302	CDL	OB8-CB7-C71	2.48	119.41	111.83
29	I	301	CDL	OB8-CB7-C71	2.48	119.41	111.83
29	L	302	CDL	OB8-CB7-C71	2.48	119.41	111.83
29	I	301	CDL	OA8-CA7-C31	2.48	119.40	111.83
29	B3	401	CDL	OA8-CA7-C31	2.48	119.39	111.83
30	G3	303	PC1	O31-C31-C32	2.47	119.38	111.83
32	i3	303	UQ8	C12-C13-C14	-2.47	121.97	127.62
29	f	302	CDL	OB8-CB7-C71	2.47	119.37	111.83
35	L	303	PEE	O3-C30-C31	2.47	119.36	111.83
37	B2	1002	ADP	C5-C4-N9	2.47	108.50	105.81
29	f3	304	CDL	OA8-CA7-C31	2.47	119.36	111.83
37	B5	1002	ADP	C4'-O4'-C1'	-2.46	104.03	109.47
37	B2	1002	ADP	O4'-C1'-N9	2.46	112.82	108.09
29	A3	501	CDL	OB8-CB7-C71	2.46	119.34	111.83
37	B4	1002	ADP	C4'-O4'-C1'	-2.46	104.04	109.47
29	B	401	CDL	OA8-CA7-C31	2.45	119.32	111.83
37	B4	1002	ADP	C5-C4-N9	2.43	108.46	105.81
29	f	304	CDL	OB8-CB7-C71	2.43	119.25	111.83
37	B1	1002	ADP	C4'-O4'-C1'	-2.42	104.12	109.47
32	i3	303	UQ8	C7-C6-C1	-2.42	120.75	124.89
32	I	303	UQ8	C15-C14-C16	2.41	119.42	115.23
29	a3	501	CDL	OA8-CA7-C31	2.41	119.19	111.83
32	i3	303	UQ8	C35-C34-C36	2.41	119.41	115.23
29	B	403	CDL	OA8-CA7-C31	2.41	119.18	111.83
29	I3	302	CDL	OB8-CB7-C71	2.40	119.16	111.83
37	B1	1002	ADP	C5-C4-N9	2.40	108.43	105.81
37	B5	1002	ADP	C5-C4-N9	2.40	108.42	105.81
37	B2	1002	ADP	C4-C5-N7	-2.40	107.84	110.58
37	B4	1002	ADP	O4'-C1'-N9	2.39	112.69	108.09
29	L	302	CDL	OA8-CA7-C31	2.39	119.13	111.83
29	J3	302	CDL	OA8-CA7-C31	2.39	119.11	111.83
29	j	302	CDL	OA8-CA7-C31	2.39	119.11	111.83
29	f	304	CDL	OA8-CA7-C31	2.38	119.11	111.83
37	D2	501	ADP	C4-C5-N7	-2.38	107.86	110.58
33	B1	1003	ATP	C3'-C2'-C1'	2.37	105.95	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D5	501	ADP	C4-C5-N7	-2.37	107.87	110.58
32	i	302	UQ8	C7-C6-C1	-2.37	120.83	124.89
37	B4	1002	ADP	C4-C5-N7	-2.37	107.88	110.58
32	I3	304	UQ8	C37-C38-C39	-2.36	122.22	127.62
32	I3	304	UQ8	C7-C6-C1	-2.35	120.87	124.89
33	B4	1003	ATP	C3'-C2'-C1'	2.35	105.90	101.46
33	B5	1003	ATP	C2'-C3'-C4'	2.34	107.12	102.61
29	f3	302	CDL	OB8-CB7-C71	2.32	118.92	111.83
37	B1	1002	ADP	C4-C5-N7	-2.32	107.92	110.58
29	P	201	CDL	CA4-OA6-CA5	-2.31	112.26	117.80
29	a3	502	CDL	OA8-CA7-C31	2.31	118.89	111.83
37	D1	501	ADP	C4-C5-N7	-2.31	107.94	110.58
37	B5	1002	ADP	C4-C5-N7	-2.30	107.95	110.58
37	B5	1002	ADP	O4'-C1'-N9	2.30	112.50	108.09
37	D4	501	ADP	C4-C5-N7	-2.29	107.96	110.58
33	B2	1003	ATP	C3'-C2'-C1'	2.29	105.79	101.46
33	B2	1003	ATP	C2'-C3'-C4'	2.28	107.01	102.61
37	B1	1002	ADP	O4'-C1'-N9	2.27	112.46	108.09
29	K3	202	CDL	CA4-OA6-CA5	-2.27	112.36	117.80
32	i3	303	UQ8	C46-C44-C45	2.27	119.81	114.59
33	A2	601	ATP	C3'-C2'-C1'	2.27	105.75	101.46
35	J	303	PEE	C40-C39-C38	-2.26	107.86	124.83
33	B1	1003	ATP	C2'-C3'-C4'	2.25	106.97	102.61
35	a3	503	PEE	O3-C30-C31	2.25	118.70	111.83
29	B	402	CDL	CB6-CB4-CB3	-2.23	106.58	111.78
29	a	501	CDL	OB6-CB5-OB7	-2.23	118.50	123.70
32	i	302	UQ8	C46-C44-C45	2.22	119.71	114.59
33	B4	1003	ATP	C2'-C3'-C4'	2.22	106.90	102.61
33	A1	601	ATP	C4-C5-N7	-2.22	108.05	110.58
29	B	401	CDL	OB8-CB7-C71	2.21	118.57	111.83
32	i3	303	UQ8	C42-C43-C44	-2.21	120.28	127.64
29	F	302	CDL	OA8-CA7-C31	2.20	118.56	111.83
33	A5	601	ATP	C4-C5-N7	-2.20	108.07	110.58
35	m	301	PEE	C17-C18-C19	-2.19	108.40	124.83
32	i	302	UQ8	C42-C43-C44	-2.19	120.33	127.64
29	B3	401	CDL	OB8-CB7-C71	2.19	118.52	111.83
32	I	303	UQ8	C42-C43-C44	-2.19	120.33	127.64
33	G	301	ATP	C4'-O4'-C1'	-2.19	104.63	109.47
35	m	301	PEE	C40-C39-C38	-2.19	108.43	124.83
32	i	302	UQ8	C12-C13-C14	-2.19	122.62	127.62
35	j3	303	PEE	C17-C18-C19	-2.18	108.47	124.83
32	I	303	UQ8	C46-C44-C45	2.18	119.60	114.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	B2	1003	ATP	C4-C5-N7	-2.17	108.10	110.58
33	B5	1003	ATP	C4-C5-N7	-2.17	108.10	110.58
33	A4	601	ATP	C4-C5-N7	-2.16	108.11	110.58
32	I3	304	UQ8	C15-C14-C16	2.16	118.98	115.23
33	B4	1003	ATP	C4-C5-N7	-2.15	108.12	110.58
32	I	303	UQ8	C10-C9-C11	2.15	118.96	115.23
35	L3	302	PEE	C17-C18-C19	-2.15	108.72	124.83
33	A2	601	ATP	C4-C5-N7	-2.15	108.12	110.58
32	I3	304	UQ8	C42-C43-C44	-2.15	120.48	127.64
33	A4	601	ATP	C3'-C2'-C1'	2.14	105.52	101.46
33	C4	601	ATP	C3'-C2'-C1'	2.14	105.52	101.46
35	j3	303	PEE	C40-C39-C38	-2.14	108.78	124.83
33	g3	301	ATP	C4'-O4'-C1'	-2.14	104.74	109.47
29	a3	501	CDL	OB6-CB5-OB7	-2.14	118.70	123.70
33	C5	601	ATP	C4-C5-N7	-2.13	108.14	110.58
33	C4	601	ATP	C4-C5-N7	-2.13	108.15	110.58
36	E	900	NAD	C6N-N1N-C2N	-2.13	120.07	121.88
32	I3	304	UQ8	C35-C34-C33	-2.12	118.18	123.63
33	B1	1003	ATP	C4-C5-N7	-2.12	108.16	110.58
33	G	301	ATP	C4-C5-N7	-2.12	108.16	110.58
33	C2	601	ATP	C3'-C2'-C1'	2.12	105.47	101.46
29	B3	402	CDL	OB6-CB5-OB7	-2.12	118.75	123.70
36	e3	900	NAD	C6N-N1N-C2N	-2.12	120.08	121.88
33	g3	301	ATP	C4-C5-N7	-2.11	108.17	110.58
35	L3	302	PEE	C40-C39-C38	-2.11	109.04	124.83
37	D4	501	ADP	C4-N9-C8	2.10	107.95	105.74
35	j3	303	PEE	C37-C38-C39	-2.10	109.08	124.83
32	I3	304	UQ8	C46-C44-C45	2.10	119.42	114.59
35	a3	503	PEE	C17-C18-C19	-2.10	109.11	124.83
37	B4	1002	ADP	C6-C5-C4	2.10	120.04	117.18
35	L	303	PEE	C40-C39-C38	-2.10	109.14	124.83
36	E3	900	NAD	C6N-N1N-C2N	-2.09	120.09	121.88
29	B3	404	CDL	CB6-CB4-CB3	-2.09	106.90	111.78
33	C2	601	ATP	C4-C5-N7	-2.09	108.19	110.58
29	a3	502	CDL	C41-C40-C39	-2.09	103.82	114.37
37	B4	1002	ADP	C2'-C3'-C4'	2.09	106.64	102.61
37	D5	501	ADP	C6-C5-C4	2.08	120.02	117.18
37	B1	1002	ADP	C6-C5-C4	2.08	120.02	117.18
36	e	900	NAD	C6N-N1N-C2N	-2.08	120.11	121.88
29	I3	303	CDL	CB4-OB6-CB5	-2.08	112.82	117.80
33	C1	601	ATP	C4-C5-N7	-2.08	108.21	110.58
37	B5	1002	ADP	C6-C5-C4	2.07	120.01	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D1	501	ADP	C4-N9-C8	2.07	107.92	105.74
35	J	303	PEE	C17-C18-C19	-2.07	109.30	124.83
35	a3	503	PEE	C37-C38-C39	-2.07	109.33	124.83
37	D2	501	ADP	C6-C5-C4	2.07	120.00	117.18
37	B1	1002	ADP	C2'-C3'-C4'	2.07	106.60	102.61
29	F	302	CDL	C41-C40-C39	-2.06	103.94	114.37
35	a3	503	PEE	C40-C39-C38	-2.06	109.41	124.83
29	f	303	CDL	CA6-CA4-CA3	-2.06	106.99	111.78
30	g	304	PC1	C2-O21-C21	-2.06	112.88	117.80
35	m	301	PEE	C37-C38-C39	-2.05	109.44	124.83
29	B	402	CDL	OB6-CB5-OB7	-2.05	118.91	123.70
37	B2	1002	ADP	C6-C5-C4	2.05	119.97	117.18
29	b	401	CDL	CA4-OA6-CA5	-2.04	112.91	117.80
37	D1	501	ADP	C5-C4-N9	2.04	108.03	105.81
32	i	302	UQ8	C15-C14-C16	2.04	118.77	115.23
32	I3	304	UQ8	C30-C29-C31	2.04	118.77	115.23
29	l	302	CDL	CB4-OB6-CB5	-2.03	112.93	117.80
29	B	404	CDL	CA6-CA4-CA3	-2.03	107.05	111.78
35	L	303	PEE	C37-C38-C39	-2.03	109.65	124.83
35	A	501	PEE	C17-C18-C19	-2.02	109.69	124.83
33	g	301	ATP	C4'-O4'-C1'	-2.02	105.00	109.47
35	l3	302	PEE	C40-C39-C38	-2.02	109.69	124.83
29	l3	301	CDL	CA4-OA6-CA5	-2.02	112.96	117.80
37	D4	501	ADP	C5-C4-N9	2.02	108.01	105.81
33	G3	301	ATP	C4-C5-N7	-2.01	108.28	110.58
35	A	501	PEE	C40-C39-C38	-2.01	109.76	124.83
35	L	303	PEE	C20-C19-C18	-2.01	109.77	124.83
37	B2	1002	ADP	C2'-C3'-C4'	2.01	106.49	102.61
35	l3	302	PEE	C37-C38-C39	-2.01	109.79	124.83
32	I	303	UQ8	C35-C34-C33	-2.01	118.47	123.63
29	P3	201	CDL	CA4-OA6-CA5	-2.00	113.00	117.80
37	D1	501	ADP	C6-C5-C4	2.00	119.91	117.18
35	J	303	PEE	C20-C19-C18	-2.00	109.84	124.83

There are no chirality outliers.

All (2956) 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-OB2
29	a	501	CDL	CB3-OB5-PB2-OB4
29	a	501	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
29	a	501	CDL	C51-CB5-OB6-CB4
29	b	401	CDL	CB3-OB5-PB2-OB2
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	CA2-OA2-PA1-OA4
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
29	f	304	CDL	OA5-CA3-CA4-OA6
29	f	304	CDL	C51-CB5-OB6-CB4
29	i	301	CDL	CA3-OA5-PA1-OA2
29	i	301	CDL	CA3-OA5-PA1-OA4
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	CB2-OB2-PB2-OB5
29	k	201	CDL	CB3-OB5-PB2-OB2
29	k	201	CDL	CB3-OB5-PB2-OB3
29	k	201	CDL	CB3-OB5-PB2-OB4
29	g	305	CDL	OA5-CA3-CA4-OA6
29	g	305	CDL	CB2-OB2-PB2-OB4
29	g	305	CDL	CB2-OB2-PB2-OB5
29	g	305	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
29	g	305	CDL	CB3-OB5-PB2-OB3
29	g	305	CDL	CB3-OB5-PB2-OB4
29	j	301	CDL	CB3-OB5-PB2-OB2
29	j	301	CDL	CB3-OB5-PB2-OB3
29	j	302	CDL	CA3-OA5-PA1-OA2
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	301	CDL	CA3-OA5-PA1-OA2
29	l	301	CDL	CA3-OA5-PA1-OA4
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	r	201	CDL	CB2-OB2-PB2-OB5
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	CA2-OA2-PA1-OA4
29	B	401	CDL	CA2-OA2-PA1-OA5
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
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

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Mol	Chain	Res	Type	Atoms
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	CA3-OA5-PA1-OA3
29	F	303	CDL	CB2-OB2-PB2-OB3
29	F	303	CDL	CB2-OB2-PB2-OB5
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	OB7-CB5-OB6-CB4
29	I	301	CDL	CB2-C1-CA2-OA2
29	I	301	CDL	CA3-OA5-PA1-OA2
29	I	301	CDL	CA3-OA5-PA1-OA3
29	I	301	CDL	CA3-OA5-PA1-OA4
29	I	301	CDL	CB3-OB5-PB2-OB2
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	201	CDL	CB2-OB2-PB2-OB5
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	CA2-OA2-PA1-OA3
29	J	301	CDL	OB7-CB5-OB6-CB4
29	J	301	CDL	C51-CB5-OB6-CB4
29	J	302	CDL	CA3-OA5-PA1-OA2
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	301	CDL	CA3-OA5-PA1-OA2
29	L	301	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
29	L	301	CDL	C11-CA5-OA6-CA4
29	L	301	CDL	CB3-OB5-PB2-OB2
29	L	301	CDL	CB3-OB5-PB2-OB3
29	L	302	CDL	CA3-OA5-PA1-OA2
29	L	302	CDL	CA3-OA5-PA1-OA3
29	L	302	CDL	CA3-OA5-PA1-OA4
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
29	a3	501	CDL	OA5-CA3-CA4-OA6
29	a3	501	CDL	CB3-OB5-PB2-OB2
29	a3	501	CDL	CB3-OB5-PB2-OB4
29	a3	501	CDL	OB7-CB5-OB6-CB4
29	a3	501	CDL	C51-CB5-OB6-CB4
29	a3	502	CDL	CA3-OA5-PA1-OA3
29	b3	401	CDL	CB3-OB5-PB2-OB2
29	b3	401	CDL	CB3-OB5-PB2-OB4
29	b3	401	CDL	OB7-CB5-OB6-CB4
29	b3	401	CDL	C51-CB5-OB6-CB4
29	f3	302	CDL	C1-CA2-OA2-PA1
29	f3	302	CDL	CA2-OA2-PA1-OA4
29	f3	302	CDL	CA4-CA3-OA5-PA1
29	f3	302	CDL	C11-CA5-OA6-CA4
29	f3	302	CDL	CB2-OB2-PB2-OB3
29	f3	302	CDL	CB2-OB2-PB2-OB4
29	f3	302	CDL	CB2-OB2-PB2-OB5
29	f3	302	CDL	CB3-OB5-PB2-OB2
29	f3	302	CDL	CB3-OB5-PB2-OB3
29	f3	302	CDL	CB3-OB5-PB2-OB4
29	f3	303	CDL	OA7-CA5-OA6-CA4
29	f3	303	CDL	CB3-OB5-PB2-OB2
29	f3	303	CDL	CB3-OB5-PB2-OB3
29	f3	303	CDL	CB3-OB5-PB2-OB4
29	f3	303	CDL	OB6-CB4-CB6-OB8
29	f3	303	CDL	C51-CB5-OB6-CB4
29	f3	304	CDL	C1-CA2-OA2-PA1
29	f3	304	CDL	CA3-OA5-PA1-OA3
29	f3	304	CDL	OA5-CA3-CA4-OA6
29	f3	304	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
29	i3	301	CDL	CA3-OA5-PA1-OA2
29	i3	301	CDL	CB2-OB2-PB2-OB3
29	i3	301	CDL	CB2-OB2-PB2-OB5
29	i3	302	CDL	CA3-OA5-PA1-OA2
29	i3	302	CDL	CA3-OA5-PA1-OA4
29	i3	302	CDL	CB3-OB5-PB2-OB2
29	i3	302	CDL	CB3-OB5-PB2-OB4
29	i3	302	CDL	OB7-CB5-OB6-CB4
29	k3	201	CDL	CA3-OA5-PA1-OA3
29	k3	201	CDL	OA7-CA5-OA6-CA4
29	k3	201	CDL	C11-CA5-OA6-CA4
29	k3	201	CDL	CB2-OB2-PB2-OB4
29	k3	201	CDL	CB2-OB2-PB2-OB5
29	k3	201	CDL	CB3-OB5-PB2-OB2
29	k3	201	CDL	CB3-OB5-PB2-OB3
29	k3	201	CDL	CB3-OB5-PB2-OB4
29	g3	305	CDL	OA5-CA3-CA4-OA6
29	g3	305	CDL	CB2-OB2-PB2-OB4
29	g3	305	CDL	CB2-OB2-PB2-OB5
29	g3	305	CDL	CB3-OB5-PB2-OB2
29	g3	305	CDL	CB3-OB5-PB2-OB3
29	g3	305	CDL	CB3-OB5-PB2-OB4
29	j3	301	CDL	CB3-OB5-PB2-OB2
29	j3	301	CDL	CB3-OB5-PB2-OB3
29	j3	302	CDL	CA3-OA5-PA1-OA2
29	j3	302	CDL	CA3-OA5-PA1-OA4
29	j3	302	CDL	CB3-OB5-PB2-OB2
29	j3	302	CDL	CB3-OB5-PB2-OB3
29	j3	302	CDL	CB3-OB5-PB2-OB4
29	l3	301	CDL	CA3-OA5-PA1-OA2
29	l3	301	CDL	CA3-OA5-PA1-OA4
29	l3	303	CDL	CB3-OB5-PB2-OB3
29	p3	201	CDL	CA2-OA2-PA1-OA3
29	p3	201	CDL	CA3-OA5-PA1-OA3
29	p3	201	CDL	C11-CA5-OA6-CA4
29	p3	201	CDL	CB2-OB2-PB2-OB3
29	p3	201	CDL	CB3-OB5-PB2-OB2
29	p3	201	CDL	CB3-OB5-PB2-OB3
29	p3	201	CDL	CB3-OB5-PB2-OB4
29	A3	501	CDL	C1-CA2-OA2-PA1
29	A3	501	CDL	C11-CA5-OA6-CA4
29	A3	501	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
29	A3	501	CDL	CB3-OB5-PB2-OB3
29	A3	501	CDL	CB3-OB5-PB2-OB4
29	A3	501	CDL	C51-CB5-OB6-CB4
29	B3	401	CDL	CA2-OA2-PA1-OA4
29	B3	401	CDL	CA2-OA2-PA1-OA5
29	B3	401	CDL	CA4-CA3-OA5-PA1
29	B3	401	CDL	C11-CA5-OA6-CA4
29	B3	402	CDL	OA7-CA5-OA6-CA4
29	B3	402	CDL	CB3-OB5-PB2-OB2
29	B3	402	CDL	CB3-OB5-PB2-OB3
29	B3	402	CDL	CB3-OB5-PB2-OB4
29	B3	402	CDL	OB7-CB5-OB6-CB4
29	B3	402	CDL	C51-CB5-OB6-CB4
29	B3	404	CDL	O1-C1-CB2-OB2
29	B3	404	CDL	CA2-C1-CB2-OB2
29	B3	404	CDL	C11-CA5-OA6-CA4
29	B3	404	CDL	OA9-CA7-OA8-CA6
29	B3	404	CDL	CB3-OB5-PB2-OB2
29	B3	404	CDL	CB3-OB5-PB2-OB3
29	B3	404	CDL	CB3-OB5-PB2-OB4
29	B3	404	CDL	OB6-CB4-CB6-OB8
29	F3	302	CDL	CB2-OB2-PB2-OB3
29	F3	302	CDL	CB2-OB2-PB2-OB5
29	F3	302	CDL	CB3-OB5-PB2-OB2
29	F3	302	CDL	CB3-OB5-PB2-OB3
29	F3	302	CDL	CB3-OB5-PB2-OB4
29	F3	302	CDL	OB7-CB5-OB6-CB4
29	I3	301	CDL	CB2-C1-CA2-OA2
29	I3	301	CDL	CA3-OA5-PA1-OA2
29	I3	301	CDL	CA3-OA5-PA1-OA3
29	I3	301	CDL	CA3-OA5-PA1-OA4
29	I3	301	CDL	CB3-OB5-PB2-OB2
29	I3	301	CDL	CB3-OB5-PB2-OB3
29	I3	301	CDL	CB3-OB5-PB2-OB4
29	I3	302	CDL	CA3-OA5-PA1-OA2
29	I3	302	CDL	CA3-OA5-PA1-OA3
29	I3	302	CDL	CA3-OA5-PA1-OA4
29	I3	303	CDL	CA3-OA5-PA1-OA2
29	I3	303	CDL	CB3-OB5-PB2-OB2
29	I3	303	CDL	CB3-OB5-PB2-OB3
29	I3	303	CDL	CB3-OB5-PB2-OB4
29	I3	303	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
29	K3	201	CDL	CA3-OA5-PA1-OA3
29	K3	201	CDL	OA7-CA5-OA6-CA4
29	K3	201	CDL	C11-CA5-OA6-CA4
29	K3	201	CDL	CB2-OB2-PB2-OB5
29	K3	202	CDL	OA5-CA3-CA4-OA6
29	K3	202	CDL	CB3-OB5-PB2-OB2
29	K3	202	CDL	CB3-OB5-PB2-OB3
29	K3	202	CDL	CB3-OB5-PB2-OB4
29	J3	301	CDL	CA2-OA2-PA1-OA3
29	J3	301	CDL	OB7-CB5-OB6-CB4
29	J3	301	CDL	C51-CB5-OB6-CB4
29	J3	302	CDL	CA3-OA5-PA1-OA2
29	J3	302	CDL	CA3-OA5-PA1-OA4
29	J3	302	CDL	CB3-OB5-PB2-OB2
29	J3	302	CDL	CB3-OB5-PB2-OB3
29	J3	302	CDL	CB3-OB5-PB2-OB4
29	L3	301	CDL	CA3-OA5-PA1-OA2
29	L3	301	CDL	CA3-OA5-PA1-OA3
29	L3	301	CDL	C11-CA5-OA6-CA4
29	L3	301	CDL	CB3-OB5-PB2-OB2
29	L3	301	CDL	CB3-OB5-PB2-OB3
29	P3	201	CDL	C11-CA5-OA6-CA4
29	P3	201	CDL	CB2-OB2-PB2-OB3
29	P3	201	CDL	CB2-OB2-PB2-OB5
29	P3	201	CDL	CB3-OB5-PB2-OB2
29	P3	201	CDL	CB3-OB5-PB2-OB3
29	P3	201	CDL	CB3-OB5-PB2-OB4
30	d	301	PC1	C1-O11-P-O14
30	d	301	PC1	C1-O11-P-O13
30	d	301	PC1	O13-C11-C12-N
30	d	301	PC1	O22-C21-O21-C2
30	g	303	PC1	C1-O11-P-O13
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	C1-O11-P-O13
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

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Mol	Chain	Res	Type	Atoms
30	G	303	PC1	C1-O11-P-O13
30	G	304	PC1	O22-C21-O21-C2
30	d3	301	PC1	C1-O11-P-O14
30	d3	301	PC1	C1-O11-P-O13
30	d3	301	PC1	O13-C11-C12-N
30	d3	301	PC1	O22-C21-O21-C2
30	g3	303	PC1	C1-O11-P-O13
30	g3	303	PC1	O13-C11-C12-N
30	g3	303	PC1	C2-C1-O11-P
30	g3	304	PC1	O22-C21-O21-C2
30	g3	304	PC1	C22-C21-O21-C2
30	D3	301	PC1	C1-O11-P-O14
30	D3	301	PC1	C1-O11-P-O13
30	D3	301	PC1	O13-C11-C12-N
30	D3	301	PC1	O22-C21-O21-C2
30	D3	301	PC1	C22-C21-O21-C2
30	G3	303	PC1	C1-O11-P-O12
30	G3	303	PC1	C1-O11-P-O13
30	G3	304	PC1	O22-C21-O21-C2
33	B1	1003	ATP	C5'-O5'-PA-O1A
33	A1	601	ATP	C5'-O5'-PA-O2A
33	A1	601	ATP	C5'-O5'-PA-O3A
33	C2	601	ATP	C5'-O5'-PA-O2A
33	C2	601	ATP	C5'-O5'-PA-O3A
33	B2	1003	ATP	C5'-O5'-PA-O1A
33	A2	601	ATP	C5'-O5'-PA-O2A
33	A2	601	ATP	C5'-O5'-PA-O3A
33	B4	1003	ATP	C5'-O5'-PA-O1A
33	A4	601	ATP	C5'-O5'-PA-O2A
33	A4	601	ATP	C5'-O5'-PA-O3A
33	C5	601	ATP	C5'-O5'-PA-O2A
33	C5	601	ATP	C5'-O5'-PA-O3A
33	B5	1003	ATP	C5'-O5'-PA-O1A
33	A5	601	ATP	C5'-O5'-PA-O2A
33	A5	601	ATP	C5'-O5'-PA-O3A
35	m	301	PEE	C1-O3P-P-O2P
35	m	301	PEE	C4-O4P-P-O3P
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	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
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-O3P
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	C1-O3P-P-O4P
35	L	303	PEE	C4-O4P-P-O1P
35	a3	503	PEE	C1-O3P-P-O2P
35	a3	503	PEE	C1-O3P-P-O1P
35	a3	503	PEE	C1-O3P-P-O4P
35	a3	503	PEE	C4-O4P-P-O1P
35	j3	303	PEE	C1-O3P-P-O2P
35	j3	303	PEE	C4-O4P-P-O3P
35	j3	303	PEE	C4-O4P-P-O2P
35	j3	303	PEE	C4-O4P-P-O1P
35	l3	302	PEE	C1-O3P-P-O2P
35	l3	302	PEE	C1-O3P-P-O1P
35	l3	302	PEE	C1-O3P-P-O4P
35	l3	302	PEE	C4-O4P-P-O1P
35	L3	302	PEE	O2-C2-C3-O3
35	L3	302	PEE	C1-O3P-P-O2P
35	L3	302	PEE	C4-O4P-P-O3P
35	L3	302	PEE	C4-O4P-P-O2P
35	L3	302	PEE	C4-O4P-P-O1P
36	e	900	NAD	O4B-C4B-C5B-O5B
36	E	900	NAD	C5B-O5B-PA-O1A
36	E	900	NAD	O4D-C4D-C5D-O5D
36	E	900	NAD	O4D-C1D-N1N-C2N
36	e3	900	NAD	O4B-C4B-C5B-O5B
36	e3	900	NAD	O4D-C1D-N1N-C2N
36	E3	900	NAD	C5B-O5B-PA-O1A
37	D1	501	ADP	C5'-O5'-PA-O1A
37	D1	501	ADP	C2'-C1'-N9-C4
37	D2	501	ADP	C5'-O5'-PA-O1A
37	B2	1002	ADP	PA-O3A-PB-O2B
37	D4	501	ADP	C5'-O5'-PA-O1A
37	D4	501	ADP	C2'-C1'-N9-C4
37	D5	501	ADP	C5'-O5'-PA-O1A
37	B5	1002	ADP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
37	B5	1002	ADP	PA-O3A-PB-O3B
29	B	403	CDL	OB9-CB7-OB8-CB6
29	I	301	CDL	OB9-CB7-OB8-CB6
29	B3	403	CDL	OB9-CB7-OB8-CB6
29	I3	301	CDL	OB9-CB7-OB8-CB6
29	B	403	CDL	C71-CB7-OB8-CB6
29	B3	403	CDL	C71-CB7-OB8-CB6
35	m	301	PEE	C31-C30-O3-C3
35	j3	303	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
29	f3	303	CDL	OA9-CA7-OA8-CA6
29	f3	303	CDL	OB9-CB7-OB8-CB6
29	i3	301	CDL	OA9-CA7-OA8-CA6
29	j3	302	CDL	OA9-CA7-OA8-CA6
29	l3	303	CDL	OB9-CB7-OB8-CB6
29	B3	404	CDL	OB9-CB7-OB8-CB6
29	I3	301	CDL	OA9-CA7-OA8-CA6
29	J3	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
35	a3	503	PEE	O5-C30-O3-C3
35	j3	303	PEE	O5-C30-O3-C3
35	l3	302	PEE	O5-C30-O3-C3
29	f	302	CDL	OA7-CA5-OA6-CA4
29	f	303	CDL	OB7-CB5-OB6-CB4
29	g	305	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	f3	302	CDL	OA7-CA5-OA6-CA4
29	f3	303	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
29	p3	201	CDL	OA7-CA5-OA6-CA4
29	A3	501	CDL	OA7-CA5-OA6-CA4
29	A3	501	CDL	OB7-CB5-OB6-CB4
29	B3	401	CDL	OA7-CA5-OA6-CA4
29	B3	404	CDL	OA7-CA5-OA6-CA4
29	L3	301	CDL	OA7-CA5-OA6-CA4
29	f	303	CDL	C31-CA7-OA8-CA6
29	f	303	CDL	C71-CB7-OB8-CB6
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
29	f3	303	CDL	C31-CA7-OA8-CA6
29	f3	303	CDL	C71-CB7-OB8-CB6
29	i3	301	CDL	C31-CA7-OA8-CA6
29	l3	303	CDL	C71-CB7-OB8-CB6
29	B3	404	CDL	C31-CA7-OA8-CA6
29	B3	404	CDL	C71-CB7-OB8-CB6
29	I3	301	CDL	C71-CB7-OB8-CB6
30	d	301	PC1	C32-C31-O31-C3
30	d3	301	PC1	C32-C31-O31-C3
29	f	303	CDL	C11-CA5-OA6-CA4
29	i	301	CDL	C51-CB5-OB6-CB4
29	g	305	CDL	C11-CA5-OA6-CA4
29	B	402	CDL	C11-CA5-OA6-CA4
29	F	303	CDL	C51-CB5-OB6-CB4
29	f3	303	CDL	C11-CA5-OA6-CA4
29	i3	302	CDL	C51-CB5-OB6-CB4
29	g3	305	CDL	C11-CA5-OA6-CA4
29	B3	402	CDL	C11-CA5-OA6-CA4
29	F3	302	CDL	C51-CB5-OB6-CB4
29	I3	303	CDL	C51-CB5-OB6-CB4
30	d	301	PC1	C22-C21-O21-C2
30	G	304	PC1	C22-C21-O21-C2
30	d3	301	PC1	C22-C21-O21-C2
30	G3	304	PC1	C22-C21-O21-C2
29	r	201	CDL	OB9-CB7-OB8-CB6
29	i3	301	CDL	OB9-CB7-OB8-CB6
29	f	304	CDL	C31-CA7-OA8-CA6
29	f	304	CDL	C71-CB7-OB8-CB6
29	j	302	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
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
29	f3	304	CDL	C31-CA7-OA8-CA6
29	f3	304	CDL	C71-CB7-OB8-CB6
29	j3	302	CDL	C31-CA7-OA8-CA6
29	I3	301	CDL	C31-CA7-OA8-CA6
29	K3	201	CDL	C71-CB7-OB8-CB6
29	K3	202	CDL	C31-CA7-OA8-CA6
29	J3	302	CDL	C31-CA7-OA8-CA6
29	L3	301	CDL	C71-CB7-OB8-CB6
35	A	501	PEE	C31-C30-O3-C3
35	L	303	PEE	C31-C30-O3-C3
35	a3	503	PEE	C31-C30-O3-C3
35	l3	302	PEE	C31-C30-O3-C3
29	f	304	CDL	OA9-CA7-OA8-CA6
29	F	302	CDL	OB9-CB7-OB8-CB6
29	K	201	CDL	OB9-CB7-OB8-CB6
29	K	202	CDL	OA9-CA7-OA8-CA6
29	a3	502	CDL	OB9-CB7-OB8-CB6
29	f3	304	CDL	OA9-CA7-OA8-CA6
29	K3	201	CDL	OB9-CB7-OB8-CB6
29	K3	202	CDL	OA9-CA7-OA8-CA6
29	f	304	CDL	OB7-CB5-OB6-CB4
29	P	201	CDL	OA7-CA5-OA6-CA4
29	f3	304	CDL	OB7-CB5-OB6-CB4
29	g3	305	CDL	OA7-CA5-OA6-CA4
29	P3	201	CDL	OA7-CA5-OA6-CA4
29	B	402	CDL	O1-C1-CA2-OA2
29	B3	402	CDL	O1-C1-CA2-OA2
29	k	201	CDL	C71-CB7-OB8-CB6
29	g	305	CDL	C31-CA7-OA8-CA6
29	r	201	CDL	C71-CB7-OB8-CB6
29	L	301	CDL	C71-CB7-OB8-CB6
29	i3	301	CDL	C71-CB7-OB8-CB6
29	k3	201	CDL	C71-CB7-OB8-CB6
29	g3	305	CDL	C31-CA7-OA8-CA6
29	k	201	CDL	OB9-CB7-OB8-CB6
29	k3	201	CDL	OB9-CB7-OB8-CB6
30	d	301	PC1	O32-C31-O31-C3
30	d3	301	PC1	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
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	i3	301	CDL	C11-CA5-OA6-CA4
29	i3	302	CDL	C11-CA5-OA6-CA4
29	K3	202	CDL	C11-CA5-OA6-CA4
29	f	304	CDL	OB9-CB7-OB8-CB6
29	f3	304	CDL	OB9-CB7-OB8-CB6
29	g3	305	CDL	OA9-CA7-OA8-CA6
33	A1	601	ATP	O4'-C4'-C5'-O5'
33	A1	601	ATP	C3'-C4'-C5'-O5'
33	A2	601	ATP	O4'-C4'-C5'-O5'
33	A2	601	ATP	C3'-C4'-C5'-O5'
33	A4	601	ATP	O4'-C4'-C5'-O5'
33	A4	601	ATP	C3'-C4'-C5'-O5'
33	A5	601	ATP	O4'-C4'-C5'-O5'
33	A5	601	ATP	C3'-C4'-C5'-O5'
36	e	900	NAD	O4D-C4D-C5D-O5D
36	E	900	NAD	O4B-C4B-C5B-O5B
36	e3	900	NAD	O4D-C4D-C5D-O5D
36	E3	900	NAD	O4B-C4B-C5B-O5B
36	E3	900	NAD	O4D-C4D-C5D-O5D
29	F	302	CDL	C71-CB7-OB8-CB6
29	a3	502	CDL	C71-CB7-OB8-CB6
29	g	305	CDL	OA9-CA7-OA8-CA6
29	L3	301	CDL	OB9-CB7-OB8-CB6
32	i	302	UQ8	C34-C36-C37-C38
32	I	303	UQ8	C34-C36-C37-C38
32	I	303	UQ8	C29-C31-C32-C33
32	i3	303	UQ8	C34-C36-C37-C38
32	I3	304	UQ8	C34-C36-C37-C38
32	I3	304	UQ8	C29-C31-C32-C33
29	L	301	CDL	OB9-CB7-OB8-CB6
29	l	301	CDL	C31-CA7-OA8-CA6
29	l	301	CDL	C71-CB7-OB8-CB6
29	l3	301	CDL	C31-CA7-OA8-CA6
29	l3	301	CDL	C71-CB7-OB8-CB6
37	D1	501	ADP	C2'-C1'-N9-C8
37	D4	501	ADP	C2'-C1'-N9-C8
29	K	202	CDL	OA7-CA5-OA6-CA4
29	K3	202	CDL	OA7-CA5-OA6-CA4
29	B	403	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
29	F	302	CDL	CB2-C1-CA2-OA2
29	a3	502	CDL	CB2-C1-CA2-OA2
29	B3	403	CDL	CB2-C1-CA2-OA2
29	B	401	CDL	C71-CB7-OB8-CB6
29	B3	401	CDL	C71-CB7-OB8-CB6
30	D	301	PC1	C32-C31-O31-C3
30	D3	301	PC1	C32-C31-O31-C3
29	K3	201	CDL	C62-C63-C64-C65
29	K	201	CDL	C62-C63-C64-C65
29	I	302	CDL	C76-C77-C78-C79
29	I3	303	CDL	C76-C77-C78-C79
29	f	303	CDL	O1-C1-CB2-OB2
29	F	302	CDL	O1-C1-CA2-OA2
29	a3	502	CDL	O1-C1-CA2-OA2
29	f3	303	CDL	O1-C1-CB2-OB2
30	D	301	PC1	O32-C31-O31-C3
30	D3	301	PC1	O32-C31-O31-C3
29	B	404	CDL	CB7-C71-C72-C73
29	B3	404	CDL	CB7-C71-C72-C73
29	r	201	CDL	OA7-CA5-OA6-CA4
29	i3	301	CDL	OA7-CA5-OA6-CA4
29	f	304	CDL	C11-CA5-OA6-CA4
29	f3	304	CDL	C11-CA5-OA6-CA4
29	i	301	CDL	C31-CA7-OA8-CA6
29	I	302	CDL	C31-CA7-OA8-CA6
29	i3	302	CDL	C31-CA7-OA8-CA6
29	I3	303	CDL	C31-CA7-OA8-CA6
29	B	402	CDL	CA5-C11-C12-C13
29	B3	402	CDL	CA5-C11-C12-C13
29	f	304	CDL	C22-C23-C24-C25
29	I3	303	CDL	C22-C23-C24-C25
29	I	302	CDL	C22-C23-C24-C25
29	f3	304	CDL	C22-C23-C24-C25
29	B	401	CDL	OB9-CB7-OB8-CB6
36	e	900	NAD	C3B-C4B-C5B-O5B
36	E	900	NAD	C3B-C4B-C5B-O5B
36	e3	900	NAD	C3B-C4B-C5B-O5B
36	E3	900	NAD	C3B-C4B-C5B-O5B
29	i	301	CDL	OA7-CA5-OA6-CA4
29	i3	302	CDL	OA7-CA5-OA6-CA4
29	b	401	CDL	C16-C17-C18-C19
29	b3	401	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	f	303	CDL	CB7-C71-C72-C73
29	B	404	CDL	CA5-C11-C12-C13
29	f3	303	CDL	CB7-C71-C72-C73
29	B3	404	CDL	CA5-C11-C12-C13
29	B3	401	CDL	OB9-CB7-OB8-CB6
29	l	302	CDL	CA5-C11-C12-C13
29	B	401	CDL	CA5-C11-C12-C13
29	l3	303	CDL	CA5-C11-C12-C13
29	B3	401	CDL	CA5-C11-C12-C13
29	B	403	CDL	O1-C1-CA2-OA2
29	B3	403	CDL	O1-C1-CA2-OA2
29	l	301	CDL	OA9-CA7-OA8-CA6
29	l	301	CDL	OB9-CB7-OB8-CB6
29	l3	301	CDL	OA9-CA7-OA8-CA6
29	l3	301	CDL	OB9-CB7-OB8-CB6
29	i	301	CDL	CB5-C51-C52-C53
29	i3	302	CDL	CB5-C51-C52-C53
29	f	302	CDL	CA7-C31-C32-C33
29	k	201	CDL	CA7-C31-C32-C33
29	P	201	CDL	CA5-C11-C12-C13
29	f3	302	CDL	CA7-C31-C32-C33
29	k3	201	CDL	CA7-C31-C32-C33
29	P3	201	CDL	CA5-C11-C12-C13
30	G	304	PC1	C32-C31-O31-C3
30	G3	304	PC1	C32-C31-O31-C3
29	J	301	CDL	C11-CA5-OA6-CA4
29	J3	301	CDL	C11-CA5-OA6-CA4
29	i	301	CDL	OA9-CA7-OA8-CA6
29	I	302	CDL	OA9-CA7-OA8-CA6
29	i3	302	CDL	OA9-CA7-OA8-CA6
30	g	304	PC1	C21-C22-C23-C24
30	g3	304	PC1	C21-C22-C23-C24
29	l	301	CDL	C54-C55-C56-C57
35	m	301	PEE	C43-C44-C45-C46
35	j3	303	PEE	C43-C44-C45-C46
29	I3	303	CDL	OA9-CA7-OA8-CA6
29	l3	301	CDL	C54-C55-C56-C57
29	B	401	CDL	CB5-C51-C52-C53
29	B3	401	CDL	CB5-C51-C52-C53
29	f	304	CDL	OA7-CA5-OA6-CA4
29	J	301	CDL	OA7-CA5-OA6-CA4
29	f3	304	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
29	J3	301	CDL	OA7-CA5-OA6-CA4
29	g	305	CDL	C71-CB7-OB8-CB6
29	j	302	CDL	C71-CB7-OB8-CB6
29	K	202	CDL	C71-CB7-OB8-CB6
29	g3	305	CDL	C71-CB7-OB8-CB6
29	j3	302	CDL	C71-CB7-OB8-CB6
29	K3	202	CDL	C71-CB7-OB8-CB6
30	g	303	PC1	C31-C32-C33-C34
30	g3	303	PC1	C31-C32-C33-C34
29	a	501	CDL	C11-CA5-OA6-CA4
29	f	302	CDL	C51-CB5-OB6-CB4
29	j	302	CDL	C11-CA5-OA6-CA4
29	F	302	CDL	C11-CA5-OA6-CA4
29	I	301	CDL	C11-CA5-OA6-CA4
29	I	302	CDL	C11-CA5-OA6-CA4
29	a3	501	CDL	C11-CA5-OA6-CA4
29	a3	502	CDL	C11-CA5-OA6-CA4
29	f3	302	CDL	C51-CB5-OB6-CB4
29	j3	302	CDL	C11-CA5-OA6-CA4
29	I3	301	CDL	C11-CA5-OA6-CA4
29	I3	303	CDL	C11-CA5-OA6-CA4
35	J	303	PEE	C11-C10-O2-C2
35	L3	302	PEE	C11-C10-O2-C2
29	a	501	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
29	a3	501	CDL	OA7-CA5-OA6-CA4
29	a3	502	CDL	OA7-CA5-OA6-CA4
29	j3	302	CDL	OA7-CA5-OA6-CA4
29	I3	301	CDL	OA7-CA5-OA6-CA4
29	I3	303	CDL	OA7-CA5-OA6-CA4
35	J	303	PEE	O4-C10-O2-C2
35	L3	302	PEE	O4-C10-O2-C2
32	i	302	UQ8	C29-C31-C32-C33
32	i3	303	UQ8	C29-C31-C32-C33
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	b3	401	CDL	O1-C1-CA2-OA2
29	I3	301	CDL	O1-C1-CA2-OA2
29	I3	303	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
29	F	302	CDL	CA5-C11-C12-C13
29	a3	502	CDL	CA5-C11-C12-C13
29	a	501	CDL	CA7-C31-C32-C33
29	a3	501	CDL	CA7-C31-C32-C33
29	l	302	CDL	C20-C21-C22-C23
29	L	301	CDL	C81-C82-C83-C84
29	l3	303	CDL	C20-C21-C22-C23
29	I3	302	CDL	C40-C41-C42-C43
29	L3	301	CDL	C81-C82-C83-C84
29	L	302	CDL	C40-C41-C42-C43
29	F	302	CDL	OA7-CA5-OA6-CA4
29	j	301	CDL	C11-CA5-OA6-CA4
29	j3	301	CDL	C11-CA5-OA6-CA4
29	j	302	CDL	CA7-C31-C32-C33
30	g	304	PC1	C32-C31-O31-C3
30	g3	304	PC1	C32-C31-O31-C3
29	j3	302	CDL	CA7-C31-C32-C33
35	A	501	PEE	C10-C11-C12-C13
35	L	303	PEE	C10-C11-C12-C13
35	a3	503	PEE	C10-C11-C12-C13
35	l3	302	PEE	C10-C11-C12-C13
29	g	305	CDL	OB9-CB7-OB8-CB6
29	j	302	CDL	OB9-CB7-OB8-CB6
29	g3	305	CDL	OB9-CB7-OB8-CB6
29	j3	302	CDL	OB9-CB7-OB8-CB6
29	f	302	CDL	C62-C63-C64-C65
29	j	302	CDL	C36-C37-C38-C39
29	B	402	CDL	C54-C55-C56-C57
29	P	201	CDL	C54-C55-C56-C57
29	j3	302	CDL	C36-C37-C38-C39
29	B3	402	CDL	C54-C55-C56-C57
29	P3	201	CDL	C54-C55-C56-C57
29	B	403	CDL	C18-C19-C20-C21
29	K	202	CDL	C83-C84-C85-C86
29	K3	202	CDL	C83-C84-C85-C86
30	g	303	PC1	C2D-C2E-C2F-C2G
30	g3	303	PC1	C2D-C2E-C2F-C2G
35	J	303	PEE	C41-C42-C43-C44
35	L3	302	PEE	C41-C42-C43-C44
35	J	303	PEE	C17-C18-C19-C20
35	L3	302	PEE	C17-C18-C19-C20
29	F	303	CDL	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
29	I	302	CDL	C13-C14-C15-C16
29	K	202	CDL	C74-C75-C76-C77
29	f3	302	CDL	C62-C63-C64-C65
29	B3	403	CDL	C18-C19-C20-C21
29	F3	302	CDL	C35-C36-C37-C38
29	I3	303	CDL	C13-C14-C15-C16
29	K3	202	CDL	C74-C75-C76-C77
30	G	304	PC1	O32-C31-O31-C3
30	G3	304	PC1	O32-C31-O31-C3
29	b	401	CDL	C71-CB7-OB8-CB6
29	b3	401	CDL	C71-CB7-OB8-CB6
29	b	401	CDL	C81-C82-C83-C84
29	f	302	CDL	C35-C36-C37-C38
29	j	302	CDL	C41-C42-C43-C44
29	l	302	CDL	C22-C23-C24-C25
29	l	302	CDL	C74-C75-C76-C77
29	A	502	CDL	C56-C57-C58-C59
29	J	301	CDL	C35-C36-C37-C38
29	J	302	CDL	C77-C78-C79-C80
29	b3	401	CDL	C81-C82-C83-C84
29	j3	302	CDL	C41-C42-C43-C44
29	l3	303	CDL	C22-C23-C24-C25
29	A3	501	CDL	C56-C57-C58-C59
29	J3	301	CDL	C35-C36-C37-C38
29	f	302	CDL	OB7-CB5-OB6-CB4
29	j	301	CDL	OA7-CA5-OA6-CA4
29	f3	302	CDL	OB7-CB5-OB6-CB4
29	j3	301	CDL	OA7-CA5-OA6-CA4
29	g	305	CDL	C74-C75-C76-C77
29	j	302	CDL	C54-C55-C56-C57
29	J	301	CDL	C72-C73-C74-C75
29	f3	302	CDL	C35-C36-C37-C38
29	g3	305	CDL	C74-C75-C76-C77
29	l3	303	CDL	C74-C75-C76-C77
29	B3	403	CDL	C76-C77-C78-C79
29	J3	301	CDL	C72-C73-C74-C75
29	J3	302	CDL	C77-C78-C79-C80
29	P3	201	CDL	C74-C75-C76-C77
29	i	301	CDL	CB7-C71-C72-C73
29	i3	302	CDL	CB7-C71-C72-C73
29	A3	501	CDL	CB5-C51-C52-C53
29	B	403	CDL	C76-C77-C78-C79

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Mol	Chain	Res	Type	Atoms
29	P	201	CDL	C74-C75-C76-C77
29	j3	302	CDL	C54-C55-C56-C57
29	K	202	CDL	C58-C59-C60-C61
29	B3	401	CDL	C41-C42-C43-C44
35	a3	503	PEE	C34-C35-C36-C37
29	j	301	CDL	C51-CB5-OB6-CB4
29	j3	301	CDL	C51-CB5-OB6-CB4
29	j3	301	CDL	C22-C23-C24-C25
29	j3	301	CDL	C31-C32-C33-C34
29	L3	301	CDL	C74-C75-C76-C77
29	a	501	CDL	C60-C61-C62-C63
29	j	301	CDL	C22-C23-C24-C25
29	j	301	CDL	C31-C32-C33-C34
29	A	502	CDL	C14-C15-C16-C17
29	B	401	CDL	C41-C42-C43-C44
29	L	301	CDL	C71-C72-C73-C74
29	L	302	CDL	C21-C22-C23-C24
29	a3	501	CDL	C53-C54-C55-C56
29	A3	501	CDL	C14-C15-C16-C17
29	L3	301	CDL	C71-C72-C73-C74
35	L	303	PEE	C34-C35-C36-C37
29	B	403	CDL	CA5-C11-C12-C13
29	B3	403	CDL	CA5-C11-C12-C13
36	e	900	NAD	C3D-C4D-C5D-O5D
36	e3	900	NAD	C3D-C4D-C5D-O5D
29	f	303	CDL	C76-C77-C78-C79
29	j	301	CDL	C72-C73-C74-C75
29	B	402	CDL	C83-C84-C85-C86
29	K	201	CDL	C74-C75-C76-C77
29	L	301	CDL	C74-C75-C76-C77
29	f3	303	CDL	C76-C77-C78-C79
29	j3	301	CDL	C72-C73-C74-C75
29	B3	402	CDL	C83-C84-C85-C86
29	I3	302	CDL	C21-C22-C23-C24
29	K3	201	CDL	C74-C75-C76-C77
29	K3	202	CDL	C58-C59-C60-C61
29	J3	302	CDL	C38-C39-C40-C41
29	K3	202	CDL	OB9-CB7-OB8-CB6
29	a	501	CDL	C53-C54-C55-C56
29	b	401	CDL	C11-C12-C13-C14
29	f	303	CDL	C51-C52-C53-C54
29	j	301	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	J	302	CDL	C38-C39-C40-C41
29	a3	501	CDL	C60-C61-C62-C63
29	j3	301	CDL	C11-C12-C13-C14
30	D3	301	PC1	C27-C28-C29-C2A
29	L	301	CDL	C83-C84-C85-C86
29	b3	401	CDL	C11-C12-C13-C14
29	L3	301	CDL	C83-C84-C85-C86
30	D	301	PC1	C27-C28-C29-C2A
29	r	201	CDL	CB4-CB6-OB8-CB7
29	i3	301	CDL	CB4-CB6-OB8-CB7
29	A	502	CDL	CB5-C51-C52-C53
29	F	303	CDL	CB5-C51-C52-C53
29	F3	302	CDL	CB5-C51-C52-C53
29	g	305	CDL	C19-C20-C21-C22
29	f3	303	CDL	C51-C52-C53-C54
29	g3	305	CDL	C19-C20-C21-C22
29	K	202	CDL	OB9-CB7-OB8-CB6
29	i	301	CDL	C74-C75-C76-C77
29	k	201	CDL	C36-C37-C38-C39
29	B	402	CDL	C22-C23-C24-C25
29	B	404	CDL	C12-C13-C14-C15
29	I	302	CDL	C72-C73-C74-C75
29	L	301	CDL	C37-C38-C39-C40
29	k3	201	CDL	C36-C37-C38-C39
29	l3	303	CDL	C55-C56-C57-C58
29	B3	402	CDL	C22-C23-C24-C25
29	I3	303	CDL	C72-C73-C74-C75
29	I3	303	CDL	C82-C83-C84-C85
29	L3	301	CDL	C37-C38-C39-C40
29	l	301	CDL	C21-C22-C23-C24
29	l	302	CDL	C83-C84-C85-C86
29	I	302	CDL	C82-C83-C84-C85
29	i3	302	CDL	C74-C75-C76-C77
29	l3	303	CDL	C83-C84-C85-C86
29	B3	404	CDL	C12-C13-C14-C15
29	F3	302	CDL	C78-C79-C80-C81
29	J3	302	CDL	CA3-CA4-CA6-OA8
29	a	501	CDL	C58-C59-C60-C61
29	l	301	CDL	C34-C35-C36-C37
29	l	302	CDL	C55-C56-C57-C58
29	F	303	CDL	C52-C53-C54-C55
29	F	303	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
29	a3	501	CDL	C58-C59-C60-C61
29	l3	301	CDL	C34-C35-C36-C37
29	F3	302	CDL	C52-C53-C54-C55
29	P3	201	CDL	C23-C24-C25-C26
29	r	201	CDL	CA7-C31-C32-C33
29	K	202	CDL	CA5-C11-C12-C13
29	i3	301	CDL	CA7-C31-C32-C33
29	K3	202	CDL	CA5-C11-C12-C13
29	k	201	CDL	C37-C38-C39-C40
29	B	403	CDL	C81-C82-C83-C84
29	K	201	CDL	C54-C55-C56-C57
29	P	201	CDL	C23-C24-C25-C26
29	k3	201	CDL	C37-C38-C39-C40
29	j3	301	CDL	C37-C38-C39-C40
29	l3	301	CDL	C21-C22-C23-C24
29	l3	303	CDL	C36-C37-C38-C39
29	B3	401	CDL	C81-C82-C83-C84
29	B3	403	CDL	C81-C82-C83-C84
29	B3	404	CDL	C35-C36-C37-C38
29	J3	301	CDL	C63-C64-C65-C66
30	g	303	PC1	C2C-C2D-C2E-C2F
30	g3	303	PC1	C2C-C2D-C2E-C2F
30	g	304	PC1	O32-C31-O31-C3
30	g3	304	PC1	O32-C31-O31-C3
29	f	302	CDL	C56-C57-C58-C59
29	f	304	CDL	C11-C12-C13-C14
29	j	301	CDL	C37-C38-C39-C40
29	l	302	CDL	C36-C37-C38-C39
29	p	201	CDL	C54-C55-C56-C57
29	B	401	CDL	C81-C82-C83-C84
29	B	404	CDL	C35-C36-C37-C38
29	J	301	CDL	C63-C64-C65-C66
29	L	301	CDL	C31-C32-C33-C34
29	L	302	CDL	C83-C84-C85-C86
29	f3	302	CDL	C56-C57-C58-C59
29	f3	304	CDL	C11-C12-C13-C14
29	p3	201	CDL	C54-C55-C56-C57
29	I3	302	CDL	C83-C84-C85-C86
29	K3	201	CDL	C54-C55-C56-C57
30	d	301	PC1	C37-C38-C39-C3A
30	G	304	PC1	C34-C35-C36-C37
29	j3	301	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
29	A3	501	CDL	C21-C22-C23-C24
29	L3	301	CDL	C31-C32-C33-C34
30	G3	304	PC1	C34-C35-C36-C37
35	l3	302	PEE	C42-C43-C44-C45
29	a	501	CDL	C38-C39-C40-C41
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	C33-C34-C35-C36
29	A	502	CDL	C21-C22-C23-C24
29	I	301	CDL	C60-C61-C62-C63
29	L	301	CDL	C54-C55-C56-C57
29	a3	501	CDL	C38-C39-C40-C41
29	b3	401	CDL	C40-C41-C42-C43
29	k3	201	CDL	C76-C77-C78-C79
29	I3	301	CDL	C60-C61-C62-C63
29	L3	301	CDL	C54-C55-C56-C57
30	d3	301	PC1	C37-C38-C39-C3A
35	A	501	PEE	C42-C43-C44-C45
29	r	201	CDL	CB7-C71-C72-C73
29	i3	301	CDL	CB7-C71-C72-C73
29	b	401	CDL	C40-C41-C42-C43
29	i3	302	CDL	C19-C20-C21-C22
29	l3	301	CDL	C11-CA5-OA6-CA4
29	a	501	CDL	C1-CB2-OB2-PB2
29	a3	501	CDL	C1-CB2-OB2-PB2
29	A	502	CDL	C16-C17-C18-C19
29	J	301	CDL	C33-C34-C35-C36
29	f3	304	CDL	C75-C76-C77-C78
29	A3	501	CDL	C16-C17-C18-C19
29	J3	301	CDL	C33-C34-C35-C36
29	j3	301	CDL	C16-C17-C18-C19
30	d	301	PC1	C28-C29-C2A-C2B
30	d3	301	PC1	C28-C29-C2A-C2B
29	f	304	CDL	CA7-C31-C32-C33
29	f	304	CDL	CB5-C51-C52-C53
29	f	303	CDL	C35-C36-C37-C38
29	j	301	CDL	C16-C17-C18-C19
29	K	202	CDL	C43-C44-C45-C46
29	J	302	CDL	C13-C14-C15-C16
29	f3	303	CDL	C35-C36-C37-C38
29	K3	202	CDL	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
29	J3	302	CDL	C13-C14-C15-C16
29	b	401	CDL	OB9-CB7-OB8-CB6
29	b3	401	CDL	OB9-CB7-OB8-CB6
29	B3	401	CDL	C38-C39-C40-C41
29	f	302	CDL	C19-C20-C21-C22
29	j	302	CDL	C13-C14-C15-C16
29	l	301	CDL	C37-C38-C39-C40
29	f3	302	CDL	C19-C20-C21-C22
29	j3	302	CDL	C13-C14-C15-C16
29	l3	301	CDL	C37-C38-C39-C40
29	p3	201	CDL	C73-C74-C75-C76
29	B3	401	CDL	C22-C23-C24-C25
30	d	301	PC1	C35-C36-C37-C38
30	d3	301	PC1	C35-C36-C37-C38
29	a	501	CDL	C51-C52-C53-C54
29	j	301	CDL	C82-C83-C84-C85
29	l	302	CDL	C15-C16-C17-C18
29	A	502	CDL	C80-C81-C82-C83
29	B	401	CDL	C22-C23-C24-C25
29	B	401	CDL	C38-C39-C40-C41
29	j3	301	CDL	C82-C83-C84-C85
29	A3	501	CDL	C80-C81-C82-C83
29	K	202	CDL	CB5-C51-C52-C53
29	f3	304	CDL	CA7-C31-C32-C33
29	f3	304	CDL	CB5-C51-C52-C53
29	K3	202	CDL	CB5-C51-C52-C53
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	j3	301	CDL	C31-CA7-OA8-CA6
29	I3	303	CDL	C71-CB7-OB8-CB6
29	P3	201	CDL	C31-CA7-OA8-CA6
29	j	302	CDL	C52-C53-C54-C55
29	p	201	CDL	C73-C74-C75-C76
29	F	303	CDL	C38-C39-C40-C41
29	I	301	CDL	C74-C75-C76-C77
29	a3	501	CDL	C51-C52-C53-C54
29	l3	303	CDL	C15-C16-C17-C18
29	B3	404	CDL	C43-C44-C45-C46
29	F3	302	CDL	C38-C39-C40-C41
29	L3	301	CDL	C38-C39-C40-C41
29	B	404	CDL	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
29	L	301	CDL	C38-C39-C40-C41
29	L	301	CDL	C78-C79-C80-C81
29	f3	302	CDL	C17-C18-C19-C20
29	j3	302	CDL	C52-C53-C54-C55
29	p3	201	CDL	C22-C23-C24-C25
29	B3	402	CDL	C75-C76-C77-C78
29	L3	301	CDL	C78-C79-C80-C81
29	f	302	CDL	C17-C18-C19-C20
29	B	402	CDL	C75-C76-C77-C78
29	I3	301	CDL	C74-C75-C76-C77
29	b	401	CDL	C53-C54-C55-C56
29	i	301	CDL	C81-C82-C83-C84
29	p	201	CDL	C22-C23-C24-C25
29	B	401	CDL	C63-C64-C65-C66
29	b3	401	CDL	C53-C54-C55-C56
29	j3	301	CDL	C20-C21-C22-C23
29	B3	401	CDL	C63-C64-C65-C66
29	I3	303	CDL	C74-C75-C76-C77
29	f	304	CDL	CA5-C11-C12-C13
29	F	303	CDL	CB7-C71-C72-C73
29	f3	302	CDL	CA5-C11-C12-C13
29	f3	304	CDL	CA5-C11-C12-C13
29	b	401	CDL	C56-C57-C58-C59
29	j	301	CDL	C20-C21-C22-C23
29	F	302	CDL	C37-C38-C39-C40
29	I	302	CDL	C74-C75-C76-C77
29	a3	502	CDL	C37-C38-C39-C40
29	b3	401	CDL	C56-C57-C58-C59
29	i3	302	CDL	C81-C82-C83-C84
30	G	304	PC1	C2C-C2D-C2E-C2F
30	G3	304	PC1	C2C-C2D-C2E-C2F
29	B	404	CDL	O1-C1-CA2-OA2
29	B3	404	CDL	O1-C1-CA2-OA2
29	A	502	CDL	C72-C73-C74-C75
29	A3	501	CDL	C72-C73-C74-C75
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
29	j3	302	CDL	C51-CB5-OB6-CB4
29	B3	403	CDL	C11-CA5-OA6-CA4
29	J3	302	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
35	m	301	PEE	C11-C10-O2-C2
35	j3	303	PEE	C11-C10-O2-C2
29	f	302	CDL	CA5-C11-C12-C13
29	F3	302	CDL	CB7-C71-C72-C73
29	f	302	CDL	C23-C24-C25-C26
29	f	303	CDL	C77-C78-C79-C80
29	J	302	CDL	C16-C17-C18-C19
29	f3	302	CDL	C23-C24-C25-C26
29	f3	302	CDL	C42-C43-C44-C45
29	f3	302	CDL	C78-C79-C80-C81
29	f3	303	CDL	C77-C78-C79-C80
29	J3	302	CDL	C52-C53-C54-C55
29	j	301	CDL	OB7-CB5-OB6-CB4
29	j	302	CDL	OB7-CB5-OB6-CB4
29	B	403	CDL	OA7-CA5-OA6-CA4
29	j3	301	CDL	OB7-CB5-OB6-CB4
29	j3	302	CDL	OB7-CB5-OB6-CB4
29	B3	403	CDL	OA7-CA5-OA6-CA4
35	m	301	PEE	O4-C10-O2-C2
35	j3	303	PEE	O4-C10-O2-C2
29	f	302	CDL	C42-C43-C44-C45
29	J	301	CDL	C21-C22-C23-C24
29	J3	301	CDL	C21-C22-C23-C24
29	J3	302	CDL	C16-C17-C18-C19
35	m	301	PEE	C19-C20-C21-C22
35	j3	303	PEE	C19-C20-C21-C22
29	F	303	CDL	C39-C40-C41-C42
29	J	302	CDL	C52-C53-C54-C55
29	p3	201	CDL	C52-C53-C54-C55
29	p3	201	CDL	C58-C59-C60-C61
29	F3	302	CDL	C39-C40-C41-C42
29	f	302	CDL	C78-C79-C80-C81
29	p	201	CDL	C52-C53-C54-C55
29	p	201	CDL	C58-C59-C60-C61
36	E	900	NAD	C3D-C4D-C5D-O5D
36	E3	900	NAD	C3D-C4D-C5D-O5D
29	l	301	CDL	C60-C61-C62-C63
29	l3	301	CDL	C60-C61-C62-C63
29	f	303	CDL	C80-C81-C82-C83
29	f3	303	CDL	C80-C81-C82-C83
30	g	304	PC1	C24-C25-C26-C27
30	g3	304	PC1	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
35	m	301	PEE	C14-C15-C16-C17
35	j3	303	PEE	C14-C15-C16-C17
32	I	303	UQ8	C40-C39-C41-C42
32	I3	304	UQ8	C40-C39-C41-C42
29	f	303	CDL	CA5-C11-C12-C13
29	F	302	CDL	C51-C52-C53-C54
29	J	302	CDL	C74-C75-C76-C77
29	a3	502	CDL	C51-C52-C53-C54
29	a	501	CDL	C21-C22-C23-C24
29	l	302	CDL	C62-C63-C64-C65
29	F	303	CDL	C20-C21-C22-C23
29	a3	501	CDL	C21-C22-C23-C24
29	l3	303	CDL	C62-C63-C64-C65
29	J3	302	CDL	C74-C75-C76-C77
30	G	304	PC1	C29-C2A-C2B-C2C
30	G3	304	PC1	C29-C2A-C2B-C2C
35	L3	302	PEE	C23-C24-C25-C26
29	B	404	CDL	C57-C58-C59-C60
29	K	201	CDL	C40-C41-C42-C43
29	i3	302	CDL	C76-C77-C78-C79
29	B3	404	CDL	C57-C58-C59-C60
29	F3	302	CDL	C20-C21-C22-C23
29	K3	201	CDL	C40-C41-C42-C43
35	J	303	PEE	C23-C24-C25-C26
29	g	305	CDL	CA5-C11-C12-C13
29	f3	303	CDL	CA5-C11-C12-C13
29	g3	305	CDL	CA5-C11-C12-C13
29	i	301	CDL	C76-C77-C78-C79
30	g	303	PC1	C37-C38-C39-C3A
30	g3	303	PC1	C37-C38-C39-C3A
29	i3	302	CDL	OB5-CB3-CB4-OB6
29	J	301	CDL	C52-C53-C54-C55
29	J3	301	CDL	C52-C53-C54-C55
29	A	502	CDL	C35-C36-C37-C38
29	f3	302	CDL	C38-C39-C40-C41
29	i3	302	CDL	C61-C62-C63-C64
29	A3	501	CDL	C35-C36-C37-C38
29	a	501	CDL	C43-C44-C45-C46
29	f	302	CDL	C38-C39-C40-C41
29	i	301	CDL	C61-C62-C63-C64
29	a3	501	CDL	C43-C44-C45-C46
35	l3	302	PEE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
29	L3	301	CDL	CA5-C11-C12-C13
29	A	502	CDL	C74-C75-C76-C77
29	A3	501	CDL	C74-C75-C76-C77
29	L3	301	CDL	C52-C53-C54-C55
35	A	501	PEE	C32-C33-C34-C35
29	j	302	CDL	C74-C75-C76-C77
29	L	301	CDL	C52-C53-C54-C55
29	j3	302	CDL	C74-C75-C76-C77
29	I	302	CDL	C56-C57-C58-C59
29	f3	302	CDL	C80-C81-C82-C83
29	f3	304	CDL	C18-C19-C20-C21
29	I3	303	CDL	C56-C57-C58-C59
29	L	301	CDL	CA5-C11-C12-C13
29	f	302	CDL	C80-C81-C82-C83
29	f	304	CDL	C18-C19-C20-C21
29	j	302	CDL	C72-C73-C74-C75
29	K	201	CDL	C56-C57-C58-C59
29	J	302	CDL	C31-C32-C33-C34
29	a3	501	CDL	C83-C84-C85-C86
29	k3	201	CDL	C18-C19-C20-C21
29	j3	302	CDL	C72-C73-C74-C75
29	K3	201	CDL	C56-C57-C58-C59
29	J3	302	CDL	C31-C32-C33-C34
29	a	501	CDL	C56-C57-C58-C59
29	k	201	CDL	C18-C19-C20-C21
29	A	502	CDL	C83-C84-C85-C86
29	F	302	CDL	C57-C58-C59-C60
29	a3	502	CDL	C22-C23-C24-C25
29	a3	502	CDL	C57-C58-C59-C60
29	B	401	CDL	C1-CA2-OA2-PA1
29	B3	401	CDL	C1-CA2-OA2-PA1
29	a	501	CDL	C83-C84-C85-C86
29	F	302	CDL	C22-C23-C24-C25
29	I	302	CDL	C79-C80-C81-C82
29	a3	501	CDL	C56-C57-C58-C59
29	A3	501	CDL	C83-C84-C85-C86
29	B3	402	CDL	C60-C61-C62-C63
29	I3	302	CDL	C72-C73-C74-C75
29	I3	303	CDL	C79-C80-C81-C82
29	B	402	CDL	C60-C61-C62-C63
29	L	302	CDL	C72-C73-C74-C75
30	D3	301	PC1	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
29	l	302	CDL	C17-C18-C19-C20
29	a3	501	CDL	C74-C75-C76-C77
29	f3	302	CDL	C81-C82-C83-C84
29	i3	302	CDL	C36-C37-C38-C39
29	l3	303	CDL	C17-C18-C19-C20
30	D	301	PC1	C28-C29-C2A-C2B
29	a	501	CDL	C74-C75-C76-C77
29	f	302	CDL	C81-C82-C83-C84
29	i	301	CDL	C36-C37-C38-C39
29	I3	303	CDL	C60-C61-C62-C63
29	I	302	CDL	C60-C61-C62-C63
29	L	302	CDL	C74-C75-C76-C77
29	L	302	CDL	C76-C77-C78-C79
29	I3	302	CDL	C74-C75-C76-C77
29	I3	302	CDL	C76-C77-C78-C79
30	d	301	PC1	C2B-C2C-C2D-C2E
30	d3	301	PC1	C2B-C2C-C2D-C2E
29	j3	301	CDL	OA9-CA7-OA8-CA6
29	I3	303	CDL	OB9-CB7-OB8-CB6
29	P3	201	CDL	OA9-CA7-OA8-CA6
29	F	302	CDL	C43-C44-C45-C46
29	F	303	CDL	C82-C83-C84-C85
29	a3	502	CDL	C43-C44-C45-C46
29	F3	302	CDL	C82-C83-C84-C85
29	r	201	CDL	C82-C83-C84-C85
29	i3	301	CDL	C82-C83-C84-C85
29	P	201	CDL	OA9-CA7-OA8-CA6
29	l	302	CDL	C71-C72-C73-C74
29	l3	303	CDL	C71-C72-C73-C74
29	B3	402	CDL	C71-C72-C73-C74
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	F	303	CDL	OB5-CB3-CB4-CB6
29	K	202	CDL	OA5-CA3-CA4-CA6
29	a3	501	CDL	OA5-CA3-CA4-CA6
29	b3	401	CDL	OA5-CA3-CA4-CA6
29	f3	304	CDL	OA5-CA3-CA4-CA6
29	i3	301	CDL	OA5-CA3-CA4-CA6
29	j3	301	CDL	OA5-CA3-CA4-CA6
29	F3	302	CDL	OB5-CB3-CB4-CB6
29	K3	202	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
29	P3	201	CDL	OB5-CB3-CB4-CB6
35	L3	302	PEE	O3P-C1-C2-C3
29	J	302	CDL	OB7-CB5-OB6-CB4
29	J3	302	CDL	OB7-CB5-OB6-CB4
29	B	402	CDL	C71-C72-C73-C74
29	K	201	CDL	C71-C72-C73-C74
29	J	301	CDL	C31-C32-C33-C34
29	K3	201	CDL	C71-C72-C73-C74
30	g3	303	PC1	C3D-C3E-C3F-C3G
30	g	303	PC1	C3D-C3E-C3F-C3G
29	j	301	CDL	OA9-CA7-OA8-CA6
29	I	302	CDL	OB9-CB7-OB8-CB6
30	d3	301	PC1	C24-C25-C26-C27
29	J3	301	CDL	C31-C32-C33-C34
30	d	301	PC1	C24-C25-C26-C27
35	A	501	PEE	C41-C42-C43-C44
29	B	401	CDL	C36-C37-C38-C39
29	B	404	CDL	C13-C14-C15-C16
29	F	302	CDL	C76-C77-C78-C79
29	a3	502	CDL	C76-C77-C78-C79
29	B3	401	CDL	C36-C37-C38-C39
29	B3	404	CDL	C13-C14-C15-C16
35	l3	302	PEE	C41-C42-C43-C44
30	D	301	PC1	C25-C26-C27-C28
29	I	301	CDL	C78-C79-C80-C81
29	L	301	CDL	C15-C16-C17-C18
29	L	302	CDL	C42-C43-C44-C45
29	L3	301	CDL	C15-C16-C17-C18
30	D3	301	PC1	C25-C26-C27-C28
35	L	303	PEE	C32-C33-C34-C35
35	L	303	PEE	C43-C44-C45-C46
35	a3	503	PEE	C32-C33-C34-C35
35	a3	503	PEE	C43-C44-C45-C46
29	L	302	CDL	CA5-C11-C12-C13
29	I3	302	CDL	CA5-C11-C12-C13
29	l	301	CDL	OA7-CA5-OA6-CA4
29	l3	301	CDL	OA7-CA5-OA6-CA4
29	I3	301	CDL	C78-C79-C80-C81
29	b	401	CDL	CB3-CB4-CB6-OB8
29	f	303	CDL	CB3-CB4-CB6-OB8
29	r	201	CDL	CB3-CB4-CB6-OB8
29	B	404	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
29	F	303	CDL	CA3-CA4-CA6-OA8
29	I	302	CDL	CB3-CB4-CB6-OB8
29	b3	401	CDL	CB3-CB4-CB6-OB8
29	f3	303	CDL	CB3-CB4-CB6-OB8
29	i3	301	CDL	CB3-CB4-CB6-OB8
29	j3	302	CDL	CA3-CA4-CA6-OA8
29	B3	404	CDL	CB3-CB4-CB6-OB8
29	F3	302	CDL	CA3-CA4-CA6-OA8
29	P3	201	CDL	CA3-CA4-CA6-OA8
30	d	301	PC1	C1-C2-C3-O31
30	D	301	PC1	C1-C2-C3-O31
30	D3	301	PC1	C1-C2-C3-O31
29	I3	301	CDL	C71-C72-C73-C74
29	I3	302	CDL	C42-C43-C44-C45
35	m	301	PEE	C35-C36-C37-C38
35	J	303	PEE	C19-C20-C21-C22
35	j3	303	PEE	C35-C36-C37-C38
35	L3	302	PEE	C19-C20-C21-C22
29	I	301	CDL	C71-C72-C73-C74
29	l	301	CDL	C32-C33-C34-C35
29	I	301	CDL	C19-C20-C21-C22
29	l3	301	CDL	C32-C33-C34-C35
29	I3	301	CDL	C19-C20-C21-C22
29	g	305	CDL	C31-C32-C33-C34
29	L	302	CDL	C19-C20-C21-C22
29	g3	305	CDL	C31-C32-C33-C34
29	I3	302	CDL	C19-C20-C21-C22
30	g	303	PC1	C24-C25-C26-C27
30	g3	303	PC1	C24-C25-C26-C27
29	F	303	CDL	CB4-CB6-OB8-CB7
29	F3	302	CDL	CB4-CB6-OB8-CB7
29	I3	303	CDL	C36-C37-C38-C39
29	f	303	CDL	C13-C14-C15-C16
29	g	305	CDL	C40-C41-C42-C43
29	I	302	CDL	C36-C37-C38-C39
29	f3	303	CDL	C13-C14-C15-C16
30	D	301	PC1	C29-C2A-C2B-C2C
29	k	201	CDL	C40-C41-C42-C43
29	b3	401	CDL	C42-C43-C44-C45
29	g3	305	CDL	C40-C41-C42-C43
30	D3	301	PC1	C29-C2A-C2B-C2C
29	b	401	CDL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
29	k3	201	CDL	C40-C41-C42-C43
29	F3	302	CDL	C11-C12-C13-C14
29	F	303	CDL	C11-C12-C13-C14
29	F	303	CDL	C51-C52-C53-C54
29	K	202	CDL	C77-C78-C79-C80
29	f3	302	CDL	C77-C78-C79-C80
29	f	302	CDL	C77-C78-C79-C80
29	F	303	CDL	C83-C84-C85-C86
29	F3	302	CDL	C41-C42-C43-C44
29	K3	202	CDL	C77-C78-C79-C80
29	F3	302	CDL	C51-C52-C53-C54
29	F3	302	CDL	C83-C84-C85-C86
29	J3	302	CDL	C59-C60-C61-C62
37	B2	1002	ADP	PA-O3A-PB-O1B
37	B4	1002	ADP	PA-O3A-PB-O1B
29	a	501	CDL	C31-C32-C33-C34
29	j	302	CDL	C22-C23-C24-C25
29	r	201	CDL	C58-C59-C60-C61
29	B	401	CDL	C39-C40-C41-C42
29	F	303	CDL	C41-C42-C43-C44
29	a3	501	CDL	C31-C32-C33-C34
29	i3	301	CDL	C58-C59-C60-C61
29	j3	302	CDL	C22-C23-C24-C25
29	B3	401	CDL	C59-C60-C61-C62
29	f	302	CDL	C51-C52-C53-C54
29	B	401	CDL	C59-C60-C61-C62
29	f3	302	CDL	C51-C52-C53-C54
29	J3	301	CDL	C22-C23-C24-C25
29	L	302	CDL	C31-CA7-OA8-CA6
29	I3	302	CDL	C31-CA7-OA8-CA6
29	J	301	CDL	C22-C23-C24-C25
30	D	301	PC1	C39-C3A-C3B-C3C
29	b	401	CDL	C38-C39-C40-C41
29	j	302	CDL	C20-C21-C22-C23
29	B	402	CDL	C74-C75-C76-C77
29	J	302	CDL	C59-C60-C61-C62
29	b3	401	CDL	C38-C39-C40-C41
29	j3	302	CDL	C20-C21-C22-C23
29	B3	401	CDL	C39-C40-C41-C42
29	B3	402	CDL	C74-C75-C76-C77
29	B3	403	CDL	C52-C53-C54-C55
30	D3	301	PC1	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
30	G3	304	PC1	C27-C28-C29-C2A
29	j	302	CDL	C24-C25-C26-C27
29	j3	302	CDL	C24-C25-C26-C27
29	B	403	CDL	C52-C53-C54-C55
30	G	304	PC1	C27-C28-C29-C2A
29	B	402	CDL	CB2-C1-CA2-OA2
29	I	302	CDL	CB2-C1-CA2-OA2
29	B3	402	CDL	CB2-C1-CA2-OA2
29	I3	303	CDL	CB2-C1-CA2-OA2
29	f	304	CDL	OB5-CB3-CB4-OB6
29	i	301	CDL	OB5-CB3-CB4-OB6
29	A	502	CDL	OB5-CB3-CB4-OB6
29	L	302	CDL	OA5-CA3-CA4-OA6
29	B3	404	CDL	C79-C80-C81-C82
29	p	201	CDL	C31-CA7-OA8-CA6
29	J	302	CDL	C71-CB7-OB8-CB6
29	p3	201	CDL	C31-CA7-OA8-CA6
29	J3	302	CDL	C71-CB7-OB8-CB6
29	b	401	CDL	C11-CA5-OA6-CA4
29	b3	401	CDL	C11-CA5-OA6-CA4
29	p	201	CDL	C41-C42-C43-C44
29	p	201	CDL	C72-C73-C74-C75
29	B	404	CDL	C79-C80-C81-C82
35	J	303	PEE	C31-C32-C33-C34
29	f	302	CDL	C74-C75-C76-C77
29	f3	302	CDL	C74-C75-C76-C77
29	p3	201	CDL	C41-C42-C43-C44
29	p3	201	CDL	C72-C73-C74-C75
30	d3	301	PC1	C2A-C2B-C2C-C2D
35	L3	302	PEE	C31-C32-C33-C34
32	i	302	UQ8	C40-C39-C41-C42
32	i3	303	UQ8	C40-C39-C41-C42
29	p	201	CDL	C64-C65-C66-C67
29	f	302	CDL	C33-C34-C35-C36
29	f	303	CDL	C38-C39-C40-C41
29	A	502	CDL	C60-C61-C62-C63
29	F	302	CDL	C80-C81-C82-C83
29	a3	502	CDL	C80-C81-C82-C83
29	f3	302	CDL	C33-C34-C35-C36
29	f3	303	CDL	C38-C39-C40-C41
30	d	301	PC1	C2A-C2B-C2C-C2D
30	g	304	PC1	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
30	g3	304	PC1	C33-C34-C35-C36
29	a	501	CDL	C72-C73-C74-C75
29	p	201	CDL	C63-C64-C65-C66
29	a3	501	CDL	C72-C73-C74-C75
29	b3	401	CDL	C71-C72-C73-C74
29	j3	302	CDL	C16-C17-C18-C19
29	p3	201	CDL	C63-C64-C65-C66
29	p3	201	CDL	C64-C65-C66-C67
29	b	401	CDL	C71-C72-C73-C74
29	j	302	CDL	C16-C17-C18-C19
35	A	501	PEE	C33-C34-C35-C36
35	l3	302	PEE	C33-C34-C35-C36
30	G	303	PC1	C3F-C3G-C3H-C3I
29	f	302	CDL	C58-C59-C60-C61
29	l	302	CDL	C31-CA7-OA8-CA6
29	B	402	CDL	C71-CB7-OB8-CB6
29	l3	303	CDL	C31-CA7-OA8-CA6
29	B3	402	CDL	C71-CB7-OB8-CB6
29	I	301	CDL	CB4-CB6-OB8-CB7
30	D3	301	PC1	C3F-C3G-C3H-C3I
30	G3	303	PC1	C3F-C3G-C3H-C3I
29	f3	302	CDL	C58-C59-C60-C61
29	A3	501	CDL	C60-C61-C62-C63
30	D	301	PC1	C3F-C3G-C3H-C3I
29	B	401	CDL	C32-C31-CA7-OA8
29	B3	401	CDL	C32-C31-CA7-OA8
29	a	501	CDL	C11-C12-C13-C14
29	I	301	CDL	C17-C18-C19-C20
29	a3	501	CDL	C11-C12-C13-C14
30	G	303	PC1	C22-C23-C24-C25
30	g	303	PC1	C3F-C3G-C3H-C3I
29	F	303	CDL	C74-C75-C76-C77
29	F3	302	CDL	C74-C75-C76-C77
29	I3	301	CDL	C17-C18-C19-C20
30	g3	303	PC1	C3F-C3G-C3H-C3I
29	I	301	CDL	C53-C54-C55-C56
29	I	302	CDL	C81-C82-C83-C84
29	J	302	CDL	C18-C19-C20-C21
29	a3	502	CDL	C58-C59-C60-C61
30	G3	303	PC1	C22-C23-C24-C25
30	G	303	PC1	C31-C32-C33-C34
29	g	305	CDL	C79-C80-C81-C82

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Mol	Chain	Res	Type	Atoms
29	F	302	CDL	C58-C59-C60-C61
29	g3	305	CDL	C79-C80-C81-C82
29	J3	302	CDL	C18-C19-C20-C21
29	B3	401	CDL	C31-CA7-OA8-CA6
29	I3	301	CDL	CB4-CB6-OB8-CB7
29	f	302	CDL	C44-C45-C46-C47
29	f3	302	CDL	C44-C45-C46-C47
29	r	201	CDL	C74-C75-C76-C77
29	i3	301	CDL	C74-C75-C76-C77
29	I3	301	CDL	C53-C54-C55-C56
29	L	302	CDL	C51-CB5-OB6-CB4
29	I3	302	CDL	C51-CB5-OB6-CB4
29	F	302	CDL	C24-C25-C26-C27
29	a3	502	CDL	C24-C25-C26-C27
29	l	302	CDL	C76-C77-C78-C79
29	I3	303	CDL	C81-C82-C83-C84
30	g	304	PC1	C27-C28-C29-C2A
29	f	304	CDL	C35-C36-C37-C38
29	f3	304	CDL	C35-C36-C37-C38
29	l3	303	CDL	C76-C77-C78-C79
29	p	201	CDL	CA7-C31-C32-C33
29	p3	201	CDL	CA7-C31-C32-C33
30	G3	303	PC1	C31-C32-C33-C34
29	J3	301	CDL	C78-C79-C80-C81
32	I	303	UQ8	C30-C29-C31-C32
32	I3	304	UQ8	C30-C29-C31-C32
29	J	301	CDL	C78-C79-C80-C81
29	B	401	CDL	C31-CA7-OA8-CA6
29	K	201	CDL	C78-C79-C80-C81
29	A3	501	CDL	C38-C39-C40-C41
29	K3	201	CDL	C78-C79-C80-C81
30	g3	304	PC1	C27-C28-C29-C2A
29	A	502	CDL	C38-C39-C40-C41
29	B	403	CDL	C1-CB2-OB2-PB2
29	B3	403	CDL	C1-CB2-OB2-PB2
29	a	501	CDL	C16-C17-C18-C19
29	f	302	CDL	C36-C37-C38-C39
29	f3	303	CDL	C73-C74-C75-C76
29	f	302	CDL	C84-C85-C86-C87
29	f3	302	CDL	C84-C85-C86-C87
29	j	301	CDL	C12-C13-C14-C15
29	K	202	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
29	L	302	CDL	C59-C60-C61-C62
29	a3	501	CDL	C16-C17-C18-C19
29	f3	302	CDL	C36-C37-C38-C39
29	j3	301	CDL	C12-C13-C14-C15
29	I3	303	CDL	C58-C59-C60-C61
29	f	302	CDL	OA5-CA3-CA4-CA6
29	i	301	CDL	OB5-CB3-CB4-CB6
29	r	201	CDL	OA5-CA3-CA4-CA6
29	B	401	CDL	OB5-CB3-CB4-CB6
29	B	404	CDL	OA5-CA3-CA4-CA6
29	I	301	CDL	OA5-CA3-CA4-CA6
29	L	302	CDL	OA5-CA3-CA4-CA6
29	P	201	CDL	OB5-CB3-CB4-CB6
29	f3	302	CDL	OA5-CA3-CA4-CA6
29	i3	302	CDL	OB5-CB3-CB4-CB6
29	B3	404	CDL	OA5-CA3-CA4-CA6
29	I3	302	CDL	OA5-CA3-CA4-CA6
35	m	301	PEE	O3P-C1-C2-C3
35	J	303	PEE	O3P-C1-C2-C3
29	f	303	CDL	C58-C59-C60-C61
29	F	302	CDL	C41-C42-C43-C44
29	J	301	CDL	C12-C13-C14-C15
29	f3	303	CDL	C58-C59-C60-C61
29	B3	404	CDL	C77-C78-C79-C80
29	I3	302	CDL	C59-C60-C61-C62
29	K3	202	CDL	C51-C52-C53-C54
29	J3	301	CDL	C12-C13-C14-C15
29	L3	301	CDL	C44-C45-C46-C47
29	I	302	CDL	C58-C59-C60-C61
29	k3	201	CDL	C38-C39-C40-C41
29	L	301	CDL	C44-C45-C46-C47
29	f	303	CDL	C73-C74-C75-C76
29	k	201	CDL	C38-C39-C40-C41
29	B	404	CDL	C77-C78-C79-C80
29	L	302	CDL	CA7-C31-C32-C33
29	I3	302	CDL	CA7-C31-C32-C33
33	C4	601	ATP	O4'-C4'-C5'-O5'
33	C4	601	ATP	C3'-C4'-C5'-O5'
29	a3	502	CDL	C41-C42-C43-C44
29	L3	301	CDL	C16-C17-C18-C19
29	B	401	CDL	C84-C85-C86-C87
29	B3	401	CDL	C84-C85-C86-C87

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Mol	Chain	Res	Type	Atoms
29	L	301	CDL	C16-C17-C18-C19
30	g	304	PC1	C23-C24-C25-C26
30	g3	304	PC1	C23-C24-C25-C26
29	L	301	CDL	C33-C34-C35-C36
32	I	303	UQ8	C38-C39-C41-C42
29	L3	301	CDL	C33-C34-C35-C36
29	L	302	CDL	OA9-CA7-OA8-CA6
29	I3	302	CDL	OA9-CA7-OA8-CA6
29	r	201	CDL	C52-C53-C54-C55
29	L	302	CDL	C11-C12-C13-C14
29	I3	302	CDL	C11-C12-C13-C14
29	A	502	CDL	CB2-C1-CA2-OA2
29	A3	501	CDL	CB2-C1-CA2-OA2
29	i3	301	CDL	C52-C53-C54-C55
29	i3	302	CDL	C22-C23-C24-C25
29	j	301	CDL	CB3-CB4-CB6-OB8
29	I	301	CDL	CB3-CB4-CB6-OB8
29	J	302	CDL	CA3-CA4-CA6-OA8
29	I3	301	CDL	CB3-CB4-CB6-OB8
29	I3	303	CDL	CB3-CB4-CB6-OB8
29	K3	202	CDL	CB3-CB4-CB6-OB8
30	g	303	PC1	C1-C2-C3-O31
30	G	303	PC1	C1-C2-C3-O31
30	d3	301	PC1	C1-C2-C3-O31
30	g3	303	PC1	C1-C2-C3-O31
30	G3	303	PC1	C1-C2-C3-O31
35	J	303	PEE	C1-C2-C3-O3
35	L3	302	PEE	C1-C2-C3-O3
29	i	301	CDL	C22-C23-C24-C25
30	G	304	PC1	C2F-C2G-C2H-C2I
30	G3	304	PC1	C2F-C2G-C2H-C2I
29	k	201	CDL	C16-C17-C18-C19
29	j3	301	CDL	C74-C75-C76-C77
30	G	304	PC1	C3D-C3E-C3F-C3G
29	j	301	CDL	C74-C75-C76-C77
29	k3	201	CDL	C16-C17-C18-C19
29	J3	301	CDL	C74-C75-C76-C77
30	G3	304	PC1	C3D-C3E-C3F-C3G
29	k3	201	CDL	CB4-CB6-OB8-CB7
29	j3	302	CDL	CB5-C51-C52-C53
29	J	301	CDL	C74-C75-C76-C77
32	I	303	UQ8	C28-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
32	I3	304	UQ8	C38-C39-C41-C42
29	p	201	CDL	C61-C62-C63-C64
35	a3	503	PEE	C14-C15-C16-C17
29	b	401	CDL	OA5-CA3-CA4-OA6
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	B	403	CDL	OB5-CB3-CB4-OB6
29	F	302	CDL	OA5-CA3-CA4-OA6
29	F	302	CDL	OB5-CB3-CB4-OB6
29	F	303	CDL	OB5-CB3-CB4-OB6
29	a3	502	CDL	OA5-CA3-CA4-OA6
29	a3	502	CDL	OB5-CB3-CB4-OB6
29	b3	401	CDL	OA5-CA3-CA4-OA6
29	f3	302	CDL	OA5-CA3-CA4-OA6
29	A3	501	CDL	OB5-CB3-CB4-OB6
29	B3	403	CDL	OA5-CA3-CA4-OA6
29	I3	302	CDL	OA5-CA3-CA4-OA6
35	L3	302	PEE	O3P-C1-C2-O2
29	l	302	CDL	C58-C59-C60-C61
35	L	303	PEE	C14-C15-C16-C17
29	K	202	CDL	C64-C65-C66-C67
29	l3	303	CDL	C58-C59-C60-C61
29	B3	404	CDL	C32-C33-C34-C35
29	L	302	CDL	CA4-CA3-OA5-PA1
29	I3	302	CDL	CA4-CA3-OA5-PA1
29	K3	202	CDL	C64-C65-C66-C67
29	j	302	CDL	CB5-C51-C52-C53
29	f	304	CDL	C40-C41-C42-C43
29	i	301	CDL	C51-C52-C53-C54
29	B	404	CDL	C32-C33-C34-C35
29	a3	501	CDL	C13-C14-C15-C16
29	f3	304	CDL	C63-C64-C65-C66
29	p3	201	CDL	C61-C62-C63-C64
29	a	501	CDL	C13-C14-C15-C16
29	f	304	CDL	C63-C64-C65-C66
29	p	201	CDL	C59-C60-C61-C62
29	K	201	CDL	C52-C53-C54-C55
29	f3	304	CDL	C40-C41-C42-C43
29	K3	201	CDL	C52-C53-C54-C55
29	l	302	CDL	C64-C65-C66-C67
29	l3	303	CDL	C64-C65-C66-C67

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Mol	Chain	Res	Type	Atoms
29	F	302	CDL	C52-C53-C54-C55
29	a	501	CDL	OB6-CB4-CB6-OB8
29	r	201	CDL	OB6-CB4-CB6-OB8
29	F	303	CDL	OA6-CA4-CA6-OA8
29	I	301	CDL	OB6-CB4-CB6-OB8
29	I	302	CDL	OB6-CB4-CB6-OB8
29	K	201	CDL	OA6-CA4-CA6-OA8
29	a3	501	CDL	OB6-CB4-CB6-OB8
29	i3	301	CDL	OB6-CB4-CB6-OB8
29	F3	302	CDL	OA6-CA4-CA6-OA8
29	I3	301	CDL	OB6-CB4-CB6-OB8
29	I3	303	CDL	OB6-CB4-CB6-OB8
30	d	301	PC1	O21-C2-C3-O31
30	d3	301	PC1	O21-C2-C3-O31
29	p3	201	CDL	C59-C60-C61-C62
29	i3	302	CDL	C51-C52-C53-C54
29	L3	301	CDL	C61-C62-C63-C64
29	k3	201	CDL	C24-C25-C26-C27
29	B	402	CDL	C40-C41-C42-C43
29	I	301	CDL	C21-C22-C23-C24
29	l3	301	CDL	C44-C45-C46-C47
29	i3	301	CDL	C35-C36-C37-C38
29	l3	303	CDL	C77-C78-C79-C80
29	I3	301	CDL	C21-C22-C23-C24
29	A	502	CDL	CA7-C31-C32-C33
29	k	201	CDL	C24-C25-C26-C27
29	l	301	CDL	C44-C45-C46-C47
29	p	201	CDL	OA9-CA7-OA8-CA6
29	l	301	CDL	C11-C12-C13-C14
29	l	302	CDL	C77-C78-C79-C80
29	r	201	CDL	C35-C36-C37-C38
29	a3	502	CDL	C52-C53-C54-C55
29	j3	301	CDL	C61-C62-C63-C64
35	A	501	PEE	C14-C15-C16-C17
32	I3	304	UQ8	C28-C29-C31-C32
35	L	303	PEE	C44-C45-C46-C47
35	a3	503	PEE	C44-C45-C46-C47
29	f	303	CDL	C79-C80-C81-C82
29	L	301	CDL	C61-C62-C63-C64
29	l3	301	CDL	C11-C12-C13-C14
29	B3	403	CDL	C57-C58-C59-C60
35	l3	302	PEE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	k	201	CDL	CB4-CB6-OB8-CB7
29	k	201	CDL	C54-C55-C56-C57
29	j	301	CDL	C61-C62-C63-C64
29	B	403	CDL	C57-C58-C59-C60
29	B	404	CDL	C74-C75-C76-C77
29	P	201	CDL	C58-C59-C60-C61
29	f3	303	CDL	C79-C80-C81-C82
29	B3	404	CDL	C74-C75-C76-C77
35	J	303	PEE	C34-C35-C36-C37
35	L3	302	PEE	C34-C35-C36-C37
29	A3	501	CDL	CA7-C31-C32-C33
29	f	303	CDL	C16-C17-C18-C19
29	I	301	CDL	C76-C77-C78-C79
29	k3	201	CDL	C54-C55-C56-C57
29	j3	301	CDL	C80-C81-C82-C83
29	I3	301	CDL	C76-C77-C78-C79
29	P3	201	CDL	C58-C59-C60-C61
29	F3	302	CDL	C11-CA5-OA6-CA4
29	f3	303	CDL	C16-C17-C18-C19
29	j	301	CDL	C80-C81-C82-C83
35	l3	302	PEE	C35-C36-C37-C38
29	B3	402	CDL	C40-C41-C42-C43
36	e	900	NAD	PA-O3-PN-O5D
36	E	900	NAD	PA-O3-PN-O5D
36	e3	900	NAD	PA-O3-PN-O5D
36	E3	900	NAD	PA-O3-PN-O5D
29	p3	201	CDL	OA9-CA7-OA8-CA6
29	l	301	CDL	C24-C25-C26-C27
29	l3	301	CDL	C24-C25-C26-C27
29	r	201	CDL	C16-C17-C18-C19
29	i3	301	CDL	C16-C17-C18-C19
29	p3	201	CDL	C23-C24-C25-C26
29	p	201	CDL	C23-C24-C25-C26
29	r	201	CDL	C64-C65-C66-C67
29	i3	301	CDL	C64-C65-C66-C67
32	I	303	UQ8	C15-C14-C16-C17
32	I3	304	UQ8	C15-C14-C16-C17
29	k	201	CDL	C75-C76-C77-C78
29	l3	301	CDL	C62-C63-C64-C65
29	f	302	CDL	C72-C71-CB7-OB8
29	f3	302	CDL	C72-C71-CB7-OB8
29	i3	302	CDL	C84-C85-C86-C87

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Mol	Chain	Res	Type	Atoms
29	p	201	CDL	C51-CB5-OB6-CB4
29	F	303	CDL	C11-CA5-OA6-CA4
29	p3	201	CDL	C51-CB5-OB6-CB4
29	i	301	CDL	C84-C85-C86-C87
29	B3	401	CDL	C12-C13-C14-C15
29	a3	502	CDL	CA7-C31-C32-C33
29	B	401	CDL	C12-C13-C14-C15
29	k3	201	CDL	C75-C76-C77-C78
29	j3	301	CDL	C52-C53-C54-C55
29	j	301	CDL	C52-C53-C54-C55
29	l	301	CDL	C62-C63-C64-C65
29	F3	302	CDL	C40-C41-C42-C43
29	l	302	CDL	OA9-CA7-OA8-CA6
29	J	302	CDL	OB9-CB7-OB8-CB6
29	l3	303	CDL	OA9-CA7-OA8-CA6
29	J3	302	CDL	OB9-CB7-OB8-CB6
29	p	201	CDL	C71-CB7-OB8-CB6
29	L	302	CDL	C71-CB7-OB8-CB6
29	p3	201	CDL	C71-CB7-OB8-CB6
29	l3	302	CDL	C71-CB7-OB8-CB6
29	F	303	CDL	C40-C41-C42-C43
29	a	501	CDL	C33-C34-C35-C36
29	i	301	CDL	C41-C42-C43-C44
29	f	302	CDL	OB5-CB3-CB4-CB6
29	f	304	CDL	OB5-CB3-CB4-CB6
29	g	305	CDL	OA5-CA3-CA4-CA6
29	j	301	CDL	OA5-CA3-CA4-CA6
29	A	502	CDL	OB5-CB3-CB4-CB6
29	B	403	CDL	OB5-CB3-CB4-CB6
29	J	301	CDL	OA5-CA3-CA4-CA6
29	f3	302	CDL	OB5-CB3-CB4-CB6
29	g3	305	CDL	OA5-CA3-CA4-CA6
29	l3	301	CDL	OA5-CA3-CA4-CA6
29	J3	301	CDL	OA5-CA3-CA4-CA6
30	G	303	PC1	O11-C1-C2-C3
30	G3	304	PC1	O11-C1-C2-C3
29	a3	501	CDL	C33-C34-C35-C36
29	b	401	CDL	C23-C24-C25-C26
29	J	302	CDL	C72-C73-C74-C75
29	F	302	CDL	CA7-C31-C32-C33
29	f	303	CDL	C11-C12-C13-C14
29	i3	302	CDL	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
30	D	301	PC1	C32-C33-C34-C35
30	D3	301	PC1	C32-C33-C34-C35
29	f	303	CDL	C12-C13-C14-C15
29	k	201	CDL	C22-C23-C24-C25
29	B	402	CDL	C63-C64-C65-C66
29	b3	401	CDL	C23-C24-C25-C26
29	B3	402	CDL	C63-C64-C65-C66
29	k3	201	CDL	C22-C23-C24-C25
29	B	402	CDL	OB9-CB7-OB8-CB6
29	B3	402	CDL	OB9-CB7-OB8-CB6
29	f3	303	CDL	C11-C12-C13-C14
30	d3	301	PC1	C33-C34-C35-C36
29	b3	401	CDL	OA7-CA5-OA6-CA4
29	l	301	CDL	C40-C41-C42-C43
29	f3	303	CDL	C12-C13-C14-C15
29	l3	301	CDL	C40-C41-C42-C43
30	d	301	PC1	C33-C34-C35-C36
32	i	302	UQ8	C15-C14-C16-C17
32	i3	303	UQ8	C15-C14-C16-C17
29	l	302	CDL	C32-C31-CA7-OA8
29	B	402	CDL	C32-C31-CA7-OA8
29	l3	303	CDL	C32-C31-CA7-OA8
29	l3	301	CDL	C75-C76-C77-C78
29	l	301	CDL	C75-C76-C77-C78
29	J3	302	CDL	C72-C73-C74-C75
29	j	302	CDL	CA6-CA4-OA6-CA5
29	B	401	CDL	CA3-CA4-OA6-CA5
29	B	403	CDL	CA6-CA4-OA6-CA5
29	F	302	CDL	CA6-CA4-OA6-CA5
29	I	301	CDL	CA6-CA4-OA6-CA5
29	J	302	CDL	CA6-CA4-OA6-CA5
29	i3	301	CDL	CA6-CA4-OA6-CA5
29	j3	302	CDL	CA6-CA4-OA6-CA5
29	B3	401	CDL	CA3-CA4-OA6-CA5
29	B3	403	CDL	CA6-CA4-OA6-CA5
29	I3	301	CDL	CA6-CA4-OA6-CA5
29	J3	302	CDL	CA6-CA4-OA6-CA5
29	B	401	CDL	OA9-CA7-OA8-CA6
29	F	303	CDL	C57-C58-C59-C60
29	J3	302	CDL	C41-C42-C43-C44
35	A	501	PEE	C35-C36-C37-C38
35	L	303	PEE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
35	a3	503	PEE	C35-C36-C37-C38
29	A	502	CDL	C84-C85-C86-C87
29	j3	302	CDL	C34-C35-C36-C37
29	F3	302	CDL	C57-C58-C59-C60
29	l	301	CDL	C61-C62-C63-C64
29	J	302	CDL	C41-C42-C43-C44
30	G	304	PC1	C37-C38-C39-C3A
30	G3	304	PC1	C37-C38-C39-C3A
29	A3	501	CDL	C84-C85-C86-C87
29	i3	302	CDL	C31-C32-C33-C34
29	l3	301	CDL	C61-C62-C63-C64
29	B3	401	CDL	OA9-CA7-OA8-CA6
29	f	304	CDL	O1-C1-CA2-OA2
29	A	502	CDL	O1-C1-CA2-OA2
29	f3	304	CDL	O1-C1-CA2-OA2
29	A3	501	CDL	O1-C1-CA2-OA2
29	i	301	CDL	C31-C32-C33-C34
29	J3	301	CDL	C82-C83-C84-C85
29	j	302	CDL	C34-C35-C36-C37
29	J	301	CDL	C82-C83-C84-C85
35	m	301	PEE	C40-C41-C42-C43
29	b	401	CDL	OA7-CA5-OA6-CA4
29	L	302	CDL	OB7-CB5-OB6-CB4
29	I3	302	CDL	OB7-CB5-OB6-CB4
29	B3	402	CDL	C32-C31-CA7-OA8
29	f	302	CDL	OB5-CB3-CB4-OB6
29	r	201	CDL	OA5-CA3-CA4-OA6
29	B	401	CDL	OB5-CB3-CB4-OB6
29	B	404	CDL	OA5-CA3-CA4-OA6
29	I	302	CDL	OB5-CB3-CB4-OB6
29	J	301	CDL	OA5-CA3-CA4-OA6
29	f3	304	CDL	OB5-CB3-CB4-OB6
29	i3	301	CDL	OA5-CA3-CA4-OA6
29	j3	301	CDL	OA5-CA3-CA4-OA6
29	j3	301	CDL	OB5-CB3-CB4-OB6
29	B3	403	CDL	OB5-CB3-CB4-OB6
29	B3	404	CDL	OA5-CA3-CA4-OA6
29	F3	302	CDL	OB5-CB3-CB4-OB6
29	I3	301	CDL	OA5-CA3-CA4-OA6
29	I3	303	CDL	OB5-CB3-CB4-OB6
29	J3	301	CDL	OA5-CA3-CA4-OA6
29	P3	201	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
30	G	303	PC1	O11-C1-C2-O21
35	J	303	PEE	O3P-C1-C2-O2
29	b	401	CDL	C75-C76-C77-C78
29	b3	401	CDL	C75-C76-C77-C78
35	j3	303	PEE	C40-C41-C42-C43
29	k	201	CDL	CB3-CB4-CB6-OB8
29	j	302	CDL	CA3-CA4-CA6-OA8
29	p	201	CDL	CA3-CA4-CA6-OA8
29	F	303	CDL	CB3-CB4-CB6-OB8
29	K	202	CDL	CB3-CB4-CB6-OB8
29	a3	501	CDL	CB3-CB4-CB6-OB8
29	f3	304	CDL	CA3-CA4-CA6-OA8
29	k3	201	CDL	CB3-CB4-CB6-OB8
29	j3	301	CDL	CB3-CB4-CB6-OB8
29	f	304	CDL	C78-C79-C80-C81
29	i3	301	CDL	C20-C21-C22-C23
29	B3	403	CDL	C72-C73-C74-C75
29	f3	304	CDL	C78-C79-C80-C81
32	i	302	UQ8	C38-C39-C41-C42
32	i	302	UQ8	C13-C14-C16-C17
32	I	303	UQ8	C13-C14-C16-C17
32	i3	303	UQ8	C13-C14-C16-C17
32	I3	304	UQ8	C13-C14-C16-C17
29	B	403	CDL	C72-C73-C74-C75
29	k	201	CDL	OB6-CB4-CB6-OB8
29	j	301	CDL	OB6-CB4-CB6-OB8
29	A	502	CDL	OB6-CB4-CB6-OB8
29	k3	201	CDL	OB6-CB4-CB6-OB8
29	j3	302	CDL	OA6-CA4-CA6-OA8
29	K3	202	CDL	OB6-CB4-CB6-OB8
29	J3	302	CDL	OA6-CA4-CA6-OA8
29	J3	302	CDL	OB6-CB4-CB6-OB8
29	P3	201	CDL	OA6-CA4-CA6-OA8
30	g	303	PC1	O21-C2-C3-O31
30	G	303	PC1	O21-C2-C3-O31
30	g3	303	PC1	O21-C2-C3-O31
30	G3	303	PC1	O21-C2-C3-O31
29	K	202	CDL	C81-C82-C83-C84
29	B3	402	CDL	C33-C34-C35-C36
29	K3	202	CDL	C81-C82-C83-C84
29	I3	302	CDL	C72-C71-CB7-OB8
29	r	201	CDL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
29	I	301	CDL	C22-C23-C24-C25
29	A3	501	CDL	C34-C35-C36-C37
30	G	303	PC1	C3E-C3F-C3G-C3H
30	G3	303	PC1	C3E-C3F-C3G-C3H
29	L	302	CDL	OB9-CB7-OB8-CB6
29	j	301	CDL	C63-C64-C65-C66
29	l	301	CDL	C80-C81-C82-C83
29	A	502	CDL	C34-C35-C36-C37
29	I3	301	CDL	C22-C23-C24-C25
29	B	402	CDL	C33-C34-C35-C36
29	j3	301	CDL	C63-C64-C65-C66
29	j	302	CDL	CA5-C11-C12-C13
29	J	301	CDL	CA5-C11-C12-C13
29	j3	302	CDL	CA5-C11-C12-C13
29	J3	301	CDL	CA5-C11-C12-C13
29	f3	304	CDL	C39-C40-C41-C42
29	I3	302	CDL	OB9-CB7-OB8-CB6
29	B	401	CDL	C56-C57-C58-C59
29	l3	301	CDL	C80-C81-C82-C83
29	L3	301	CDL	C77-C78-C79-C80
29	L	302	CDL	C72-C71-CB7-OB8
29	g	305	CDL	C83-C84-C85-C86
29	L	301	CDL	C77-C78-C79-C80
29	f3	304	CDL	C13-C14-C15-C16
29	g3	305	CDL	C83-C84-C85-C86
30	G	304	PC1	C3B-C3C-C3D-C3E
29	F	302	CDL	CB4-CB3-OB5-PB2
29	f	304	CDL	C13-C14-C15-C16
29	P	201	CDL	C11-C12-C13-C14
36	e	900	NAD	C2B-C1B-N9A-C8A
36	e3	900	NAD	C2B-C1B-N9A-C8A
29	f	304	CDL	C39-C40-C41-C42
29	f	304	CDL	C54-C55-C56-C57
29	F3	302	CDL	C72-C73-C74-C75
30	g	304	PC1	O13-C11-C12-N
30	G	304	PC1	O13-C11-C12-N
30	g3	304	PC1	O13-C11-C12-N
30	G3	304	PC1	O13-C11-C12-N
29	P3	201	CDL	C11-C12-C13-C14
30	G3	304	PC1	C3B-C3C-C3D-C3E
29	i	301	CDL	C72-C71-CB7-OB8
29	f3	304	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
29	F	303	CDL	OA7-CA5-OA6-CA4
29	F3	302	CDL	OA7-CA5-OA6-CA4
29	i	301	CDL	O1-C1-CA2-OA2
29	i3	302	CDL	O1-C1-CA2-OA2
29	F	303	CDL	C72-C73-C74-C75
29	L	302	CDL	C78-C79-C80-C81
29	B3	401	CDL	C56-C57-C58-C59
29	B	403	CDL	CB5-C51-C52-C53
29	B3	403	CDL	CB5-C51-C52-C53
30	G	303	PC1	C35-C36-C37-C38
35	A	501	PEE	C43-C44-C45-C46
35	l3	302	PEE	C43-C44-C45-C46
29	I3	302	CDL	C78-C79-C80-C81
30	G3	303	PC1	C35-C36-C37-C38
30	D	301	PC1	C2A-C2B-C2C-C2D
30	D3	301	PC1	C2A-C2B-C2C-C2D
29	j	301	CDL	CB5-C51-C52-C53
29	j3	301	CDL	CB5-C51-C52-C53
29	J	301	CDL	C72-C71-CB7-OB8
29	i3	302	CDL	C72-C71-CB7-OB8
29	J3	301	CDL	C72-C71-CB7-OB8
29	I	302	CDL	C20-C21-C22-C23
32	i3	303	UQ8	C38-C39-C41-C42
29	i3	301	CDL	C33-C34-C35-C36
29	I3	303	CDL	C20-C21-C22-C23
29	f3	304	CDL	C51-C52-C53-C54
29	p	201	CDL	OB9-CB7-OB8-CB6
29	r	201	CDL	C33-C34-C35-C36
29	f	304	CDL	C51-C52-C53-C54
29	F	302	CDL	OB5-CB3-CB4-CB6
29	a3	502	CDL	OB5-CB3-CB4-CB6
29	f3	304	CDL	OB5-CB3-CB4-CB6
29	A3	501	CDL	OB5-CB3-CB4-CB6
29	B3	401	CDL	OB5-CB3-CB4-CB6
29	B3	403	CDL	OA5-CA3-CA4-CA6
29	B3	403	CDL	OB5-CB3-CB4-CB6
30	g	304	PC1	O11-C1-C2-C3
30	G	304	PC1	O11-C1-C2-C3
29	f	304	CDL	C42-C43-C44-C45
29	f3	304	CDL	C42-C43-C44-C45
29	f	302	CDL	C31-C32-C33-C34
29	f3	302	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
29	I	301	CDL	C39-C40-C41-C42
29	I3	301	CDL	C39-C40-C41-C42
29	i	301	CDL	C57-C58-C59-C60
29	a3	502	CDL	C75-C76-C77-C78
29	p3	201	CDL	OB9-CB7-OB8-CB6
29	F	302	CDL	C75-C76-C77-C78
33	C1	601	ATP	C3'-C4'-C5'-O5'
29	A	502	CDL	C71-CB7-OB8-CB6
29	A3	501	CDL	C71-CB7-OB8-CB6
29	B	404	CDL	C22-C23-C24-C25
29	i3	302	CDL	C57-C58-C59-C60
29	B3	401	CDL	C72-C73-C74-C75
29	B3	404	CDL	C22-C23-C24-C25
29	I3	303	CDL	C38-C39-C40-C41
29	B	401	CDL	C72-C73-C74-C75
29	I	302	CDL	C38-C39-C40-C41
29	f	304	CDL	CA4-CA3-OA5-PA1
29	a3	502	CDL	CB4-CB3-OB5-PB2
29	f3	304	CDL	CA4-CA3-OA5-PA1
30	G	303	PC1	C2-C1-O11-P
30	G3	303	PC1	C2-C1-O11-P
29	p3	201	CDL	C39-C40-C41-C42
29	L3	301	CDL	C76-C77-C78-C79
29	p	201	CDL	C39-C40-C41-C42
29	L	301	CDL	C76-C77-C78-C79
30	G3	303	PC1	C2F-C2G-C2H-C2I
29	p	201	CDL	OB7-CB5-OB6-CB4
29	l3	303	CDL	OA7-CA5-OA6-CA4
29	p3	201	CDL	OB7-CB5-OB6-CB4
29	j	301	CDL	OA5-CA3-CA4-OA6
29	P	201	CDL	OB5-CB3-CB4-OB6
29	f3	302	CDL	OB5-CB3-CB4-OB6
29	B3	401	CDL	OB5-CB3-CB4-OB6
30	G	304	PC1	O11-C1-C2-O21
35	m	301	PEE	O3P-C1-C2-O2
30	G	303	PC1	C2F-C2G-C2H-C2I
29	g	305	CDL	C15-C16-C17-C18
29	g3	305	CDL	C15-C16-C17-C18
29	k	201	CDL	C57-C58-C59-C60
35	L	303	PEE	C12-C13-C14-C15
35	a3	503	PEE	C12-C13-C14-C15
29	j	301	CDL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
29	K	202	CDL	C61-C62-C63-C64
29	j3	301	CDL	C18-C19-C20-C21
29	b3	401	CDL	CA7-C31-C32-C33
29	k3	201	CDL	C57-C58-C59-C60
29	K3	202	CDL	C61-C62-C63-C64
29	J3	302	CDL	C20-C21-C22-C23
29	J	302	CDL	C20-C21-C22-C23
29	l	302	CDL	OA7-CA5-OA6-CA4
29	b	401	CDL	OB6-CB4-CB6-OB8
29	f	304	CDL	OA6-CA4-CA6-OA8
29	J	301	CDL	OB6-CB4-CB6-OB8
29	J	302	CDL	OA6-CA4-CA6-OA8
29	b3	401	CDL	OB6-CB4-CB6-OB8
29	f3	304	CDL	OA6-CA4-CA6-OA8
29	A3	501	CDL	OB6-CB4-CB6-OB8
29	K3	201	CDL	OA6-CA4-CA6-OA8
29	J3	301	CDL	OB6-CB4-CB6-OB8
30	D	301	PC1	O21-C2-C3-O31
30	D3	301	PC1	O21-C2-C3-O31
29	B	404	CDL	C72-C73-C74-C75
30	d3	301	PC1	C3C-C3D-C3E-C3F
29	f	304	CDL	CA3-CA4-CA6-OA8
29	g	305	CDL	CB3-CB4-CB6-OB8
29	K	201	CDL	CA3-CA4-CA6-OA8
29	P	201	CDL	CA3-CA4-CA6-OA8
29	g3	305	CDL	CB3-CB4-CB6-OB8
29	F3	302	CDL	CB3-CB4-CB6-OB8
29	B3	404	CDL	C72-C73-C74-C75
29	B	403	CDL	C19-C20-C21-C22
29	F	303	CDL	C43-C44-C45-C46
29	b	401	CDL	CA7-C31-C32-C33
29	K3	202	CDL	C31-C32-C33-C34
29	L3	301	CDL	C11-C12-C13-C14
29	l3	303	CDL	C11-CA5-OA6-CA4
29	F3	302	CDL	C43-C44-C45-C46
29	b	401	CDL	O1-C1-CB2-OB2
29	b3	401	CDL	O1-C1-CB2-OB2
29	L	301	CDL	C11-C12-C13-C14
29	B3	403	CDL	C19-C20-C21-C22
30	d	301	PC1	C3C-C3D-C3E-C3F
29	K	202	CDL	C31-C32-C33-C34
29	j	301	CDL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
29	K	202	CDL	C17-C18-C19-C20
29	j3	301	CDL	C34-C35-C36-C37
29	K3	202	CDL	C17-C18-C19-C20
29	b	401	CDL	CA3-OA5-PA1-OA2
29	b	401	CDL	CA3-OA5-PA1-OA3
29	b	401	CDL	CB3-OB5-PB2-OB3
29	f	302	CDL	CA2-OA2-PA1-OA5
29	f	303	CDL	CB2-OB2-PB2-OB3
29	f	303	CDL	CB2-OB2-PB2-OB4
29	f	303	CDL	CB2-OB2-PB2-OB5
29	f	304	CDL	CA2-OA2-PA1-OA3
29	i	301	CDL	CB3-OB5-PB2-OB3
29	k	201	CDL	CB2-OB2-PB2-OB3
29	g	305	CDL	CA2-OA2-PA1-OA3
29	j	301	CDL	CA2-OA2-PA1-OA3
29	l	301	CDL	CB3-OB5-PB2-OB2
29	l	301	CDL	CB3-OB5-PB2-OB3
29	l	301	CDL	CB3-OB5-PB2-OB4
29	l	302	CDL	CA3-OA5-PA1-OA2
29	l	302	CDL	CA3-OA5-PA1-OA4
29	l	302	CDL	CB3-OB5-PB2-OB2
29	l	302	CDL	CB3-OB5-PB2-OB4
29	p	201	CDL	CA3-OA5-PA1-OA2
29	p	201	CDL	CA3-OA5-PA1-OA4
29	r	201	CDL	CB3-OB5-PB2-OB3
29	B	401	CDL	CB3-OB5-PB2-OB2
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	B	404	CDL	CB2-OB2-PB2-OB5
29	F	302	CDL	CA3-OA5-PA1-OA2
29	F	302	CDL	CA3-OA5-PA1-OA4
29	F	303	CDL	CA2-OA2-PA1-OA4
29	F	303	CDL	CB2-OB2-PB2-OB4
29	I	301	CDL	CB2-OB2-PB2-OB3
29	I	301	CDL	CB2-OB2-PB2-OB4
29	I	301	CDL	CB2-OB2-PB2-OB5
29	K	201	CDL	CB2-OB2-PB2-OB3
29	K	201	CDL	CB3-OB5-PB2-OB4
29	K	202	CDL	CA2-OA2-PA1-OA3
29	J	301	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
29	J	301	CDL	CB3-OB5-PB2-OB3
29	J	301	CDL	CB3-OB5-PB2-OB4
29	L	301	CDL	CA3-OA5-PA1-OA4
29	L	301	CDL	CB3-OB5-PB2-OB4
29	L	302	CDL	CB3-OB5-PB2-OB2
29	L	302	CDL	CB3-OB5-PB2-OB3
29	L	302	CDL	CB3-OB5-PB2-OB4
29	P	201	CDL	CA2-OA2-PA1-OA3
29	P	201	CDL	CA3-OA5-PA1-OA2
29	P	201	CDL	CA3-OA5-PA1-OA4
29	a3	502	CDL	CA3-OA5-PA1-OA2
29	a3	502	CDL	CA3-OA5-PA1-OA4
29	b3	401	CDL	CA3-OA5-PA1-OA2
29	b3	401	CDL	CA3-OA5-PA1-OA3
29	b3	401	CDL	CB3-OB5-PB2-OB3
29	f3	302	CDL	CA2-OA2-PA1-OA5
29	f3	303	CDL	CB2-OB2-PB2-OB3
29	f3	303	CDL	CB2-OB2-PB2-OB4
29	f3	303	CDL	CB2-OB2-PB2-OB5
29	f3	304	CDL	CA2-OA2-PA1-OA3
29	i3	301	CDL	CB3-OB5-PB2-OB3
29	i3	302	CDL	CB3-OB5-PB2-OB3
29	k3	201	CDL	CB2-OB2-PB2-OB3
29	g3	305	CDL	CA2-OA2-PA1-OA3
29	j3	301	CDL	CA2-OA2-PA1-OA3
29	l3	301	CDL	CB3-OB5-PB2-OB2
29	l3	301	CDL	CB3-OB5-PB2-OB3
29	l3	301	CDL	CB3-OB5-PB2-OB4
29	l3	303	CDL	CA3-OA5-PA1-OA2
29	l3	303	CDL	CA3-OA5-PA1-OA4
29	l3	303	CDL	CB3-OB5-PB2-OB2
29	l3	303	CDL	CB3-OB5-PB2-OB4
29	p3	201	CDL	CA3-OA5-PA1-OA2
29	p3	201	CDL	CA3-OA5-PA1-OA4
29	B3	401	CDL	CB3-OB5-PB2-OB2
29	B3	401	CDL	CB3-OB5-PB2-OB3
29	B3	401	CDL	CB3-OB5-PB2-OB4
29	B3	404	CDL	CB2-OB2-PB2-OB3
29	B3	404	CDL	CB2-OB2-PB2-OB4
29	B3	404	CDL	CB2-OB2-PB2-OB5
29	F3	302	CDL	CA2-OA2-PA1-OA4
29	F3	302	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
29	I3	301	CDL	CB2-OB2-PB2-OB3
29	I3	301	CDL	CB2-OB2-PB2-OB4
29	I3	301	CDL	CB2-OB2-PB2-OB5
29	I3	302	CDL	CB3-OB5-PB2-OB2
29	I3	302	CDL	CB3-OB5-PB2-OB3
29	I3	302	CDL	CB3-OB5-PB2-OB4
29	K3	201	CDL	CB2-OB2-PB2-OB3
29	K3	201	CDL	CB3-OB5-PB2-OB4
29	K3	202	CDL	CA2-OA2-PA1-OA3
29	J3	301	CDL	CB3-OB5-PB2-OB2
29	J3	301	CDL	CB3-OB5-PB2-OB3
29	J3	301	CDL	CB3-OB5-PB2-OB4
29	J3	302	CDL	CA2-OA2-PA1-OA5
29	L3	301	CDL	CA3-OA5-PA1-OA4
29	L3	301	CDL	CB3-OB5-PB2-OB4
29	P3	201	CDL	CA2-OA2-PA1-OA3
29	P3	201	CDL	CA3-OA5-PA1-OA2
29	P3	201	CDL	CA3-OA5-PA1-OA4
30	g	303	PC1	C1-O11-P-O14
30	g	304	PC1	C1-O11-P-O14
30	G	303	PC1	C11-O13-P-O14
30	G	303	PC1	C11-O13-P-O11
30	G	303	PC1	C1-O11-P-O14
30	G	304	PC1	C1-O11-P-O14
30	g3	303	PC1	C1-O11-P-O14
30	g3	304	PC1	C1-O11-P-O14
30	G3	303	PC1	C11-O13-P-O12
30	G3	303	PC1	C11-O13-P-O14
30	G3	303	PC1	C11-O13-P-O11
30	G3	303	PC1	C1-O11-P-O14
30	G3	304	PC1	C1-O11-P-O14
33	C1	601	ATP	C5'-O5'-PA-O3A
33	C4	601	ATP	C5'-O5'-PA-O3A
35	m	301	PEE	C1-O3P-P-O1P
35	m	301	PEE	C1-O3P-P-O4P
35	m	301	PEE	O4P-C4-C5-N
35	A	501	PEE	C4-O4P-P-O3P
35	A	501	PEE	C4-O4P-P-O2P
35	J	303	PEE	C1-O3P-P-O1P
35	J	303	PEE	C1-O3P-P-O4P
35	J	303	PEE	O4P-C4-C5-N
35	L	303	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
35	L	303	PEE	C4-O4P-P-O2P
35	a3	503	PEE	C4-O4P-P-O3P
35	a3	503	PEE	C4-O4P-P-O2P
35	j3	303	PEE	C1-O3P-P-O1P
35	j3	303	PEE	C1-O3P-P-O4P
35	j3	303	PEE	O4P-C4-C5-N
35	l3	302	PEE	C4-O4P-P-O3P
35	l3	302	PEE	C4-O4P-P-O2P
35	L3	302	PEE	C1-O3P-P-O1P
35	L3	302	PEE	C1-O3P-P-O4P
35	L3	302	PEE	O4P-C4-C5-N
36	e	900	NAD	C5B-O5B-PA-O1A
36	e3	900	NAD	C5B-O5B-PA-O1A
30	G3	303	PC1	C25-C26-C27-C28
35	J	303	PEE	C33-C34-C35-C36
35	L3	302	PEE	C33-C34-C35-C36
29	A	502	CDL	C13-C14-C15-C16
29	J	302	CDL	C61-C62-C63-C64
29	L	302	CDL	C36-C37-C38-C39
30	G	303	PC1	C25-C26-C27-C28
29	p	201	CDL	C36-C37-C38-C39
29	p3	201	CDL	C36-C37-C38-C39
29	A3	501	CDL	C13-C14-C15-C16
29	J3	302	CDL	C61-C62-C63-C64
30	d	301	PC1	C38-C39-C3A-C3B
30	d3	301	PC1	C38-C39-C3A-C3B
29	B3	404	CDL	C17-C18-C19-C20
29	f	303	CDL	CA4-CA3-OA5-PA1
29	j	301	CDL	C1-CB2-OB2-PB2
29	l	302	CDL	C1-CA2-OA2-PA1
29	F	302	CDL	C1-CB2-OB2-PB2
29	J	301	CDL	C1-CB2-OB2-PB2
29	a3	502	CDL	C1-CB2-OB2-PB2
29	f3	303	CDL	CA4-CA3-OA5-PA1
29	j3	301	CDL	C1-CB2-OB2-PB2
29	l3	303	CDL	C1-CA2-OA2-PA1
29	J3	301	CDL	C1-CB2-OB2-PB2
29	A3	501	CDL	C40-C41-C42-C43
29	I3	302	CDL	C36-C37-C38-C39
29	r	201	CDL	C84-C85-C86-C87
29	f	302	CDL	C64-C65-C66-C67
29	f3	302	CDL	C64-C65-C66-C67

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Mol	Chain	Res	Type	Atoms
29	i3	301	CDL	C84-C85-C86-C87
29	B	401	CDL	C72-C71-CB7-OB8
29	B3	401	CDL	C72-C71-CB7-OB8
29	A	502	CDL	C40-C41-C42-C43
29	B	404	CDL	C17-C18-C19-C20
29	j	302	CDL	C31-C32-C33-C34
29	P	201	CDL	C34-C35-C36-C37
29	g3	305	CDL	C13-C14-C15-C16
29	j3	302	CDL	C31-C32-C33-C34
29	P3	201	CDL	C34-C35-C36-C37
29	i	301	CDL	C71-CB7-OB8-CB6
29	j	301	CDL	C13-C14-C15-C16
29	P	201	CDL	C37-C38-C39-C40
29	j3	301	CDL	C13-C14-C15-C16
29	g	305	CDL	C13-C14-C15-C16
29	P3	201	CDL	C37-C38-C39-C40
29	K3	201	CDL	C33-C34-C35-C36
29	b	401	CDL	CB7-C71-C72-C73
29	b3	401	CDL	CB7-C71-C72-C73
29	A3	501	CDL	C61-C62-C63-C64
29	K	201	CDL	C33-C34-C35-C36
29	l	302	CDL	CA6-CA4-OA6-CA5
29	p	201	CDL	CA6-CA4-OA6-CA5
29	r	201	CDL	CA6-CA4-OA6-CA5
29	B	402	CDL	CB3-CB4-OB6-CB5
29	F	303	CDL	CB3-CB4-OB6-CB5
29	a3	502	CDL	CA6-CA4-OA6-CA5
29	l3	303	CDL	CA6-CA4-OA6-CA5
29	p3	201	CDL	CA6-CA4-OA6-CA5
30	d	301	PC1	C1-C2-O21-C21
30	d3	301	PC1	C1-C2-O21-C21
29	K	202	CDL	C55-C56-C57-C58
29	J	301	CDL	C17-C18-C19-C20
29	a3	501	CDL	C75-C76-C77-C78
29	J3	301	CDL	C17-C18-C19-C20
29	l	301	CDL	C72-C71-CB7-OB8
29	I	302	CDL	C72-C71-CB7-OB8
29	l3	301	CDL	C72-C71-CB7-OB8
29	I3	303	CDL	C72-C71-CB7-OB8
29	a	501	CDL	C75-C76-C77-C78
29	A	502	CDL	C61-C62-C63-C64
29	I3	301	CDL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	K3	202	CDL	C55-C56-C57-C58
35	J	303	PEE	C14-C15-C16-C17
29	I	301	CDL	C15-C16-C17-C18
29	I	301	CDL	C44-C45-C46-C47
29	B	403	CDL	OA5-CA3-CA4-CA6
29	F	302	CDL	OA5-CA3-CA4-CA6
29	I	302	CDL	OB5-CB3-CB4-CB6
29	I3	303	CDL	OB5-CB3-CB4-CB6
29	i3	302	CDL	C71-CB7-OB8-CB6
29	I3	301	CDL	C44-C45-C46-C47
29	B	403	CDL	C22-C23-C24-C25
29	B3	402	CDL	C16-C17-C18-C19
29	B	402	CDL	C16-C17-C18-C19
29	K	201	CDL	C75-C76-C77-C78
29	B3	403	CDL	C22-C23-C24-C25
29	A3	501	CDL	OB9-CB7-OB8-CB6
29	f	303	CDL	CA2-C1-CB2-OB2
29	f3	303	CDL	CA2-C1-CB2-OB2
29	I	301	CDL	OA5-CA3-CA4-OA6
29	j3	302	CDL	OB5-CB3-CB4-OB6
29	l3	303	CDL	OB5-CB3-CB4-OB6
30	G3	304	PC1	O11-C1-C2-O21
35	L3	302	PEE	C14-C15-C16-C17
29	b3	401	CDL	C32-C31-CA7-OA8
29	I3	302	CDL	C24-C25-C26-C27
29	l	302	CDL	C11-CA5-OA6-CA4
29	A	502	CDL	OB9-CB7-OB8-CB6
29	L	302	CDL	C24-C25-C26-C27
29	L	302	CDL	C33-C34-C35-C36
29	K3	201	CDL	C75-C76-C77-C78
29	k	201	CDL	C20-C21-C22-C23
29	I3	302	CDL	C33-C34-C35-C36
29	b	401	CDL	C32-C31-CA7-OA8
35	l3	302	PEE	C12-C13-C14-C15
35	L3	302	PEE	C12-C13-C14-C15
29	k3	201	CDL	C20-C21-C22-C23
35	A	501	PEE	C12-C13-C14-C15
35	J	303	PEE	C12-C13-C14-C15
29	B	402	CDL	C1-CA2-OA2-PA1
29	B3	402	CDL	C1-CA2-OA2-PA1
29	p	201	CDL	OA6-CA4-CA6-OA8
29	B	402	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
29	K	202	CDL	OB6-CB4-CB6-OB8
29	j3	301	CDL	OB6-CB4-CB6-OB8
29	b	401	CDL	C61-C62-C63-C64
29	j3	301	CDL	C55-C56-C57-C58
29	p3	201	CDL	C11-C12-C13-C14
29	L	301	CDL	C31-CA7-OA8-CA6
29	L3	301	CDL	C31-CA7-OA8-CA6
29	a	501	CDL	C34-C35-C36-C37
29	f3	303	CDL	C72-C73-C74-C75
29	j	301	CDL	C55-C56-C57-C58
29	L	302	CDL	C34-C35-C36-C37
29	a3	501	CDL	C34-C35-C36-C37
29	p	201	CDL	C11-C12-C13-C14
29	b3	401	CDL	C61-C62-C63-C64
29	A	502	CDL	C32-C31-CA7-OA8
29	A3	501	CDL	C32-C31-CA7-OA8
29	f	303	CDL	C72-C73-C74-C75
29	L	301	CDL	OA9-CA7-OA8-CA6
29	i3	302	CDL	OB9-CB7-OB8-CB6
29	L3	301	CDL	OA9-CA7-OA8-CA6
29	j	301	CDL	C72-C71-CB7-OB8
29	j3	301	CDL	C72-C71-CB7-OB8
29	f	302	CDL	C22-C23-C24-C25
29	J3	301	CDL	CB3-CB4-CB6-OB8
29	I3	302	CDL	C34-C35-C36-C37
29	I	301	CDL	C43-C44-C45-C46
29	l3	301	CDL	C33-C34-C35-C36
29	l	301	CDL	C33-C34-C35-C36
29	I3	301	CDL	C43-C44-C45-C46
33	C2	601	ATP	PB-O3A-PA-O2A
33	C5	601	ATP	PB-O3A-PA-O2A
29	g3	305	CDL	C80-C81-C82-C83
29	f3	302	CDL	C22-C23-C24-C25
29	l	301	CDL	CA7-C31-C32-C33
29	g	305	CDL	C80-C81-C82-C83
29	a	501	CDL	C15-C16-C17-C18
29	a3	501	CDL	C15-C16-C17-C18
29	B3	404	CDL	C14-C15-C16-C17
30	g	304	PC1	C32-C33-C34-C35
29	l3	301	CDL	CA7-C31-C32-C33
30	g3	304	PC1	C3C-C3D-C3E-C3F
29	i	301	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
29	f	302	CDL	CB2-C1-CA2-OA2
29	f3	302	CDL	CB2-C1-CA2-OA2
29	I	301	CDL	C14-C15-C16-C17
30	g	304	PC1	C3C-C3D-C3E-C3F
30	g3	304	PC1	C32-C33-C34-C35
29	k	201	CDL	C31-CA7-OA8-CA6
29	k3	201	CDL	C31-CA7-OA8-CA6
29	f3	304	CDL	C53-C54-C55-C56
29	j3	302	CDL	C58-C59-C60-C61
29	F3	302	CDL	C14-C15-C16-C17
29	L	302	CDL	C44-C45-C46-C47
29	f	304	CDL	C53-C54-C55-C56
29	F	303	CDL	C14-C15-C16-C17
29	A3	501	CDL	C33-C34-C35-C36
29	j	302	CDL	C58-C59-C60-C61
29	A	502	CDL	C33-C34-C35-C36
30	G	303	PC1	C3D-C3E-C3F-C3G
29	I3	302	CDL	C44-C45-C46-C47
29	I3	303	CDL	C16-C17-C18-C19
29	j	301	CDL	OB5-CB3-CB4-OB6
29	l	302	CDL	OB5-CB3-CB4-OB6
29	A	502	CDL	OA5-CA3-CA4-OA6
30	G3	303	PC1	C3D-C3E-C3F-C3G
29	k	201	CDL	C12-C13-C14-C15
29	l	302	CDL	C16-C17-C18-C19
29	B	404	CDL	C14-C15-C16-C17
29	k	201	CDL	C14-C15-C16-C17
29	k3	201	CDL	OA9-CA7-OA8-CA6
29	I3	301	CDL	C14-C15-C16-C17
29	f3	304	CDL	C72-C73-C74-C75
29	f	303	CDL	O1-C1-CA2-OA2
29	r	201	CDL	C78-C79-C80-C81
29	i3	301	CDL	C78-C79-C80-C81
29	k3	201	CDL	C14-C15-C16-C17
29	f3	304	CDL	C36-C37-C38-C39
29	k3	201	CDL	C12-C13-C14-C15
30	G3	303	PC1	C33-C34-C35-C36
29	f	304	CDL	C72-C73-C74-C75
35	m	301	PEE	C36-C37-C38-C39
35	j3	303	PEE	C36-C37-C38-C39
29	B3	403	CDL	C56-C57-C58-C59
29	k	201	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
29	b	401	CDL	C60-C61-C62-C63
29	b3	401	CDL	C60-C61-C62-C63
29	f3	303	CDL	C23-C24-C25-C26
29	I3	303	CDL	C31-C32-C33-C34
29	J	302	CDL	OB6-CB4-CB6-OB8
29	J3	301	CDL	OA6-CA4-CA6-OA8
35	j3	303	PEE	C15-C16-C17-C18
30	G	303	PC1	C33-C34-C35-C36
29	f	303	CDL	C23-C24-C25-C26
29	f	304	CDL	C36-C37-C38-C39
29	I	302	CDL	C31-C32-C33-C34
29	J	302	CDL	C22-C23-C24-C25
29	J3	302	CDL	C22-C23-C24-C25
30	d3	301	PC1	C3B-C3C-C3D-C3E
29	B	401	CDL	C24-C25-C26-C27
30	D3	301	PC1	C34-C35-C36-C37
30	D	301	PC1	C34-C35-C36-C37
29	B3	401	CDL	C24-C25-C26-C27
29	B3	404	CDL	C20-C21-C22-C23
29	P	201	CDL	CB7-C71-C72-C73
29	B	404	CDL	C20-C21-C22-C23
29	l3	301	CDL	C17-C18-C19-C20
29	l	301	CDL	C17-C18-C19-C20
29	B	403	CDL	C56-C57-C58-C59
30	d	301	PC1	C3B-C3C-C3D-C3E
29	i3	301	CDL	C22-C23-C24-C25
29	j	302	CDL	CB4-CB3-OB5-PB2
29	l	302	CDL	CB4-CB3-OB5-PB2
29	I	302	CDL	CB4-CB3-OB5-PB2
29	L	302	CDL	C1-CA2-OA2-PA1
29	j3	302	CDL	CB4-CB3-OB5-PB2
29	l3	303	CDL	CB4-CB3-OB5-PB2
29	I3	302	CDL	C1-CA2-OA2-PA1
29	I3	303	CDL	CB4-CB3-OB5-PB2
29	r	201	CDL	C22-C23-C24-C25
29	I3	303	CDL	C34-C35-C36-C37
29	P3	201	CDL	CB7-C71-C72-C73
29	I	302	CDL	C34-C35-C36-C37
35	m	301	PEE	C15-C16-C17-C18
35	L	303	PEE	C19-C20-C21-C22
35	a3	503	PEE	C19-C20-C21-C22
29	P	201	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
29	P3	201	CDL	C72-C71-CB7-OB8
30	G	304	PC1	O31-C31-C32-C33
30	G3	304	PC1	O31-C31-C32-C33
29	L	302	CDL	C31-C32-C33-C34
29	k	201	CDL	C59-C60-C61-C62
29	I3	302	CDL	C31-C32-C33-C34
29	a	501	CDL	CB3-CB4-CB6-OB8
29	B	402	CDL	CB3-CB4-CB6-OB8
29	K3	201	CDL	CA3-CA4-CA6-OA8
30	g	304	PC1	C1-C2-C3-O31
29	k3	201	CDL	C59-C60-C61-C62
29	B	401	CDL	C32-C31-CA7-OA9
29	B3	401	CDL	C32-C31-CA7-OA9
29	g	305	CDL	C58-C59-C60-C61
29	B	403	CDL	C36-C37-C38-C39
29	B	404	CDL	C78-C79-C80-C81
30	G	303	PC1	C23-C24-C25-C26
29	I	301	CDL	CA5-C11-C12-C13
29	I3	301	CDL	CA5-C11-C12-C13
30	G3	303	PC1	C23-C24-C25-C26
33	C1	601	ATP	O4'-C4'-C5'-O5'
29	g	305	CDL	C52-C53-C54-C55
29	i3	301	CDL	C11-C12-C13-C14
29	l3	303	CDL	C14-C15-C16-C17
29	B3	403	CDL	C36-C37-C38-C39
29	B3	404	CDL	C78-C79-C80-C81
29	g3	305	CDL	C58-C59-C60-C61
29	J	302	CDL	C72-C71-CB7-OB8
29	J3	302	CDL	C72-C71-CB7-OB8
29	f	302	CDL	CA6-CA4-OA6-CA5
29	B	404	CDL	CA3-CA4-OA6-CA5
29	L	301	CDL	CA6-CA4-OA6-CA5
29	f3	302	CDL	CA6-CA4-OA6-CA5
29	B3	402	CDL	CB3-CB4-OB6-CB5
29	B3	404	CDL	CA3-CA4-OA6-CA5
29	F3	302	CDL	CB3-CB4-OB6-CB5
29	L3	301	CDL	CA6-CA4-OA6-CA5
30	d	301	PC1	C3-C2-O21-C21
30	D	301	PC1	C1-C2-O21-C21
30	D	301	PC1	C3-C2-O21-C21
30	d3	301	PC1	C3-C2-O21-C21
30	D3	301	PC1	C3-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
29	r	201	CDL	C11-C12-C13-C14
29	l	302	CDL	C14-C15-C16-C17
29	B3	401	CDL	C20-C21-C22-C23
35	J	303	PEE	C18-C19-C20-C21
35	L3	302	PEE	C18-C19-C20-C21
29	B	401	CDL	C20-C21-C22-C23
30	g3	303	PC1	C3E-C3F-C3G-C3H
29	g3	305	CDL	C52-C53-C54-C55
29	P3	201	CDL	C76-C77-C78-C79
30	g	303	PC1	C3E-C3F-C3G-C3H
29	B3	401	CDL	C71-C72-C73-C74
29	B	402	CDL	C72-C71-CB7-OB8
29	B	401	CDL	C71-C72-C73-C74
29	l3	303	CDL	C19-C20-C21-C22
29	l	302	CDL	C19-C20-C21-C22
29	b3	401	CDL	OB5-CB3-CB4-OB6
29	A3	501	CDL	OA5-CA3-CA4-OA6
29	J3	302	CDL	OB5-CB3-CB4-OB6
30	g	304	PC1	O11-C1-C2-O21
29	P	201	CDL	C76-C77-C78-C79
29	B3	402	CDL	C72-C71-CB7-OB8
29	j3	302	CDL	C18-C19-C20-C21
29	B3	403	CDL	CB4-CB3-OB5-PB2
29	j	302	CDL	C18-C19-C20-C21
29	B3	401	CDL	C11-C12-C13-C14
29	J3	301	CDL	C39-C40-C41-C42
29	B	401	CDL	C11-C12-C13-C14
29	a3	502	CDL	OA5-CA3-CA4-CA6
30	g3	304	PC1	O11-C1-C2-C3
30	G3	303	PC1	O11-C1-C2-C3
29	P	201	CDL	C40-C41-C42-C43
29	J	301	CDL	C39-C40-C41-C42
29	P3	201	CDL	C40-C41-C42-C43
35	J	303	PEE	C38-C39-C40-C41
35	L3	302	PEE	C38-C39-C40-C41
29	a	501	CDL	OA6-CA4-CA6-OA8
29	g	305	CDL	OB6-CB4-CB6-OB8
29	f3	302	CDL	OA6-CA4-CA6-OA8
29	g3	305	CDL	OB6-CB4-CB6-OB8
29	B3	401	CDL	C35-C36-C37-C38
29	B	401	CDL	C35-C36-C37-C38
29	p3	201	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
36	E	900	NAD	O4D-C1D-N1N-C6N
29	g	305	CDL	C56-C57-C58-C59
29	g3	305	CDL	C56-C57-C58-C59
29	j	302	CDL	C72-C71-CB7-OB8
29	j3	302	CDL	C72-C71-CB7-OB8
29	p	201	CDL	C37-C38-C39-C40
29	L3	301	CDL	C17-C18-C19-C20
29	f	304	CDL	CB2-C1-CA2-OA2
29	i	301	CDL	CB2-C1-CA2-OA2
29	f3	304	CDL	CB2-C1-CA2-OA2
29	i3	302	CDL	CB2-C1-CA2-OA2
29	A3	501	CDL	C20-C21-C22-C23
29	k3	201	CDL	C72-C73-C74-C75
29	k	201	CDL	C72-C73-C74-C75
29	J	302	CDL	C24-C25-C26-C27
29	J3	302	CDL	C24-C25-C26-C27
29	B	403	CDL	C11-C12-C13-C14
29	L	301	CDL	C17-C18-C19-C20
29	b	401	CDL	C21-C22-C23-C24
29	f3	303	CDL	O1-C1-CA2-OA2
29	A	502	CDL	C20-C21-C22-C23
29	a3	502	CDL	C71-C72-C73-C74
29	p3	201	CDL	C78-C79-C80-C81
29	p	201	CDL	C78-C79-C80-C81
29	A	502	CDL	C53-C54-C55-C56
29	K	201	CDL	C60-C61-C62-C63
29	B3	403	CDL	C11-C12-C13-C14
29	A3	501	CDL	C53-C54-C55-C56
29	b3	401	CDL	C21-C22-C23-C24
29	K3	201	CDL	C37-C38-C39-C40
29	K3	201	CDL	C60-C61-C62-C63
29	J3	301	CDL	C41-C42-C43-C44
30	G	304	PC1	C3A-C3B-C3C-C3D
33	A2	601	ATP	PB-O3A-PA-O1A
33	A5	601	ATP	PB-O3A-PA-O1A
29	B	404	CDL	C58-C59-C60-C61
29	K	201	CDL	C37-C38-C39-C40
29	B3	404	CDL	C58-C59-C60-C61
29	J	301	CDL	C41-C42-C43-C44
29	F	302	CDL	C71-C72-C73-C74
30	G3	304	PC1	C3A-C3B-C3C-C3D
30	d	301	PC1	C3F-C3G-C3H-C3I

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Mol	Chain	Res	Type	Atoms
30	d3	301	PC1	C3F-C3G-C3H-C3I
29	J	302	CDL	C11-C12-C13-C14
30	g3	304	PC1	C2F-C2G-C2H-C2I
29	J3	302	CDL	C11-C12-C13-C14
29	P3	201	CDL	C59-C60-C61-C62
29	l	301	CDL	CA4-CA3-OA5-PA1
29	B	403	CDL	CB4-CB3-OB5-PB2
29	L	301	CDL	C1-CA2-OA2-PA1
29	L	302	CDL	CB4-CB3-OB5-PB2
29	l3	301	CDL	CA4-CA3-OA5-PA1
29	I3	302	CDL	CB4-CB3-OB5-PB2
29	L3	301	CDL	C1-CA2-OA2-PA1
29	f	303	CDL	C20-C21-C22-C23
30	g	304	PC1	C2F-C2G-C2H-C2I
30	g	304	PC1	O31-C31-C32-C33
30	g3	304	PC1	O31-C31-C32-C33
29	f3	303	CDL	C20-C21-C22-C23
29	B3	403	CDL	C53-C54-C55-C56
29	B	403	CDL	C53-C54-C55-C56
29	P	201	CDL	C59-C60-C61-C62
29	A	502	CDL	CA3-CA4-CA6-OA8
29	A	502	CDL	CB3-CB4-CB6-OB8
29	p3	201	CDL	CA3-CA4-CA6-OA8
29	J3	302	CDL	CB3-CB4-CB6-OB8
29	j3	302	CDL	C32-C33-C34-C35
35	L	303	PEE	C20-C21-C22-C23
29	i	301	CDL	C24-C25-C26-C27
29	i3	302	CDL	C24-C25-C26-C27
35	a3	503	PEE	C20-C21-C22-C23
29	f3	304	CDL	C83-C84-C85-C86
29	j	302	CDL	C32-C33-C34-C35
29	b	401	CDL	OB5-CB3-CB4-OB6
29	f	304	CDL	C83-C84-C85-C86
35	A	501	PEE	C34-C35-C36-C37
29	r	201	CDL	C81-C82-C83-C84
29	B	402	CDL	C41-C42-C43-C44
29	B3	402	CDL	C41-C42-C43-C44
30	g3	304	PC1	C39-C3A-C3B-C3C
35	l3	302	PEE	C34-C35-C36-C37
29	K	201	CDL	C72-C73-C74-C75
29	K3	201	CDL	C72-C73-C74-C75
29	K	201	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
29	K3	201	CDL	CB2-C1-CA2-OA2
29	f	303	CDL	C14-C15-C16-C17
29	a3	502	CDL	C11-C12-C13-C14
29	f3	303	CDL	C14-C15-C16-C17
29	i3	301	CDL	C81-C82-C83-C84
30	g	304	PC1	C39-C3A-C3B-C3C
29	l3	303	CDL	OB5-CB3-CB4-CB6
35	j3	303	PEE	O3P-C1-C2-C3
29	J	302	CDL	C34-C35-C36-C37
29	j	302	CDL	OA6-CA4-CA6-OA8
29	J	301	CDL	OA6-CA4-CA6-OA8
29	L	302	CDL	OA6-CA4-CA6-OA8
29	B3	402	CDL	OB6-CB4-CB6-OB8
29	I3	302	CDL	OA6-CA4-CA6-OA8
29	f3	304	CDL	C12-C11-CA5-OA6
29	J3	301	CDL	C59-C60-C61-C62
29	f3	302	CDL	C72-C73-C74-C75
29	f	302	CDL	C72-C73-C74-C75
29	J3	302	CDL	C34-C35-C36-C37
30	G3	303	PC1	C2C-C2D-C2E-C2F
29	J	301	CDL	C59-C60-C61-C62
29	F	302	CDL	C11-C12-C13-C14
29	J3	302	CDL	C15-C16-C17-C18
30	G	303	PC1	C2C-C2D-C2E-C2F
30	d3	301	PC1	C22-C23-C24-C25
29	f	304	CDL	C12-C11-CA5-OA6
29	B	401	CDL	C12-C11-CA5-OA6
29	B3	401	CDL	C12-C11-CA5-OA6
29	A	502	CDL	C52-C53-C54-C55
29	l	301	CDL	C13-C14-C15-C16
29	K	201	CDL	C16-C17-C18-C19
29	l3	301	CDL	C13-C14-C15-C16
29	K3	201	CDL	C16-C17-C18-C19
29	J	302	CDL	C15-C16-C17-C18
29	A3	501	CDL	C36-C37-C38-C39
29	A3	501	CDL	C52-C53-C54-C55
29	p	201	CDL	C82-C83-C84-C85
29	K3	202	CDL	C73-C74-C75-C76
30	g3	303	PC1	C23-C24-C25-C26
29	K	202	CDL	C73-C74-C75-C76
30	d	301	PC1	C22-C23-C24-C25
30	g	303	PC1	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
35	L3	302	PEE	C36-C37-C38-C39
29	f	302	CDL	C24-C25-C26-C27
29	P	201	CDL	C61-C62-C63-C64
29	p3	201	CDL	C82-C83-C84-C85
29	B3	403	CDL	OB7-CB5-OB6-CB4
29	F3	302	CDL	C63-C64-C65-C66
29	f3	302	CDL	C24-C25-C26-C27
29	L	302	CDL	CB5-C51-C52-C53
29	F	303	CDL	C63-C64-C65-C66
29	k3	201	CDL	C56-C57-C58-C59
29	p	201	CDL	C72-C71-CB7-OB8
29	g	305	CDL	C53-C54-C55-C56
29	I3	302	CDL	CB5-C51-C52-C53
29	B3	402	CDL	CB6-CB4-OB6-CB5
30	D3	301	PC1	C1-C2-O21-C21
37	B1	1002	ADP	PA-O3A-PB-O3B
29	J3	301	CDL	C34-C35-C36-C37
35	J	303	PEE	C36-C37-C38-C39
35	L	303	PEE	C36-C37-C38-C39
35	a3	503	PEE	C36-C37-C38-C39
29	k	201	CDL	C56-C57-C58-C59
29	P	201	CDL	C80-C81-C82-C83
35	L3	302	PEE	C13-C14-C15-C16
29	A	502	CDL	C36-C37-C38-C39
35	J	303	PEE	C13-C14-C15-C16
29	p3	201	CDL	C72-C71-CB7-OB8
29	J	301	CDL	C34-C35-C36-C37
29	f3	302	CDL	CA4-CA6-OA8-CA7
29	g3	305	CDL	C53-C54-C55-C56
29	P3	201	CDL	C61-C62-C63-C64
29	a3	502	CDL	C55-C56-C57-C58
29	J3	302	CDL	C82-C83-C84-C85
29	F	302	CDL	C55-C56-C57-C58
29	i	301	CDL	C58-C59-C60-C61
29	B	401	CDL	C33-C34-C35-C36
29	J	302	CDL	C82-C83-C84-C85
29	i3	302	CDL	C58-C59-C60-C61
29	P3	201	CDL	C80-C81-C82-C83
29	j3	302	CDL	C1-CB2-OB2-PB2
29	B3	401	CDL	C33-C34-C35-C36
29	J3	301	CDL	C80-C81-C82-C83
29	b3	401	CDL	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
29	B	404	CDL	C54-C55-C56-C57
29	B3	404	CDL	C54-C55-C56-C57
29	K	201	CDL	CB3-CB4-CB6-OB8
29	J	301	CDL	CA3-CA4-CA6-OA8
29	J	301	CDL	CB3-CB4-CB6-OB8
29	A3	501	CDL	CA3-CA4-CA6-OA8
29	B3	402	CDL	CB3-CB4-CB6-OB8
29	J3	301	CDL	CA3-CA4-CA6-OA8
29	b	401	CDL	C44-C45-C46-C47
29	f	302	CDL	CA4-CA6-OA8-CA7
29	B3	401	CDL	C54-C55-C56-C57
29	B	401	CDL	C54-C55-C56-C57
29	l	301	CDL	C58-C59-C60-C61
29	J	301	CDL	C80-C81-C82-C83
29	F	303	CDL	C36-C37-C38-C39
29	l3	301	CDL	C58-C59-C60-C61
29	P3	201	CDL	C41-C42-C43-C44
30	G	303	PC1	O21-C21-C22-C23
30	G3	303	PC1	O21-C21-C22-C23
29	F	303	CDL	C13-C14-C15-C16
29	F3	302	CDL	C13-C14-C15-C16
29	B3	403	CDL	C63-C64-C65-C66
29	A	502	CDL	C44-C45-C46-C47
29	b	401	CDL	C72-C71-CB7-OB8
30	g3	303	PC1	O31-C31-C32-C33
29	b	401	CDL	C73-C74-C75-C76
29	B	403	CDL	C63-C64-C65-C66
36	e	900	NAD	O4B-C1B-N9A-C8A
29	A3	501	CDL	C44-C45-C46-C47
29	F	303	CDL	C22-C23-C24-C25
29	B3	404	CDL	C16-C17-C18-C19
29	F3	302	CDL	C22-C23-C24-C25
29	K	201	CDL	OB6-CB4-CB6-OB8
29	K3	201	CDL	OB6-CB4-CB6-OB8
29	l	302	CDL	C12-C13-C14-C15
29	P	201	CDL	C41-C42-C43-C44
35	A	501	PEE	C36-C37-C38-C39
35	a3	503	PEE	C38-C39-C40-C41
35	l3	302	PEE	C36-C37-C38-C39
29	b	401	CDL	C52-C51-CB5-OB6
29	g	305	CDL	C12-C11-CA5-OA6
29	L	302	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
29	b3	401	CDL	C52-C51-CB5-OB6
29	b3	401	CDL	C72-C71-CB7-OB8
29	B	403	CDL	OB7-CB5-OB6-CB4
29	j	302	CDL	OB5-CB3-CB4-CB6
29	l	302	CDL	OB5-CB3-CB4-CB6
29	j3	301	CDL	OB5-CB3-CB4-CB6
29	B3	402	CDL	C84-C85-C86-C87
29	k3	201	CDL	C42-C43-C44-C45
29	B	402	CDL	C84-C85-C86-C87
29	f	304	CDL	C16-C17-C18-C19
29	k	201	CDL	C42-C43-C44-C45
29	F3	302	CDL	C36-C37-C38-C39
29	F3	302	CDL	C60-C61-C62-C63
29	g3	305	CDL	C12-C11-CA5-OA6
30	g	303	PC1	O31-C31-C32-C33
29	l3	303	CDL	C12-C13-C14-C15
29	b3	401	CDL	C73-C74-C75-C76
29	b	401	CDL	CA5-C11-C12-C13
29	B3	403	CDL	C51-CB5-OB6-CB4
35	L	303	PEE	C38-C39-C40-C41
29	B	404	CDL	C16-C17-C18-C19
29	j	302	CDL	C1-CB2-OB2-PB2
29	f3	304	CDL	C16-C17-C18-C19
30	G	304	PC1	C22-C23-C24-C25
29	i	301	CDL	C60-C61-C62-C63
29	A3	501	CDL	C52-C51-CB5-OB6
29	I3	302	CDL	C32-C31-CA7-OA8
29	l	301	CDL	C12-C13-C14-C15
29	F	303	CDL	C60-C61-C62-C63
29	l3	301	CDL	C12-C13-C14-C15
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	C4	601	ATP	PB-O3A-PA-O2A
33	A4	601	ATP	PB-O3A-PA-O1A
33	C5	601	ATP	PB-O3A-PA-O1A
29	F	302	CDL	C53-C54-C55-C56
29	b3	401	CDL	CA5-C11-C12-C13
29	A	502	CDL	C52-C51-CB5-OB6
29	B	402	CDL	C52-C51-CB5-OB6
29	B3	402	CDL	C52-C51-CB5-OB6
29	I3	303	CDL	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
29	I	302	CDL	C41-C42-C43-C44
29	B	403	CDL	C51-CB5-OB6-CB4
29	l	302	CDL	C24-C25-C26-C27
29	l3	303	CDL	C24-C25-C26-C27
29	f	302	CDL	C52-C51-CB5-OB6
29	f3	304	CDL	C72-C71-CB7-OB8
29	i3	302	CDL	C60-C61-C62-C63
30	D	301	PC1	C24-C25-C26-C27
30	D3	301	PC1	C24-C25-C26-C27
30	G3	304	PC1	C22-C23-C24-C25
29	f	304	CDL	C72-C71-CB7-OB8
29	F	303	CDL	C72-C71-CB7-OB8
29	f3	302	CDL	C52-C51-CB5-OB6
29	f	302	CDL	C72-C71-CB7-OB9
29	f3	302	CDL	C72-C71-CB7-OB9
29	p	201	CDL	C34-C35-C36-C37
29	B3	402	CDL	C52-C53-C54-C55
29	B	402	CDL	C52-C53-C54-C55
29	p3	201	CDL	C34-C35-C36-C37
29	f	303	CDL	C72-C71-CB7-OB8
29	g	305	CDL	C72-C71-CB7-OB8
29	P	201	CDL	C12-C11-CA5-OA6
29	f3	303	CDL	C72-C71-CB7-OB8
29	g3	305	CDL	C72-C71-CB7-OB8
29	F3	302	CDL	C72-C71-CB7-OB8
29	a3	502	CDL	C53-C54-C55-C56
29	J	301	CDL	C71-C72-C73-C74
30	g	303	PC1	C2A-C2B-C2C-C2D
30	g3	303	PC1	C2A-C2B-C2C-C2D
29	P3	201	CDL	C52-C53-C54-C55
29	f	304	CDL	CB4-CB3-OB5-PB2
29	J	302	CDL	CA4-CA3-OA5-PA1
29	J3	302	CDL	CA4-CA3-OA5-PA1
29	B	404	CDL	C72-C71-CB7-OB8
29	I	301	CDL	C20-C21-C22-C23
29	P	201	CDL	C52-C53-C54-C55
29	f3	302	CDL	C59-C60-C61-C62
29	p3	201	CDL	C79-C80-C81-C82
29	i	301	CDL	CB3-CB4-CB6-OB8
29	K3	201	CDL	CB3-CB4-CB6-OB8
29	l	301	CDL	C16-C17-C18-C19
29	b3	401	CDL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
29	B	403	CDL	C51-C52-C53-C54
29	I3	301	CDL	C20-C21-C22-C23
29	J3	301	CDL	C71-C72-C73-C74
30	G	303	PC1	C3B-C3C-C3D-C3E
29	r	201	CDL	C72-C71-CB7-OB8
29	K	202	CDL	C72-C71-CB7-OB8
29	i3	301	CDL	C72-C71-CB7-OB8
29	B3	404	CDL	C72-C71-CB7-OB8
29	P3	201	CDL	C12-C11-CA5-OA6
29	l3	301	CDL	C16-C17-C18-C19
29	B3	403	CDL	C51-C52-C53-C54
29	f	302	CDL	OA6-CA4-CA6-OA8
29	l	302	CDL	OA6-CA4-CA6-OA8
29	B	401	CDL	OB6-CB4-CB6-OB8
29	F	303	CDL	OB6-CB4-CB6-OB8
29	a3	501	CDL	OA6-CA4-CA6-OA8
29	l3	303	CDL	OA6-CA4-CA6-OA8
29	B3	401	CDL	OB6-CB4-CB6-OB8
29	b	401	CDL	C20-C21-C22-C23
29	B	401	CDL	C16-C17-C18-C19
29	B3	401	CDL	C31-C32-C33-C34
29	f	302	CDL	C59-C60-C61-C62
29	P	201	CDL	C31-C32-C33-C34
29	a	501	CDL	C32-C31-CA7-OA8
29	K	202	CDL	C12-C11-CA5-OA6
29	a3	501	CDL	C32-C31-CA7-OA8
29	K3	202	CDL	C72-C71-CB7-OB8
36	E3	900	NAD	C2B-C1B-N9A-C8A
29	B3	401	CDL	C16-C17-C18-C19
29	p	201	CDL	C79-C80-C81-C82
29	K3	202	CDL	C56-C57-C58-C59
29	P3	201	CDL	C31-C32-C33-C34
30	g	303	PC1	C32-C33-C34-C35
30	G3	303	PC1	C3B-C3C-C3D-C3E
29	B	401	CDL	C31-C32-C33-C34
29	K	201	CDL	C44-C45-C46-C47
29	K3	201	CDL	C44-C45-C46-C47
29	j	301	CDL	OB5-CB3-CB4-CB6
35	L	303	PEE	O2-C10-C11-C12
35	a3	503	PEE	O2-C10-C11-C12
29	b	401	CDL	CB2-C1-CA2-OA2
32	i	302	UQ8	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
29	K	202	CDL	C56-C57-C58-C59
29	f3	304	CDL	C34-C35-C36-C37
29	L3	301	CDL	C18-C19-C20-C21
29	K3	202	CDL	C12-C11-CA5-OA6
30	g3	303	PC1	C32-C33-C34-C35
29	B3	404	CDL	C38-C39-C40-C41
29	L3	301	CDL	C59-C60-C61-C62
29	i	301	CDL	CA5-C11-C12-C13
29	f	304	CDL	C34-C35-C36-C37
29	L	301	CDL	C59-C60-C61-C62
29	B	402	CDL	CB6-CB4-OB6-CB5
29	B	404	CDL	CA6-CA4-OA6-CA5
29	B3	404	CDL	CA6-CA4-OA6-CA5
29	f3	304	CDL	C57-C58-C59-C60
30	G	303	PC1	O31-C31-C32-C33
30	G3	303	PC1	O31-C31-C32-C33
29	B	404	CDL	C38-C39-C40-C41
29	I3	302	CDL	C13-C14-C15-C16
29	L	301	CDL	C18-C19-C20-C21
29	l	302	CDL	C32-C31-CA7-OA9
29	l3	303	CDL	C32-C31-CA7-OA9
29	f	304	CDL	C57-C58-C59-C60
29	i3	302	CDL	CA5-C11-C12-C13
32	I	303	UQ8	C16-C17-C18-C19
32	i3	303	UQ8	C21-C22-C23-C24
32	I3	304	UQ8	C16-C17-C18-C19
30	G3	303	PC1	C2B-C2C-C2D-C2E
35	m	301	PEE	O2-C10-C11-C12
35	A	501	PEE	O2-C10-C11-C12
35	j3	303	PEE	O2-C10-C11-C12
35	l3	302	PEE	O2-C10-C11-C12
36	e3	900	NAD	O4B-C1B-N9A-C8A
29	f3	304	CDL	CB4-CB3-OB5-PB2
35	J	303	PEE	C2-C1-O3P-P
35	L3	302	PEE	C2-C1-O3P-P
29	I	302	CDL	C64-C65-C66-C67
29	B	402	CDL	C32-C31-CA7-OA9
29	A3	501	CDL	C52-C51-CB5-OB7
29	B3	402	CDL	C32-C31-CA7-OA9
29	a3	502	CDL	C64-C65-C66-C67
29	I3	303	CDL	C64-C65-C66-C67
29	I3	301	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
29	p	201	CDL	C75-C76-C77-C78
29	L	302	CDL	C13-C14-C15-C16
29	p3	201	CDL	C75-C76-C77-C78
29	F	302	CDL	C64-C65-C66-C67
29	B3	402	CDL	C11-C12-C13-C14
30	G	303	PC1	C2B-C2C-C2D-C2E
29	A	502	CDL	C52-C51-CB5-OB7
29	L	302	CDL	C72-C71-CB7-OB9
29	I3	302	CDL	C72-C71-CB7-OB9
29	B	402	CDL	C11-C12-C13-C14
29	I3	302	CDL	C58-C59-C60-C61
29	I	301	CDL	C72-C71-CB7-OB8
32	i	302	UQ8	C16-C17-C18-C19
32	i3	303	UQ8	C16-C17-C18-C19
35	J	303	PEE	C16-C17-C18-C19
35	L3	302	PEE	C16-C17-C18-C19
29	l	302	CDL	C53-C54-C55-C56
29	L	302	CDL	C58-C59-C60-C61
29	i3	301	CDL	C12-C13-C14-C15
29	J3	302	CDL	C83-C84-C85-C86
29	J	302	CDL	C83-C84-C85-C86
29	g	305	CDL	C12-C11-CA5-OA7
29	F	303	CDL	C72-C71-CB7-OB9
29	f3	304	CDL	C72-C71-CB7-OB9
29	F3	302	CDL	C72-C71-CB7-OB9
29	K3	202	CDL	C72-C71-CB7-OB9
29	r	201	CDL	C12-C13-C14-C15
29	a3	502	CDL	C54-C55-C56-C57
35	m	301	PEE	C32-C33-C34-C35
29	p3	201	CDL	C43-C44-C45-C46
29	l3	303	CDL	C53-C54-C55-C56
29	J3	301	CDL	C32-C33-C34-C35
29	b	401	CDL	C52-C51-CB5-OB7
29	f	304	CDL	C72-C71-CB7-OB9
29	b3	401	CDL	C52-C51-CB5-OB7
29	g3	305	CDL	C12-C11-CA5-OA7
29	I3	302	CDL	C32-C31-CA7-OA9
29	F	302	CDL	C54-C55-C56-C57
30	g3	303	PC1	O21-C21-C22-C23
29	B	402	CDL	CB5-C51-C52-C53
29	J	301	CDL	C18-C19-C20-C21
29	K	202	CDL	C72-C71-CB7-OB9

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Mol	Chain	Res	Type	Atoms
29	L	302	CDL	C32-C31-CA7-OA9
30	g	303	PC1	O32-C31-C32-C33
30	g3	303	PC1	O32-C31-C32-C33
30	D3	301	PC1	C22-C23-C24-C25
29	p	201	CDL	C43-C44-C45-C46
29	F	302	CDL	C42-C43-C44-C45
29	J3	301	CDL	C18-C19-C20-C21
35	j3	303	PEE	C32-C33-C34-C35
29	a3	502	CDL	C42-C43-C44-C45
30	g	303	PC1	O21-C21-C22-C23
29	r	201	CDL	C17-C18-C19-C20
30	G	303	PC1	O22-C21-C22-C23
30	G	303	PC1	O32-C31-C32-C33
30	G3	303	PC1	O22-C21-C22-C23
29	J	301	CDL	C32-C33-C34-C35
29	B3	402	CDL	CB5-C51-C52-C53
29	I	301	CDL	OA6-CA4-CA6-OA8
29	P	201	CDL	OA6-CA4-CA6-OA8
29	B3	402	CDL	C19-C20-C21-C22
29	B	404	CDL	C72-C71-CB7-OB9
29	P	201	CDL	C12-C11-CA5-OA7
29	B3	402	CDL	C52-C51-CB5-OB7
30	G3	303	PC1	O32-C31-C32-C33
29	f	302	CDL	C12-C11-CA5-OA6
29	f3	302	CDL	C12-C11-CA5-OA6
29	F	302	CDL	C12-C13-C14-C15
30	D	301	PC1	C22-C23-C24-C25
30	G	303	PC1	C29-C2A-C2B-C2C
35	j3	303	PEE	C12-C13-C14-C15
29	B	402	CDL	C52-C51-CB5-OB7
29	K	202	CDL	C12-C11-CA5-OA7
29	i3	301	CDL	C72-C71-CB7-OB9
29	B3	404	CDL	C72-C71-CB7-OB9
29	K3	202	CDL	C12-C11-CA5-OA7
29	B	403	CDL	C20-C21-C22-C23
29	j	302	CDL	CA4-CA3-OA5-PA1
29	I	301	CDL	C1-CA2-OA2-PA1
29	j3	302	CDL	CA4-CA3-OA5-PA1
35	m	301	PEE	C2-C1-O3P-P
35	j3	303	PEE	C2-C1-O3P-P
29	l	301	CDL	C52-C51-CB5-OB6
29	l3	301	CDL	C52-C51-CB5-OB6

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Mol	Chain	Res	Type	Atoms
35	m	301	PEE	C12-C13-C14-C15
29	a3	501	CDL	C32-C31-CA7-OA9
29	g3	305	CDL	C72-C71-CB7-OB9
29	P3	201	CDL	C12-C11-CA5-OA7
29	f3	303	CDL	C55-C56-C57-C58
29	B3	403	CDL	C20-C21-C22-C23
29	l	301	CDL	C32-C31-CA7-OA8
29	J	301	CDL	C32-C31-CA7-OA8
29	l3	301	CDL	C32-C31-CA7-OA8
29	L3	301	CDL	C14-C15-C16-C17
29	g	305	CDL	C72-C71-CB7-OB9
29	a3	502	CDL	C12-C13-C14-C15
29	i3	302	CDL	C56-C57-C58-C59
29	j3	302	CDL	OB5-CB3-CB4-CB6
29	K3	202	CDL	OB5-CB3-CB4-CB6
29	J	301	CDL	C51-C52-C53-C54
29	b3	401	CDL	C72-C73-C74-C75
29	p3	201	CDL	C31-C32-C33-C34
29	f	303	CDL	C72-C71-CB7-OB9
29	j	301	CDL	C12-C11-CA5-OA6
29	j3	301	CDL	C12-C11-CA5-OA6
29	b	401	CDL	C72-C73-C74-C75
29	i	301	CDL	C56-C57-C58-C59
29	i3	301	CDL	C17-C18-C19-C20
29	l3	301	CDL	C42-C43-C44-C45
29	A3	501	CDL	C71-C72-C73-C74
29	f	303	CDL	C55-C56-C57-C58
29	l	301	CDL	C20-C21-C22-C23
29	l3	301	CDL	C20-C21-C22-C23
29	a	501	CDL	C32-C31-CA7-OA9
29	r	201	CDL	C72-C71-CB7-OB9
29	I	301	CDL	C72-C71-CB7-OB9
29	f3	303	CDL	C72-C71-CB7-OB9
35	j3	303	PEE	O4-C10-C11-C12
29	p	201	CDL	C31-C32-C33-C34
29	I	301	CDL	C61-C62-C63-C64
29	I3	301	CDL	C61-C62-C63-C64
29	j3	301	CDL	C32-C31-CA7-OA8
29	F3	302	CDL	C52-C51-CB5-OB6
29	J3	301	CDL	C32-C31-CA7-OA8
33	C1	601	ATP	PB-O3A-PA-O1A
33	A2	601	ATP	PB-O3A-PA-O2A

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Mol	Chain	Res	Type	Atoms
33	C4	601	ATP	PB-O3A-PA-O1A
33	A5	601	ATP	PB-O3A-PA-O2A
29	I3	301	CDL	C72-C71-CB7-OB9
29	J3	301	CDL	C72-C71-CB7-OB9
29	J3	301	CDL	C51-C52-C53-C54
29	l	301	CDL	C42-C43-C44-C45
29	A	502	CDL	C71-C72-C73-C74
29	L	301	CDL	C14-C15-C16-C17
29	B	404	CDL	C32-C31-CA7-OA8
29	F	303	CDL	C52-C51-CB5-OB6
30	G3	303	PC1	C29-C2A-C2B-C2C
29	B	403	CDL	C34-C35-C36-C37

There are no ring outliers.

61 monomers are involved in 153 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	I	303	UQ8	8	0
35	L	303	PEE	1	0
33	G	301	ATP	1	0
29	f	303	CDL	3	0
36	e3	900	NAD	2	0
33	C5	601	ATP	1	0
29	b3	401	CDL	1	0
29	K3	202	CDL	1	0
32	i3	303	UQ8	5	0
29	A3	501	CDL	1	0
29	F	302	CDL	12	0
29	L	302	CDL	7	0
29	l3	303	CDL	3	0
29	a	501	CDL	2	0
33	g3	301	ATP	1	0
33	g	301	ATP	1	0
29	I	301	CDL	3	0
33	G3	301	ATP	2	0
29	r	201	CDL	1	0
29	k3	201	CDL	1	0
30	D3	301	PC1	1	0
29	f3	303	CDL	2	0
29	f	304	CDL	1	0
29	I3	301	CDL	5	0
29	i3	301	CDL	2	0

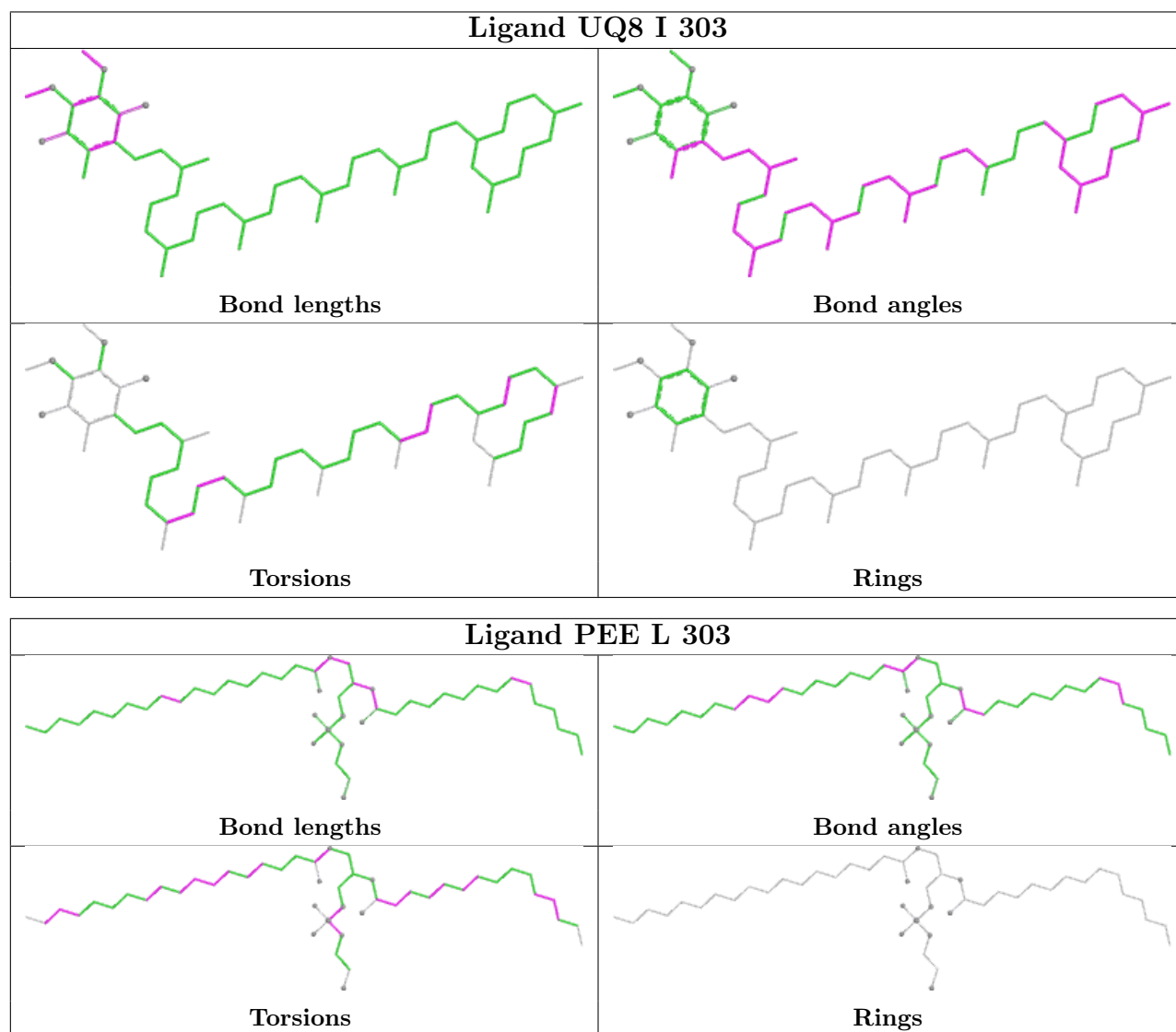
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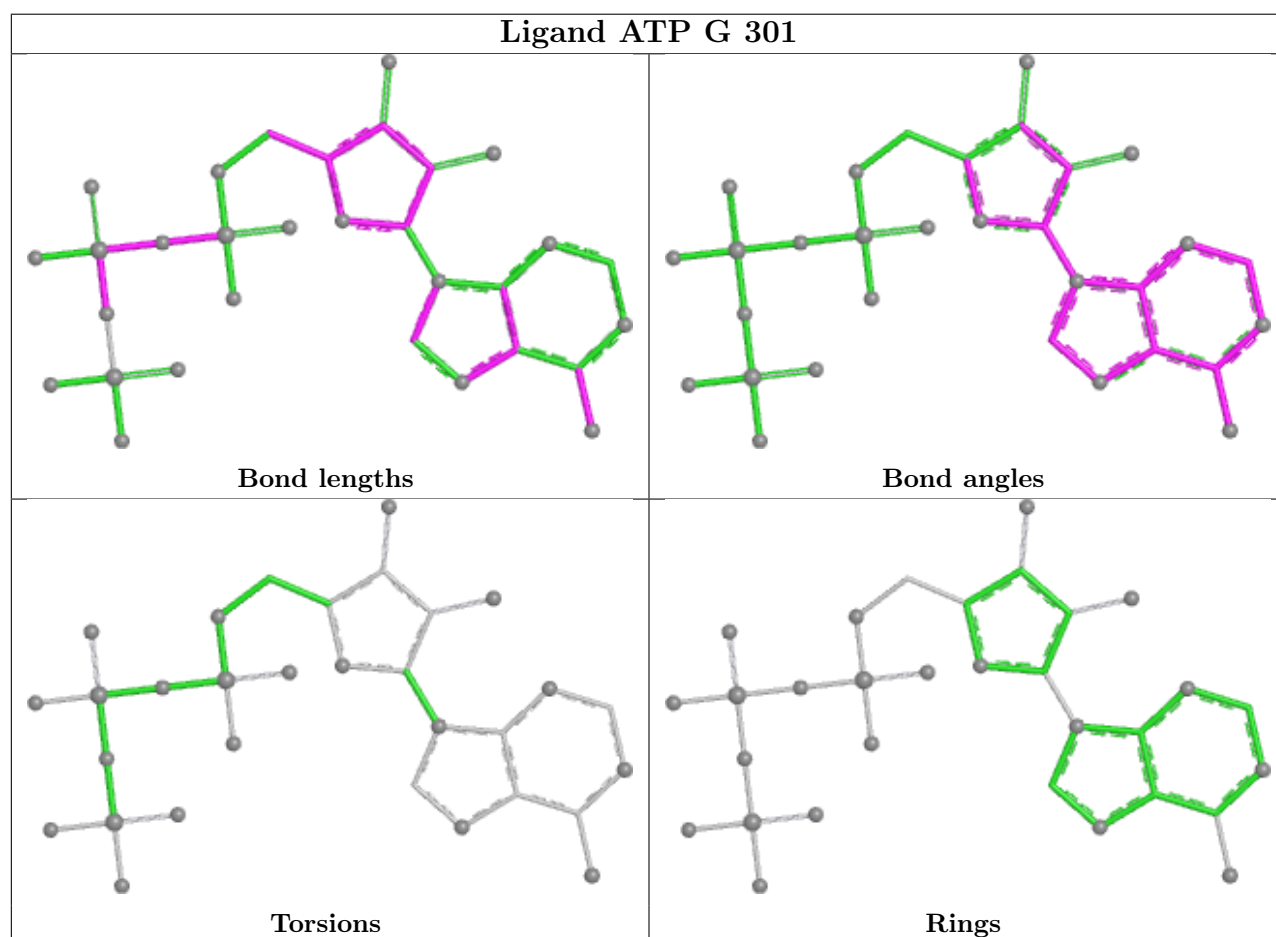
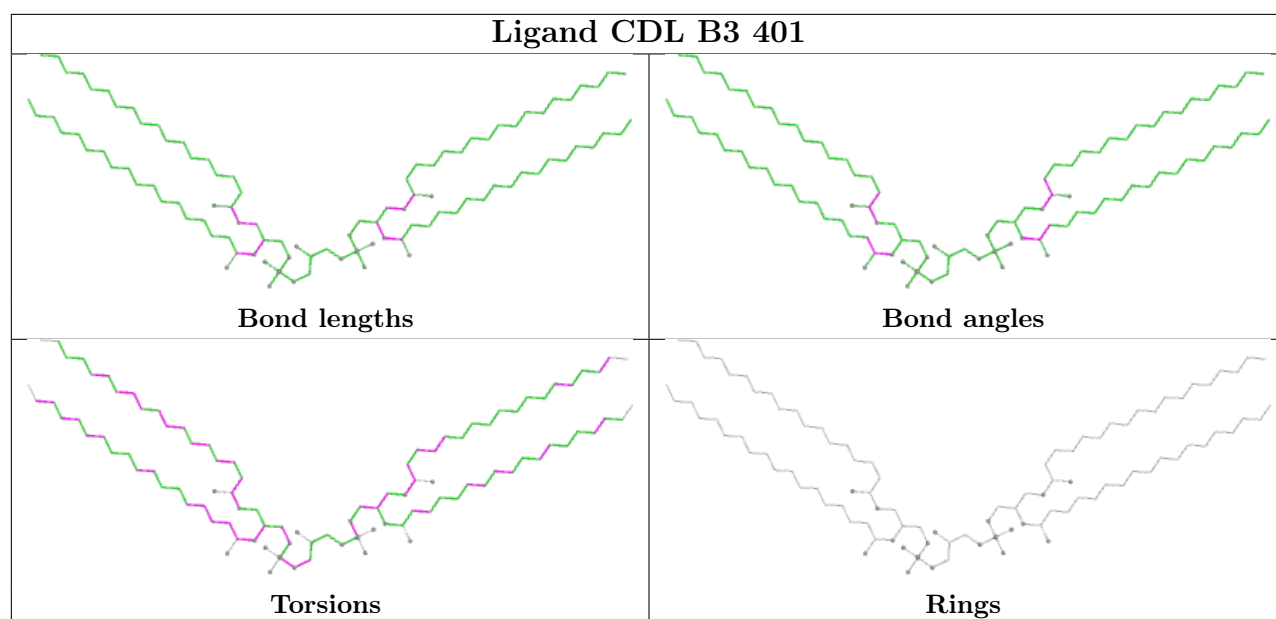
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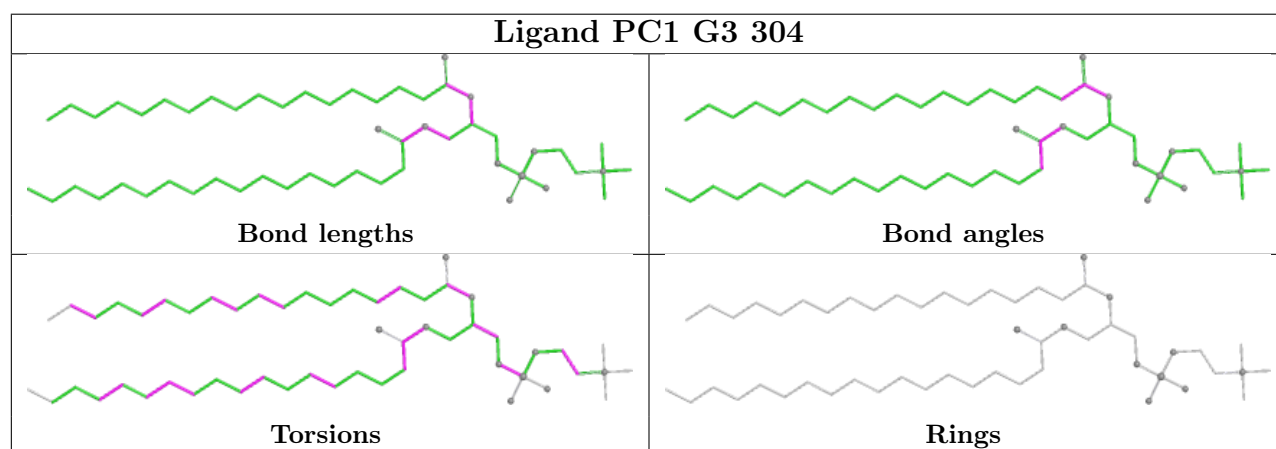
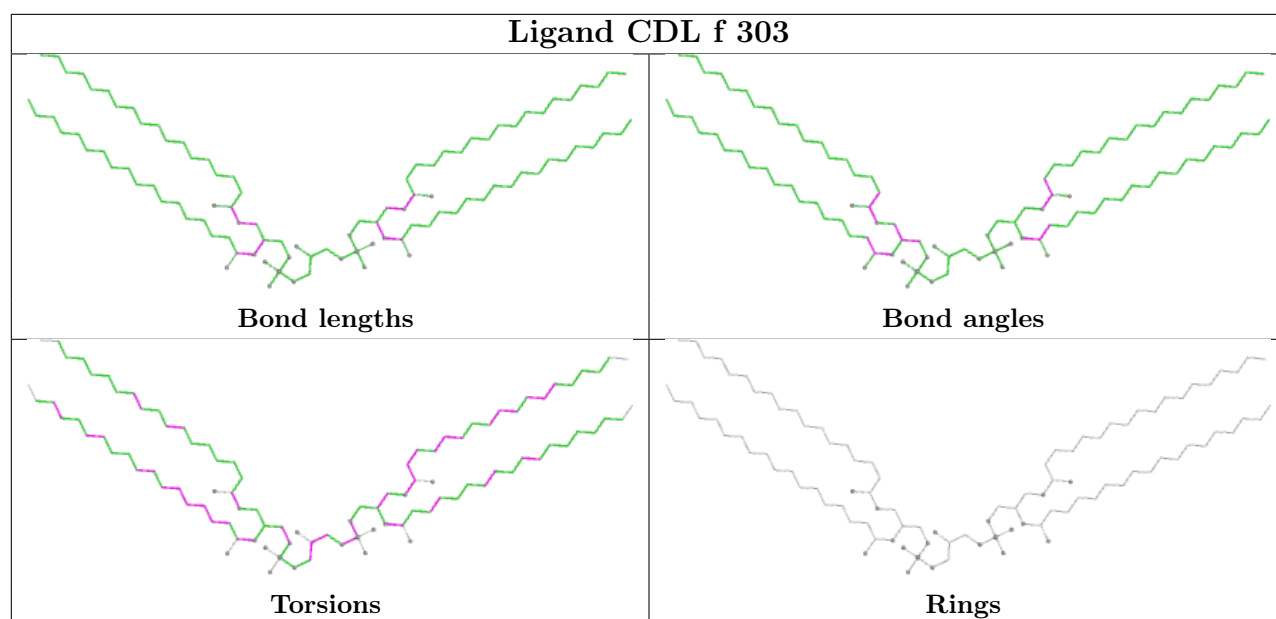
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	a3	502	CDL	14	0
31	f	301	PO4	1	0
29	B	403	CDL	1	0
29	B3	404	CDL	3	0
33	B5	1003	ATP	2	0
33	B4	1003	ATP	2	0
29	B3	402	CDL	3	0
29	g	305	CDL	1	0
29	I3	302	CDL	9	0
29	b	401	CDL	1	0
33	B1	1003	ATP	2	0
29	l	302	CDL	3	0
29	l	301	CDL	4	0
29	L	301	CDL	1	0
33	B2	1003	ATP	2	0
29	B	404	CDL	4	0
30	G	303	PC1	1	0
33	A1	601	ATP	1	0
29	I3	301	CDL	4	0
29	B	402	CDL	3	0
29	g3	305	CDL	1	0
29	K	201	CDL	1	0
29	B3	403	CDL	2	0
29	F	303	CDL	2	0
33	C2	601	ATP	1	0
37	D1	501	ADP	2	0
29	K3	201	CDL	1	0
29	F3	302	CDL	2	0
35	a3	503	PEE	1	0
32	I3	304	UQ8	7	0
36	E	900	NAD	1	0
29	L3	301	CDL	1	0
32	i	302	UQ8	5	0
29	k	201	CDL	1	0
35	J	303	PEE	1	0
30	G3	303	PC1	1	0

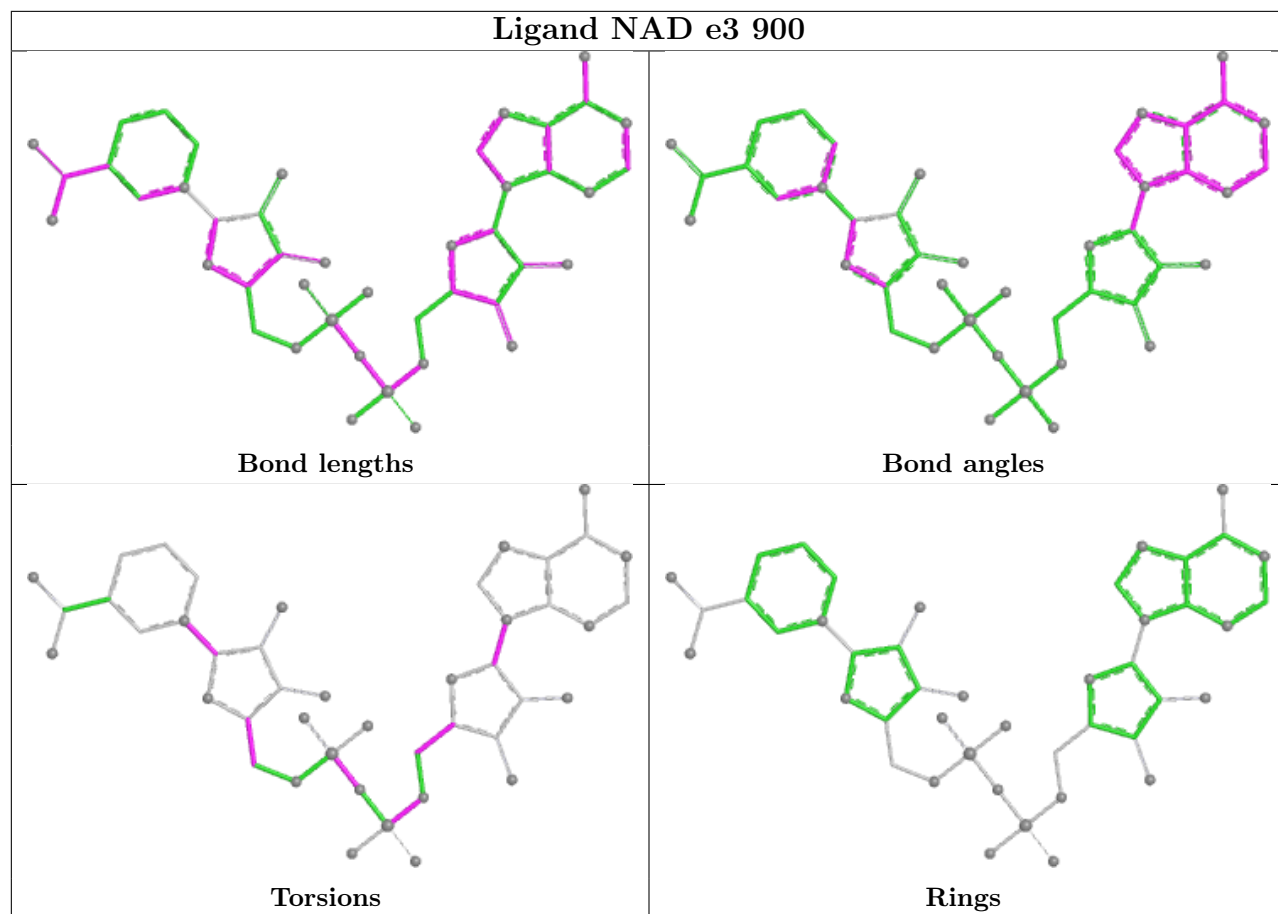
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

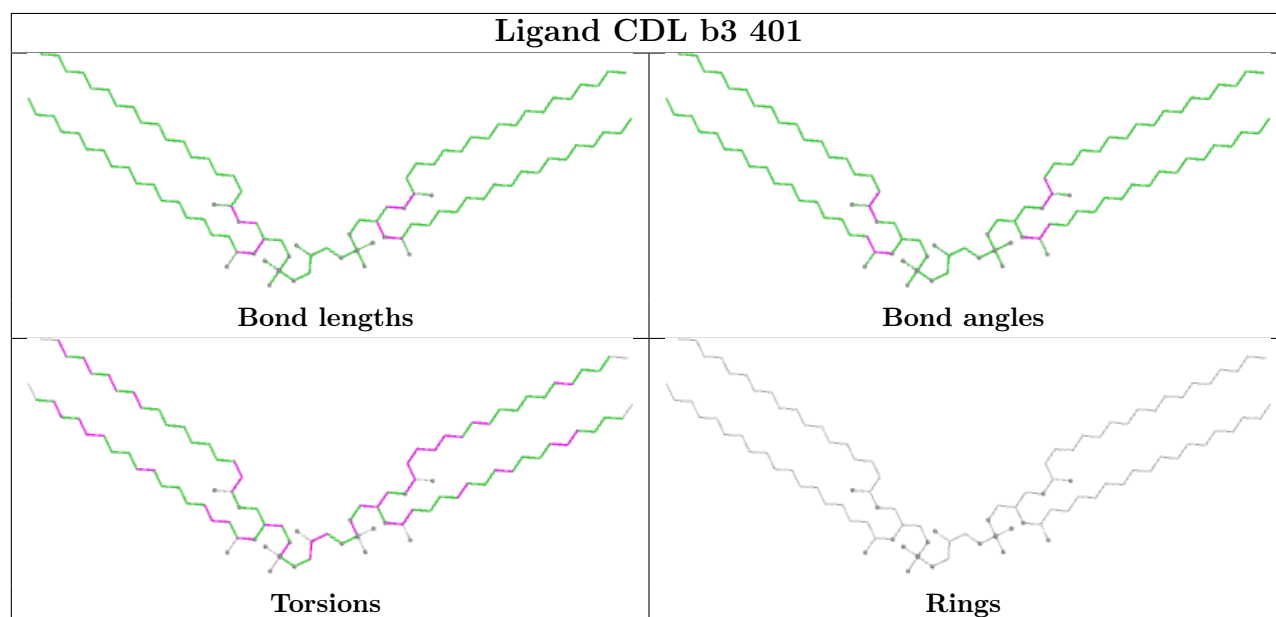
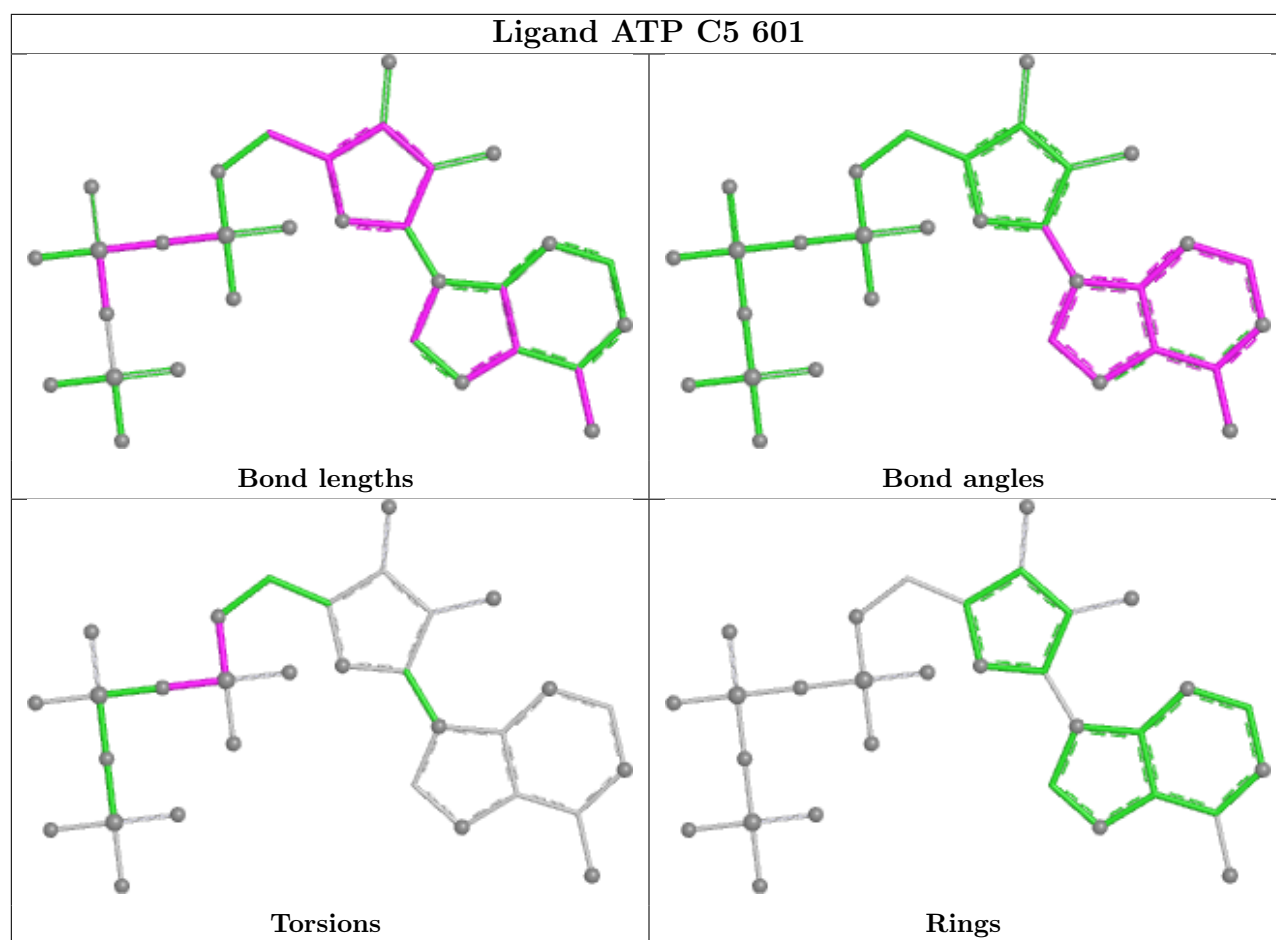
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

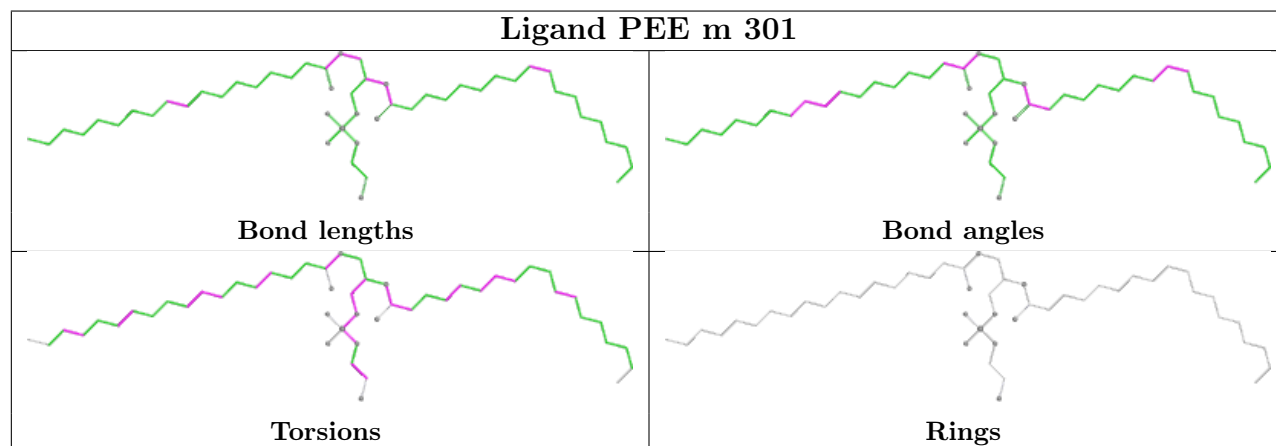
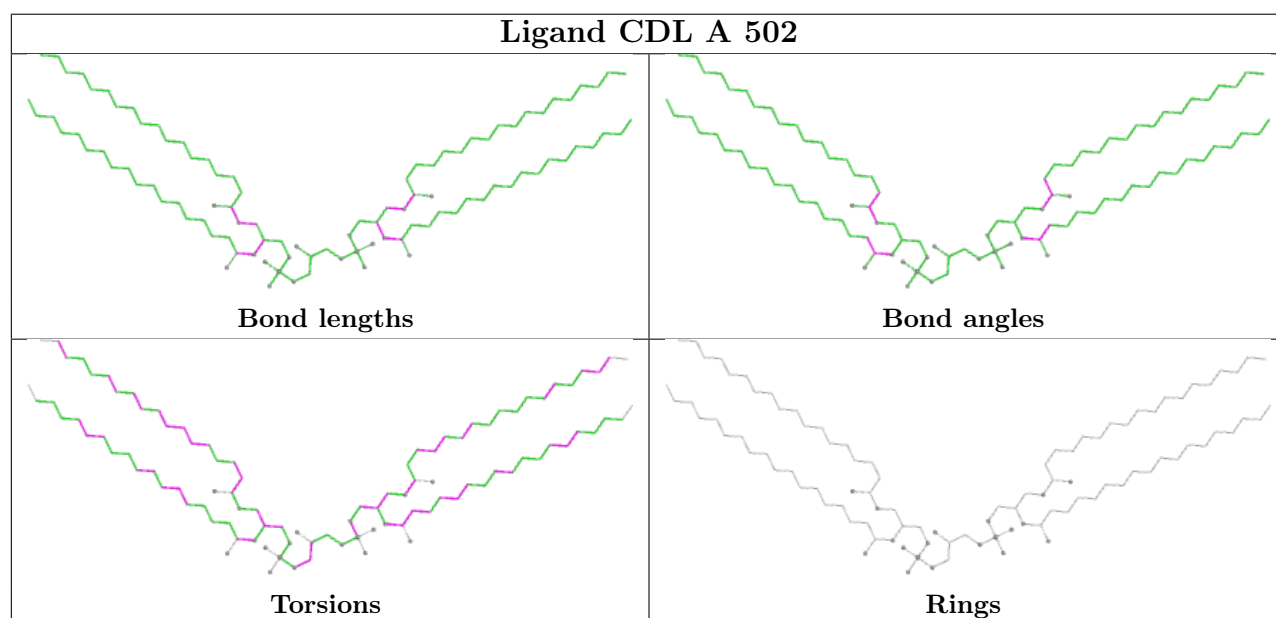
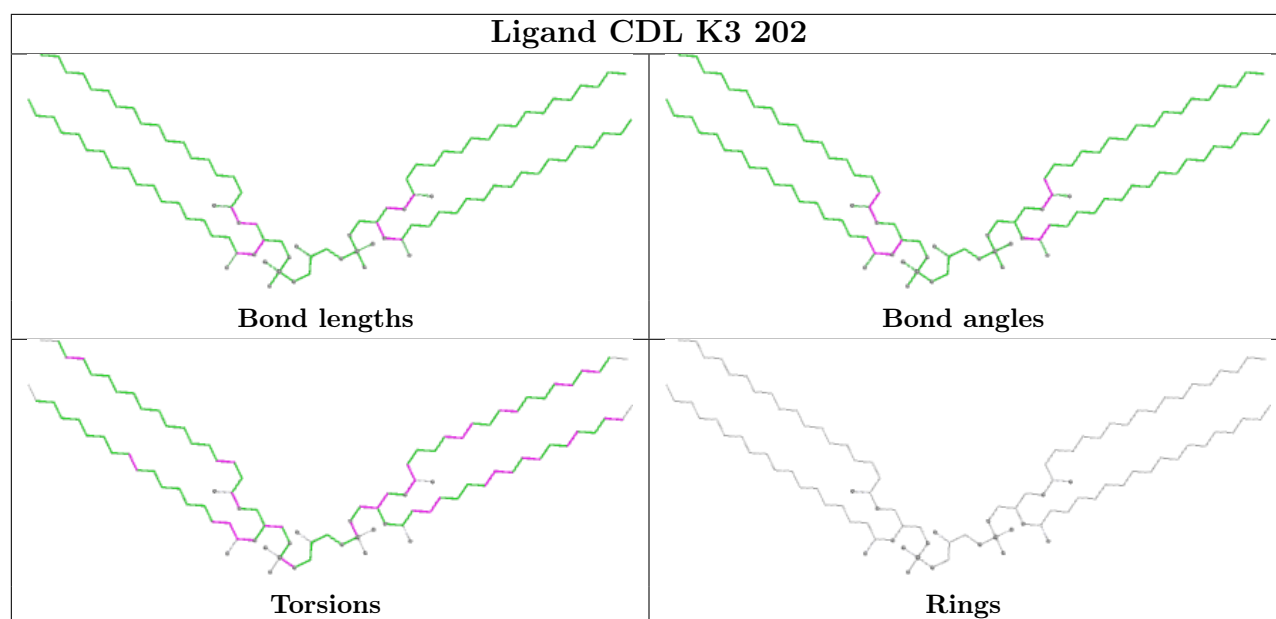


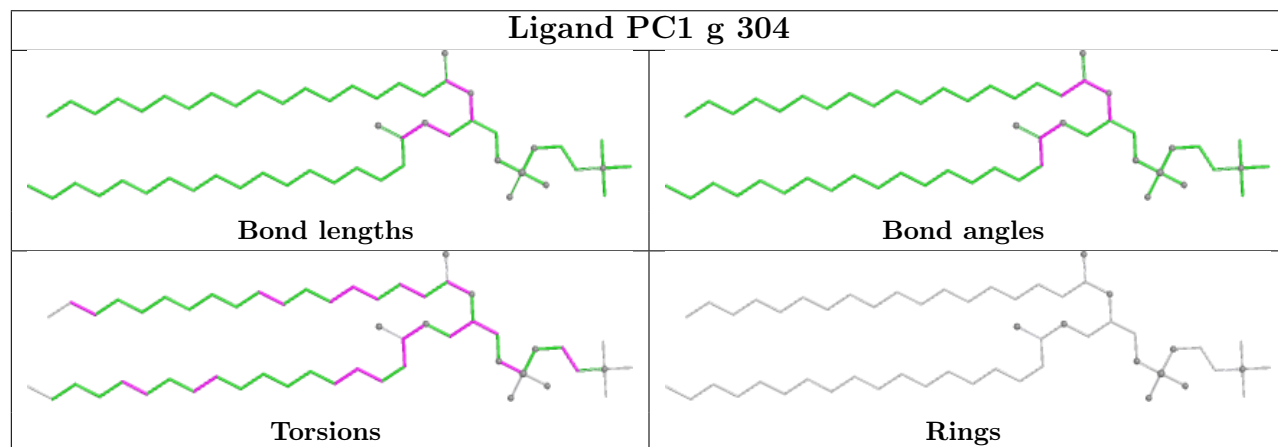
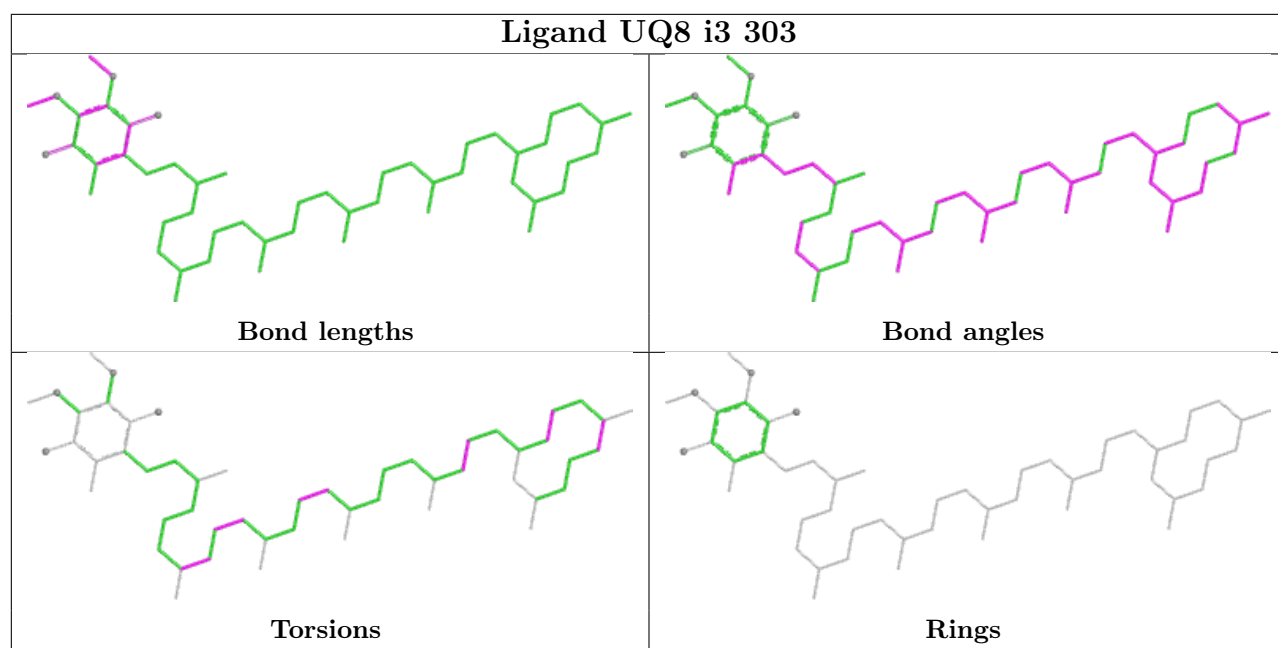


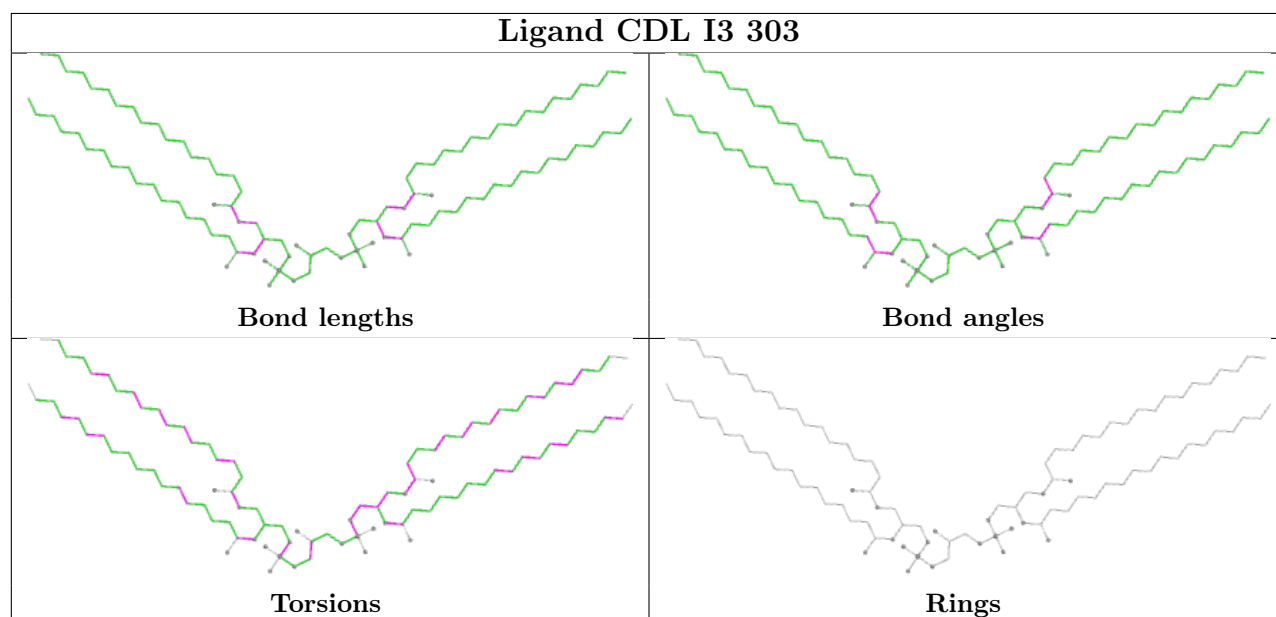
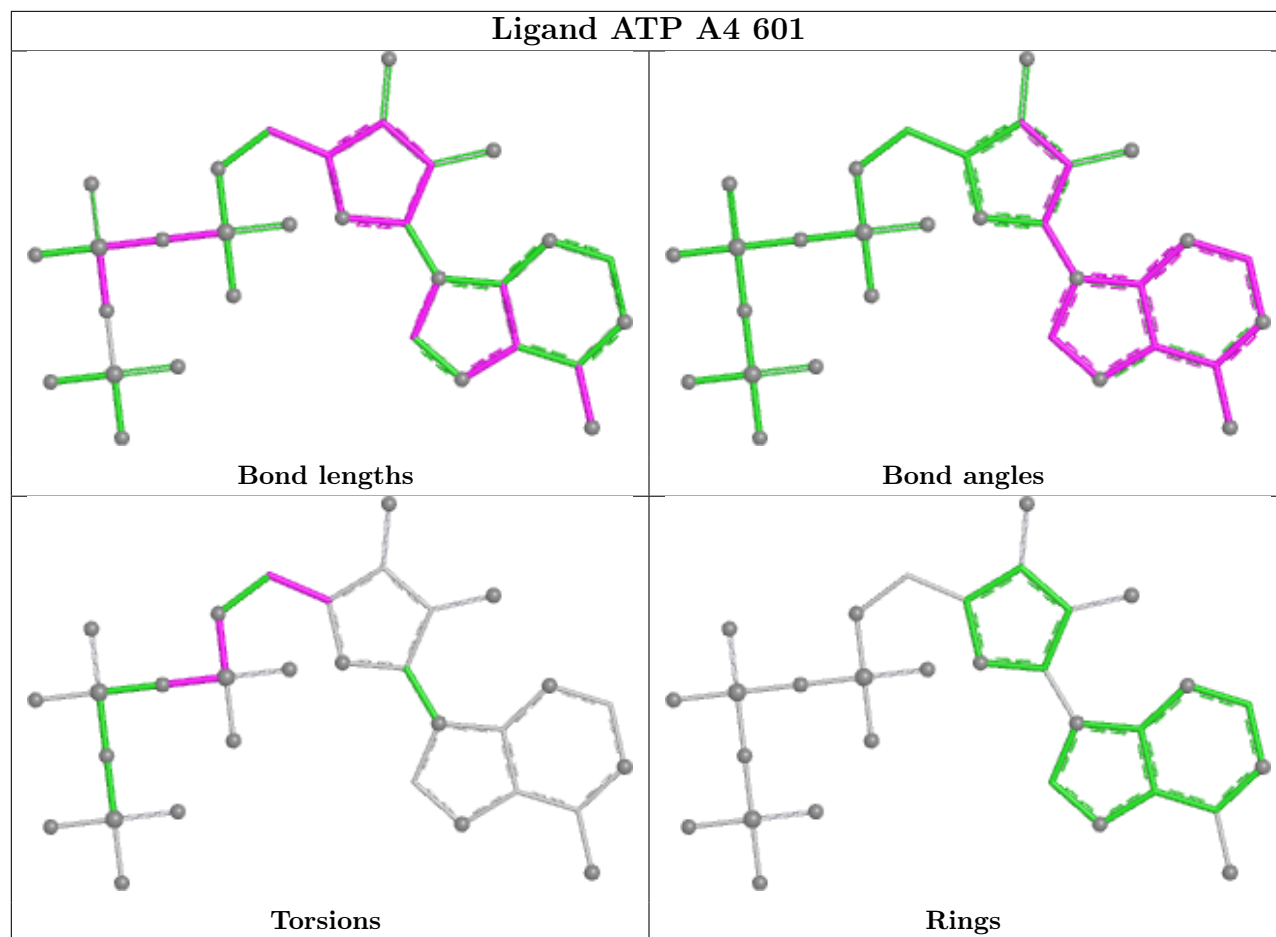


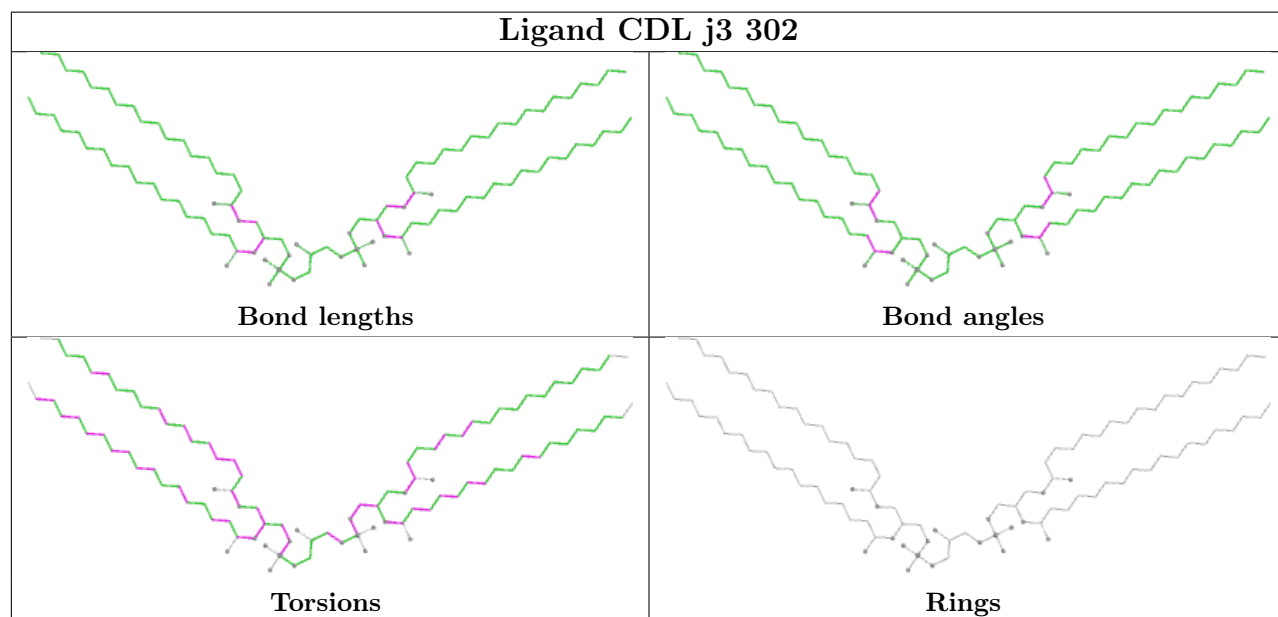
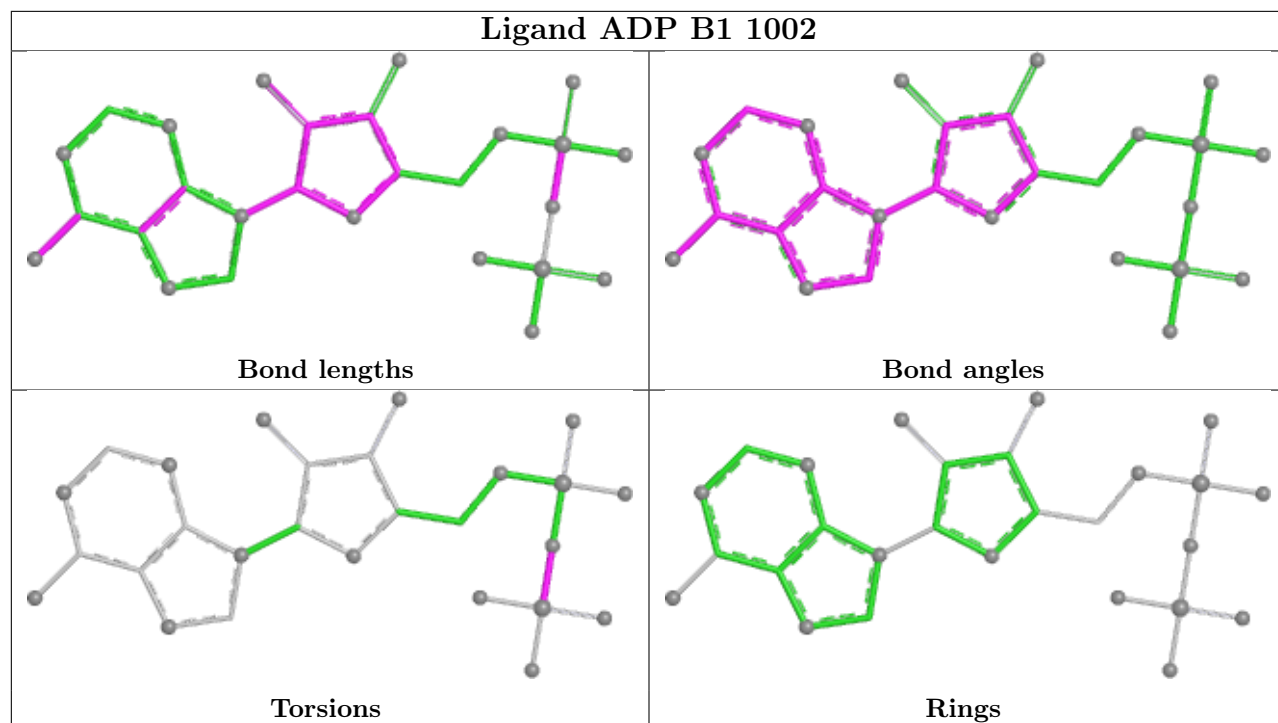


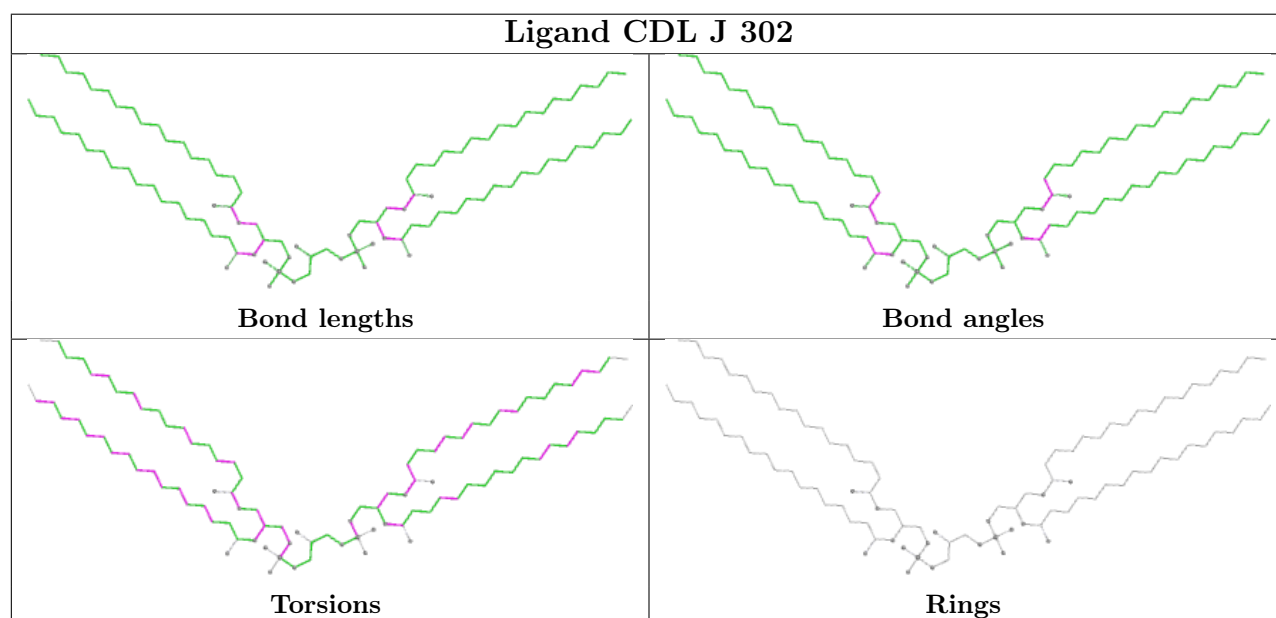
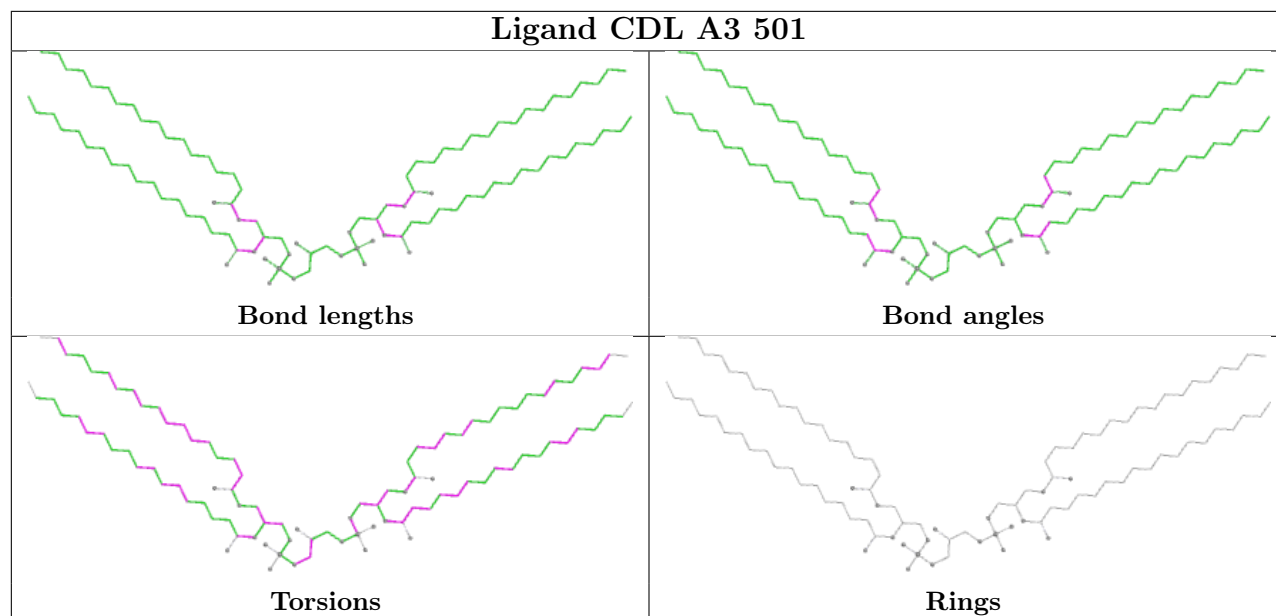


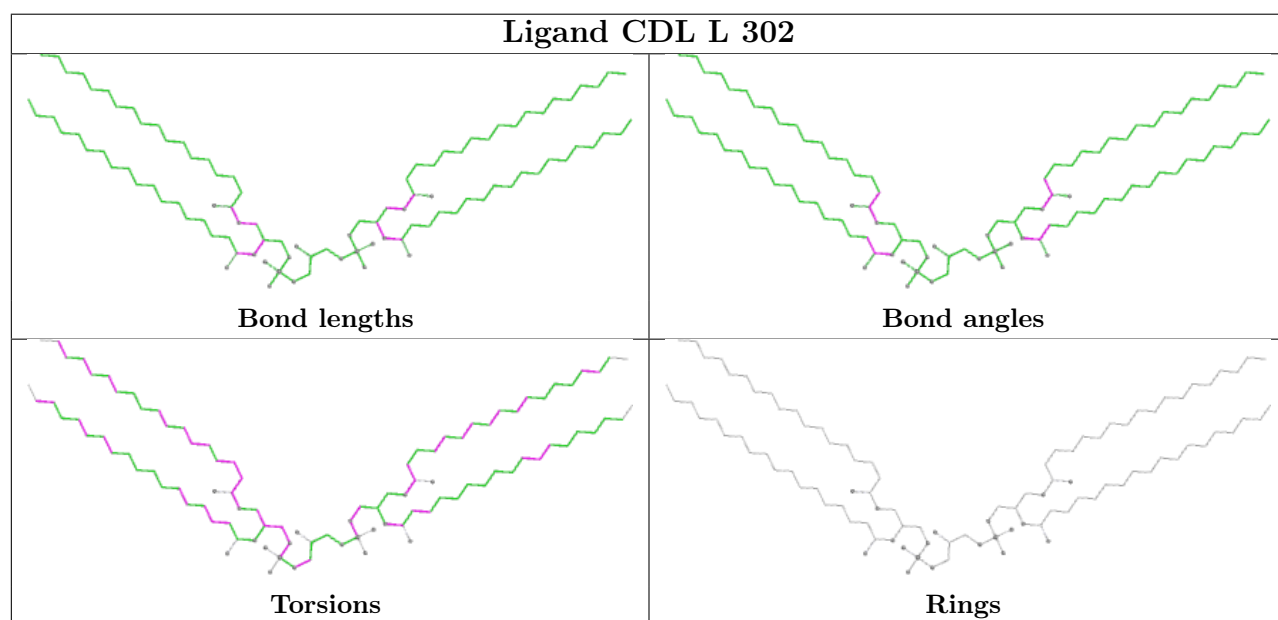
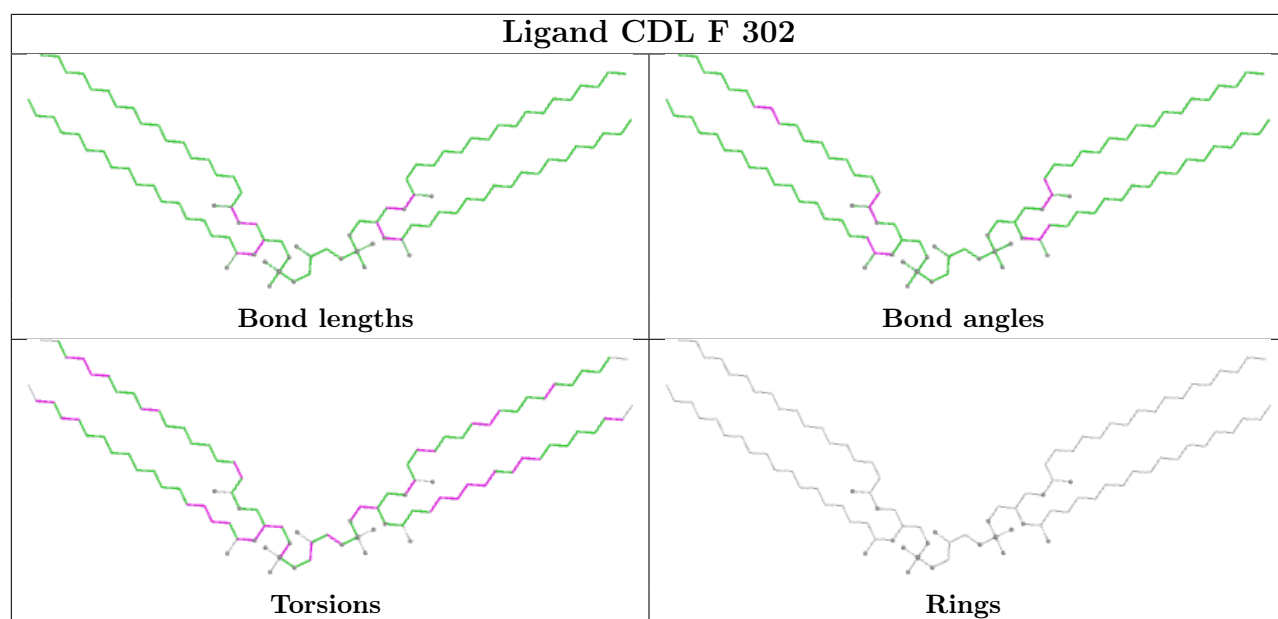


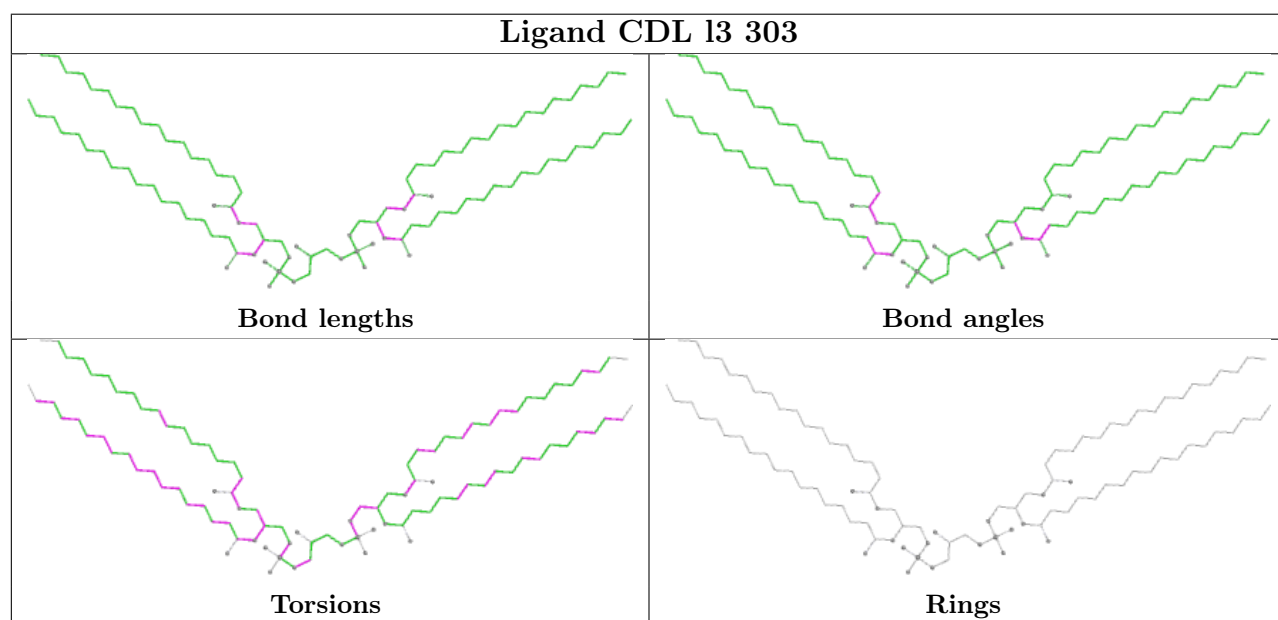
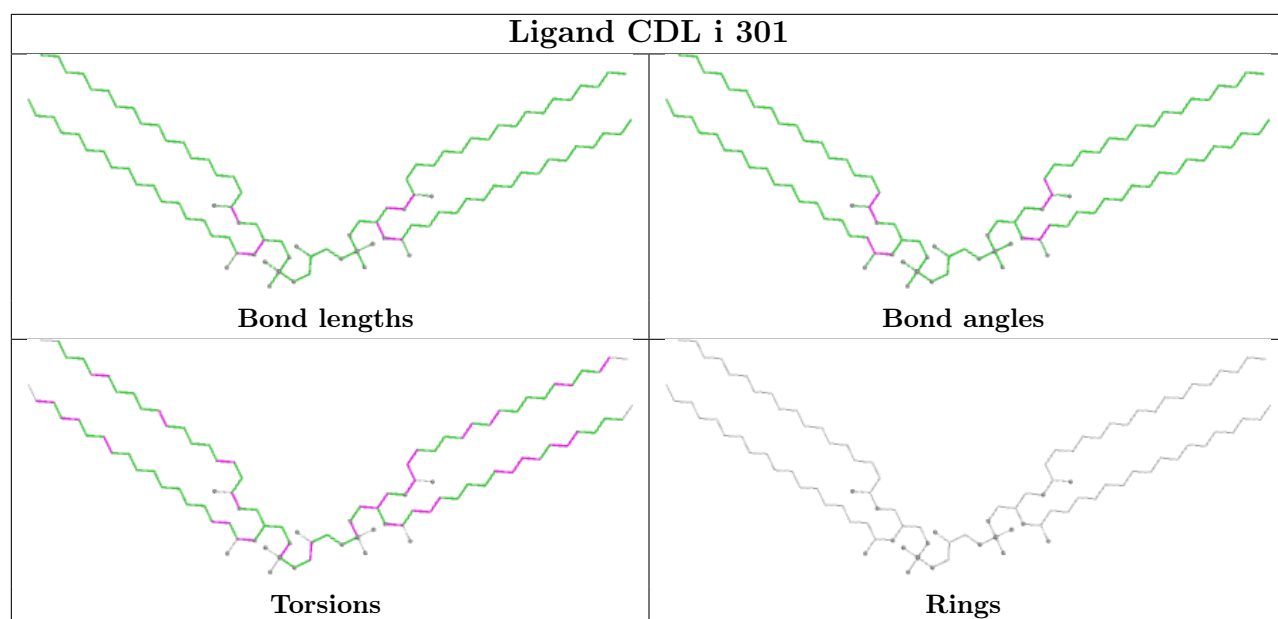


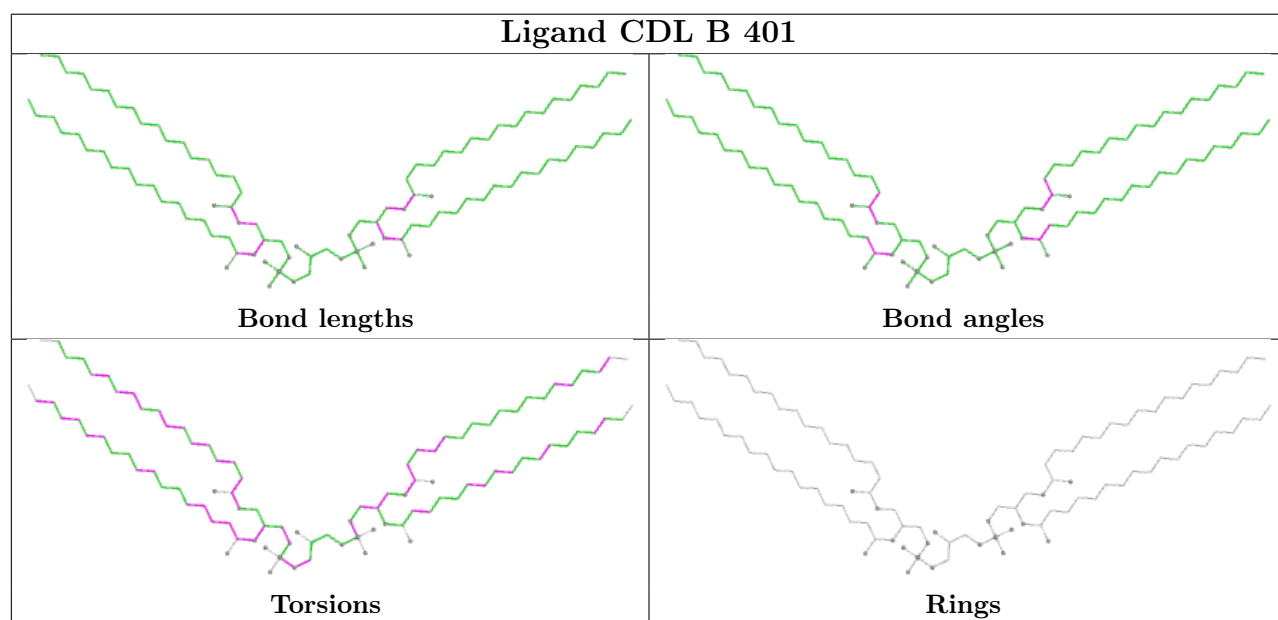
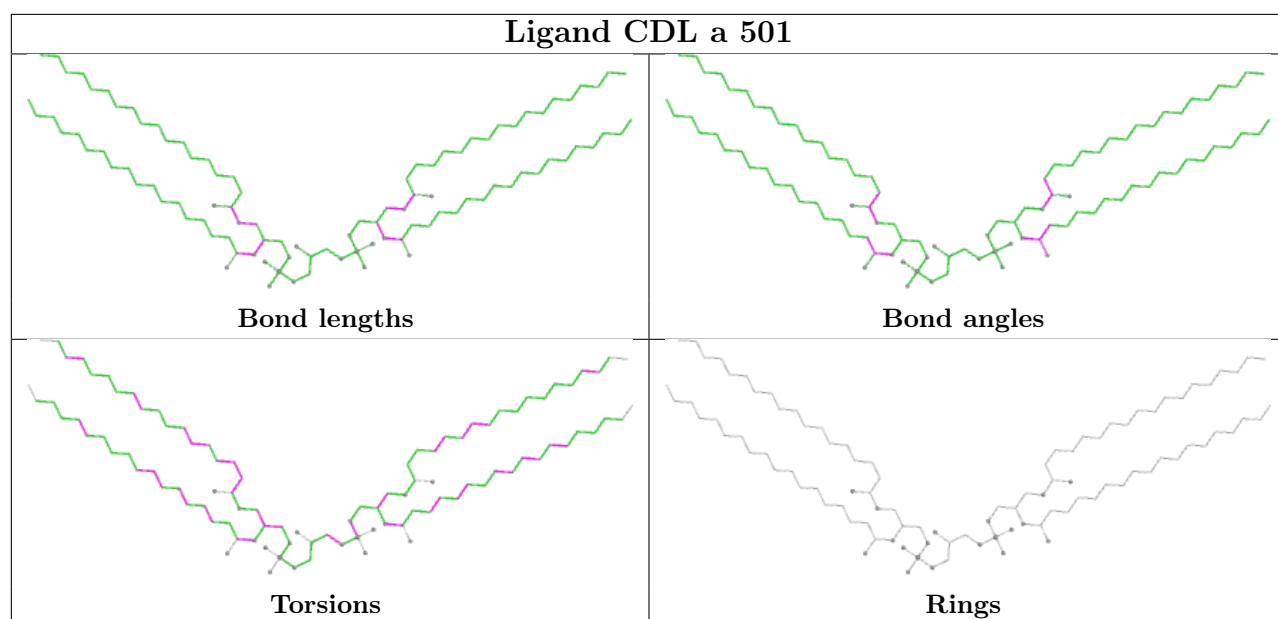


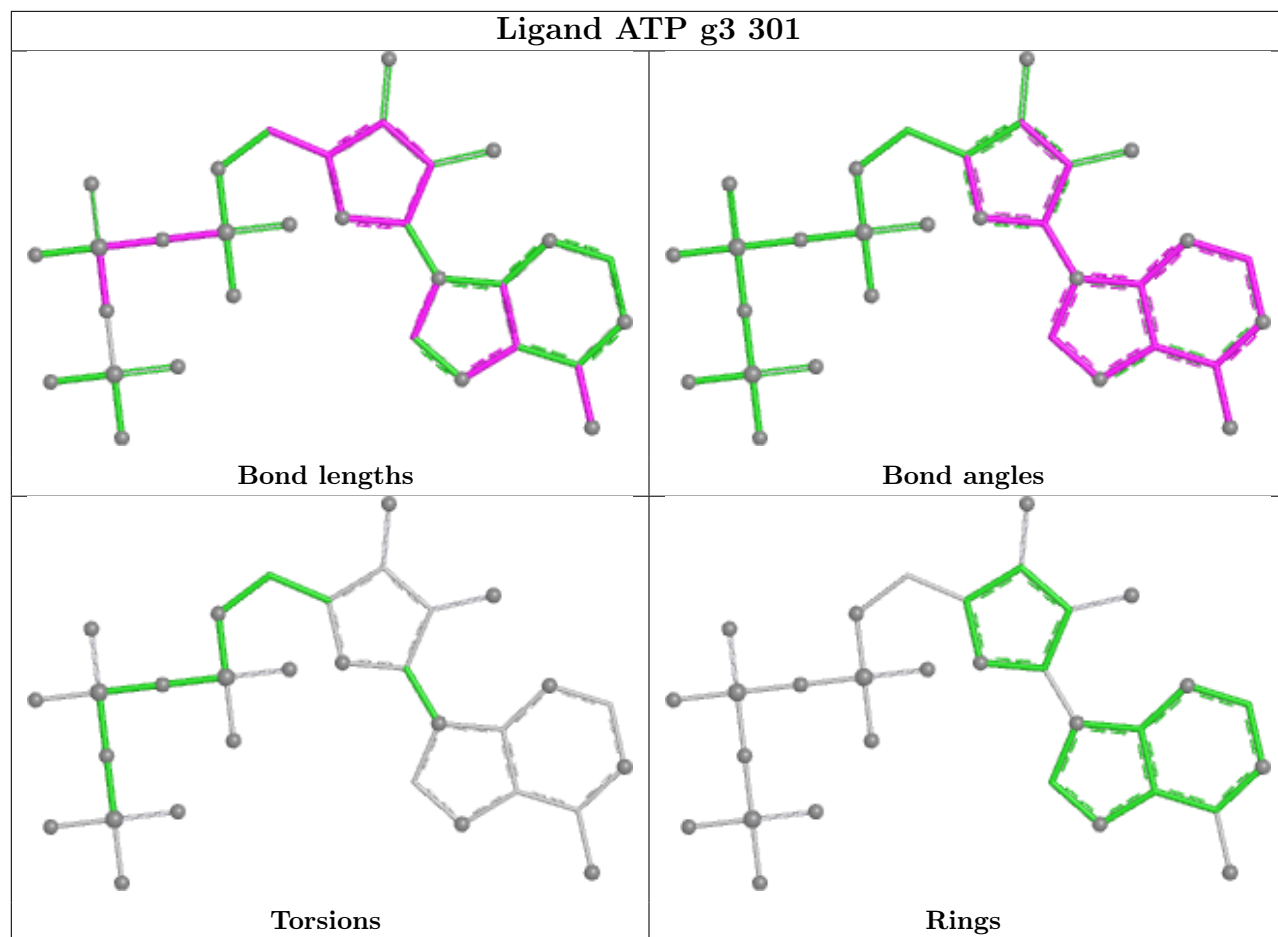




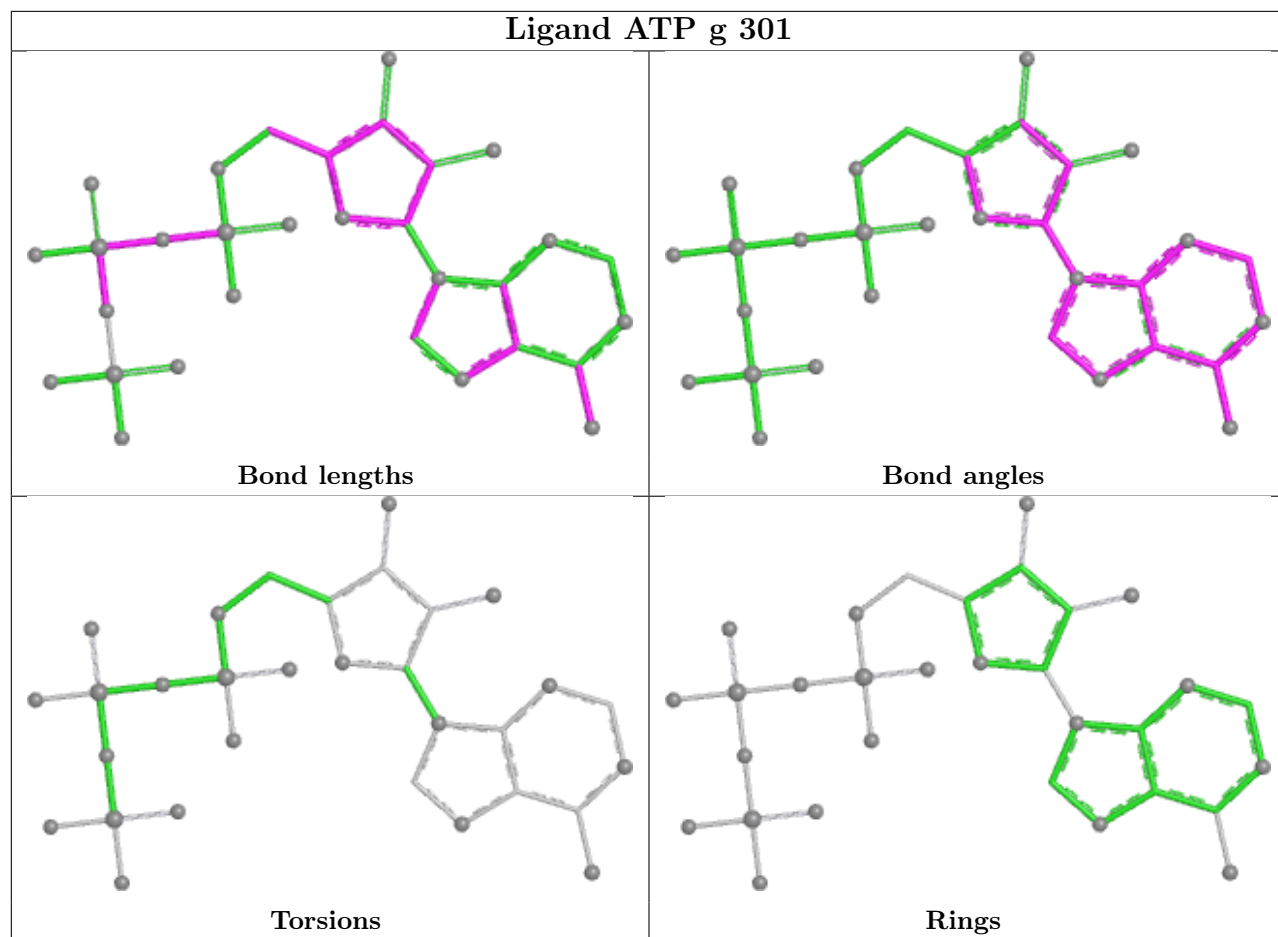




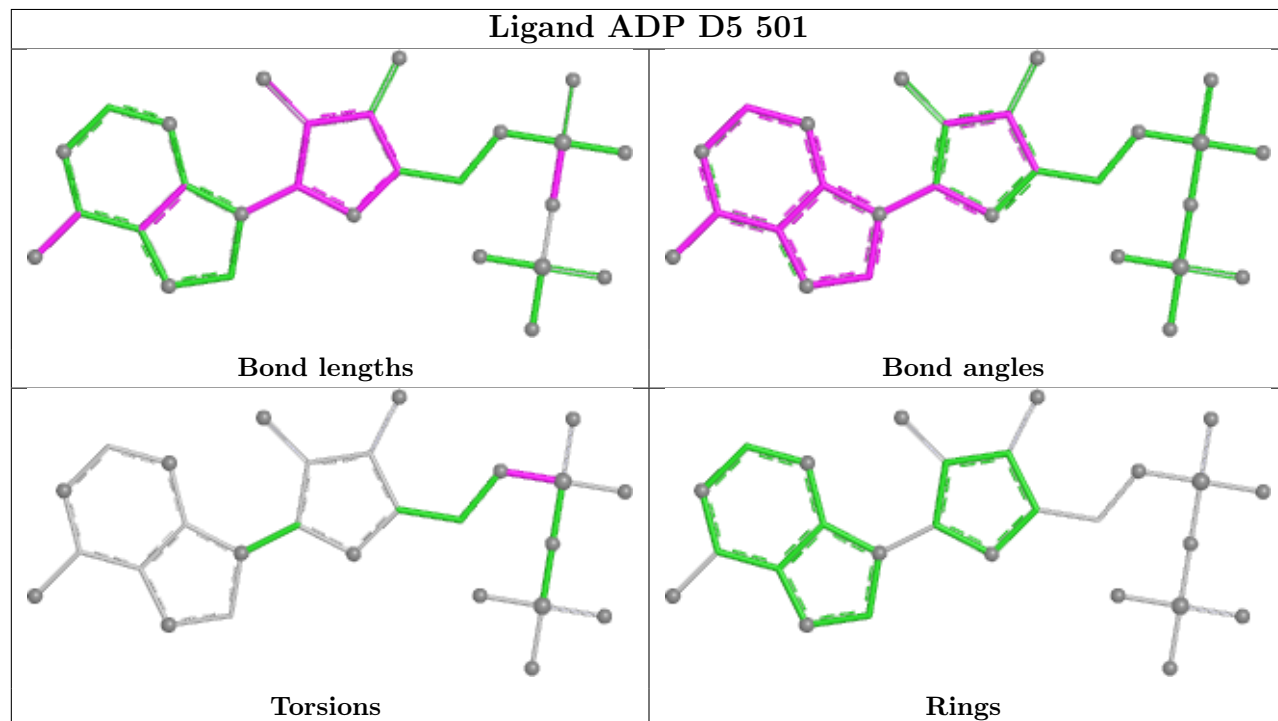


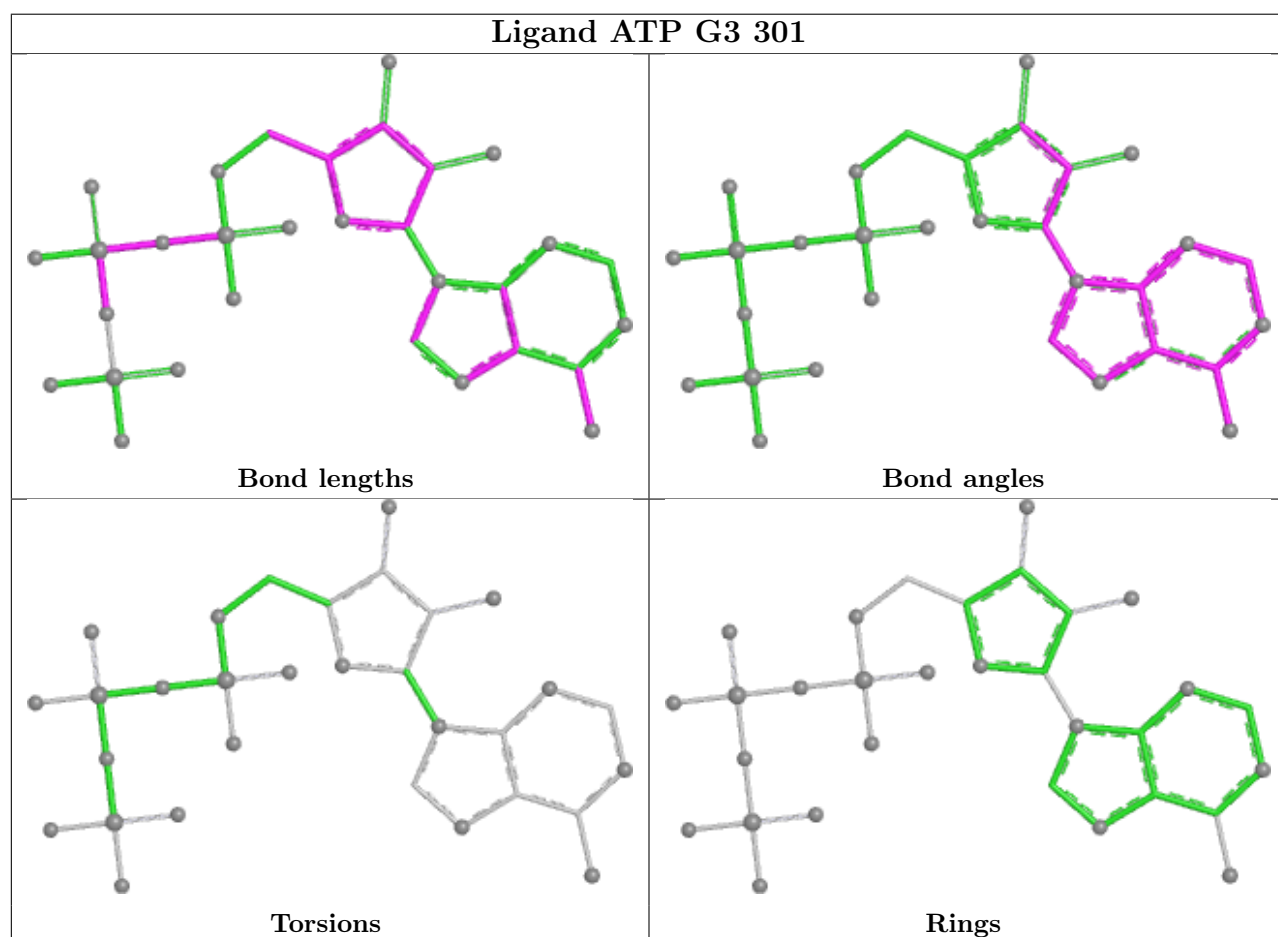
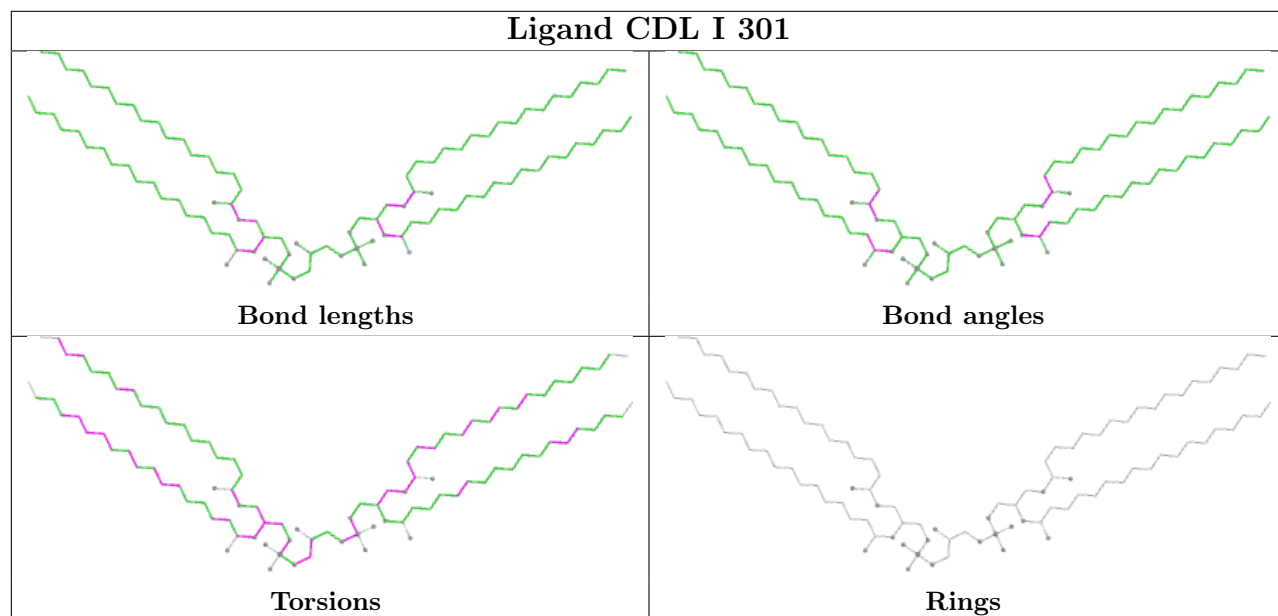


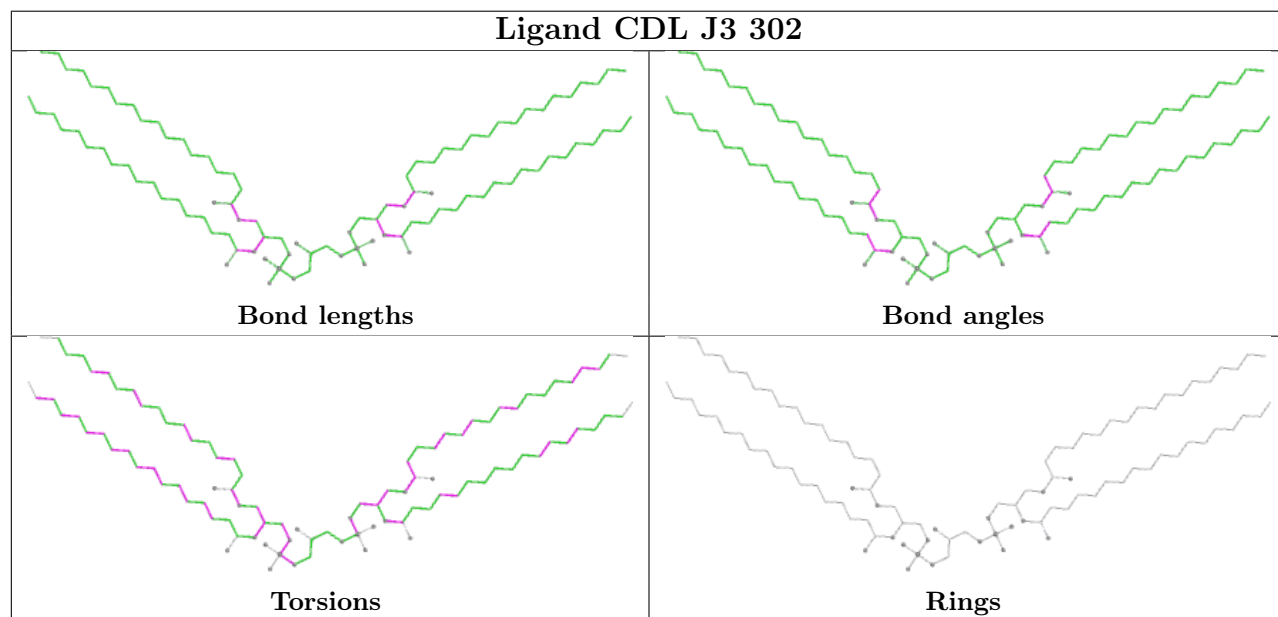
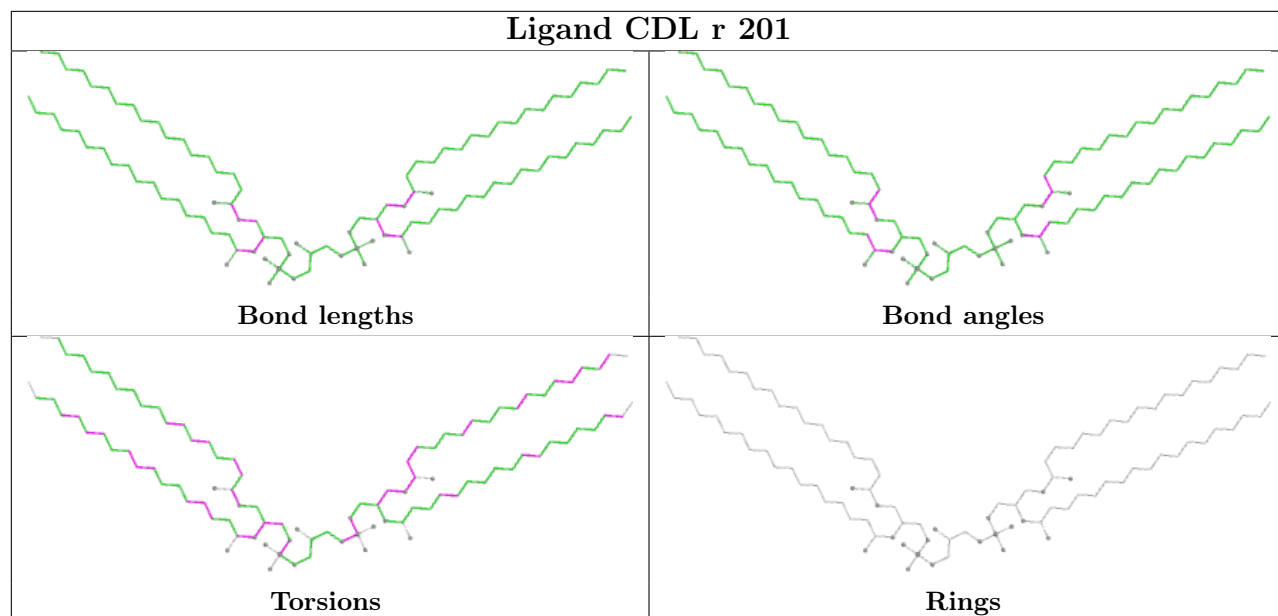
Ligand ATP g 301

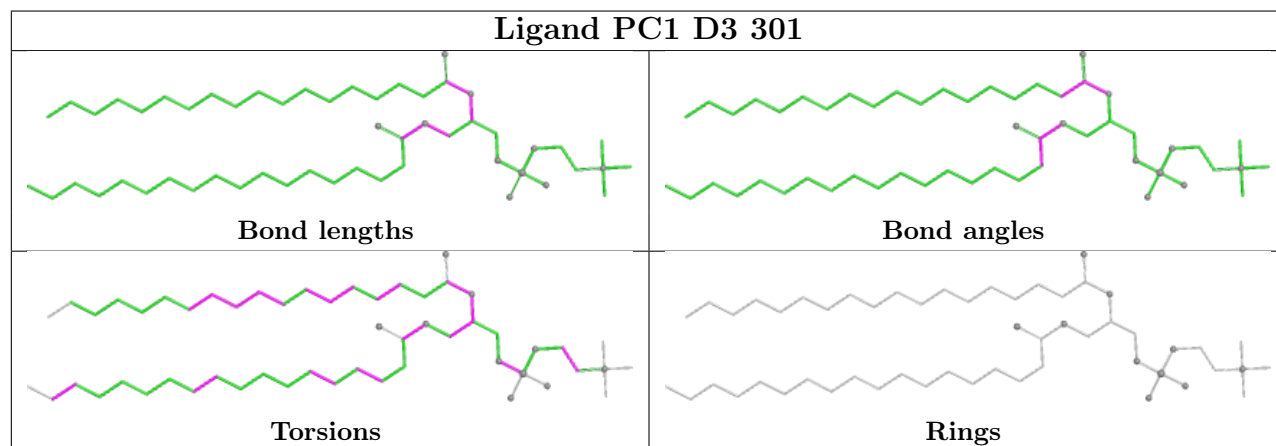
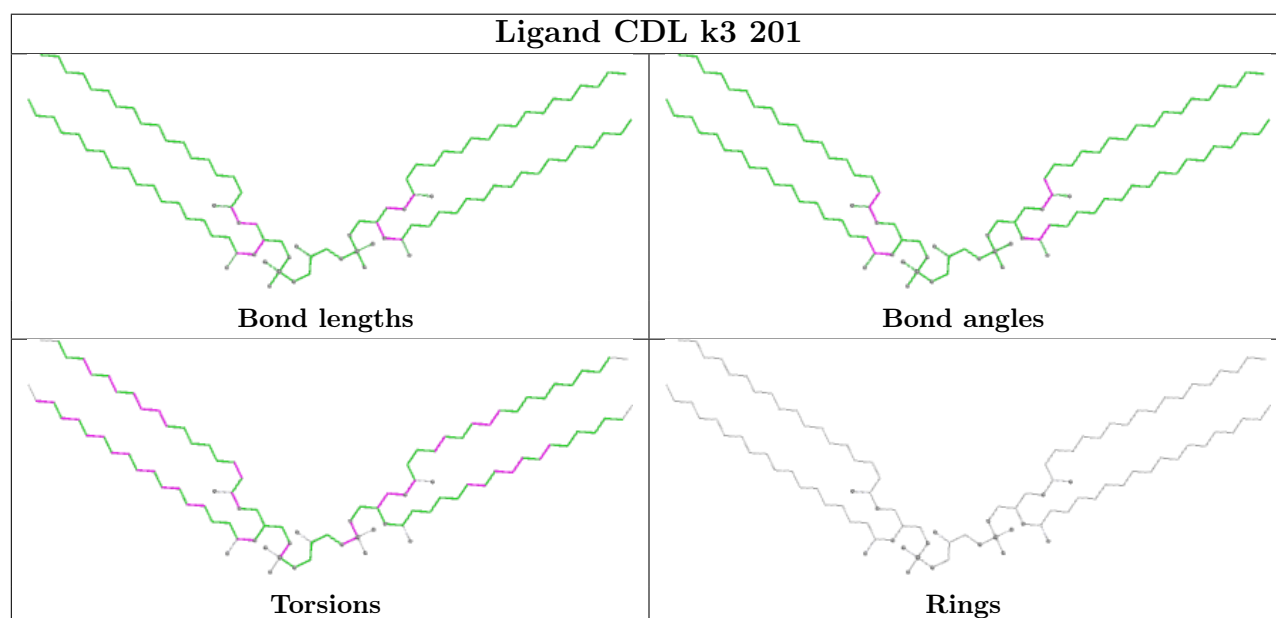
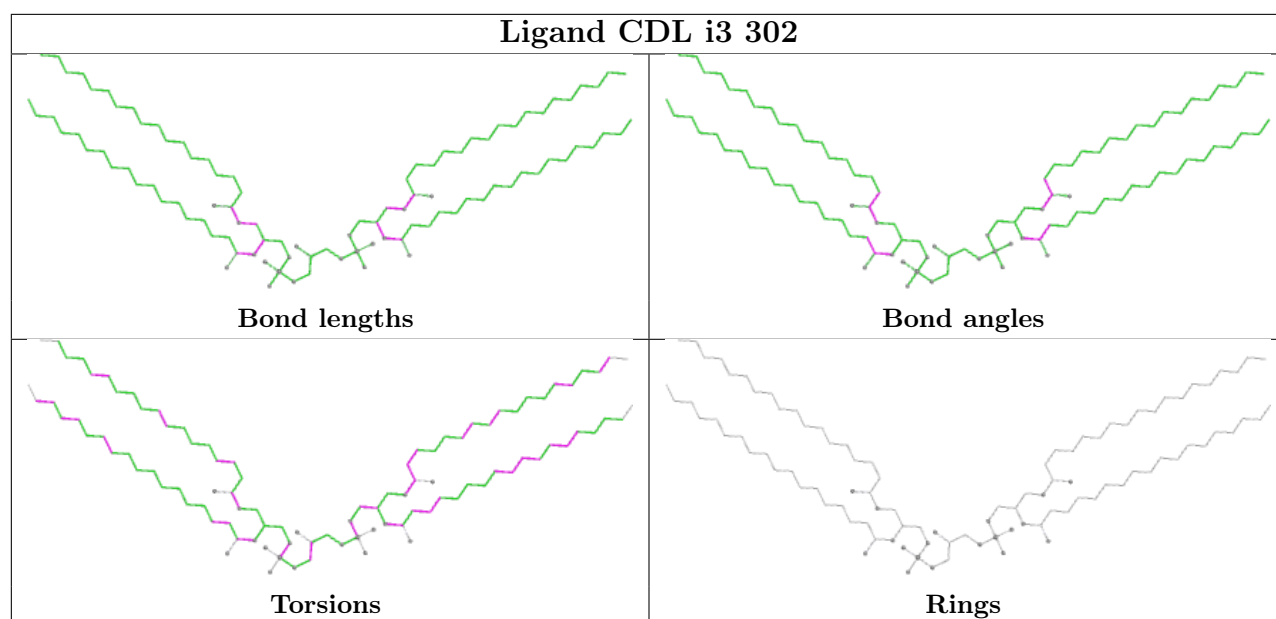


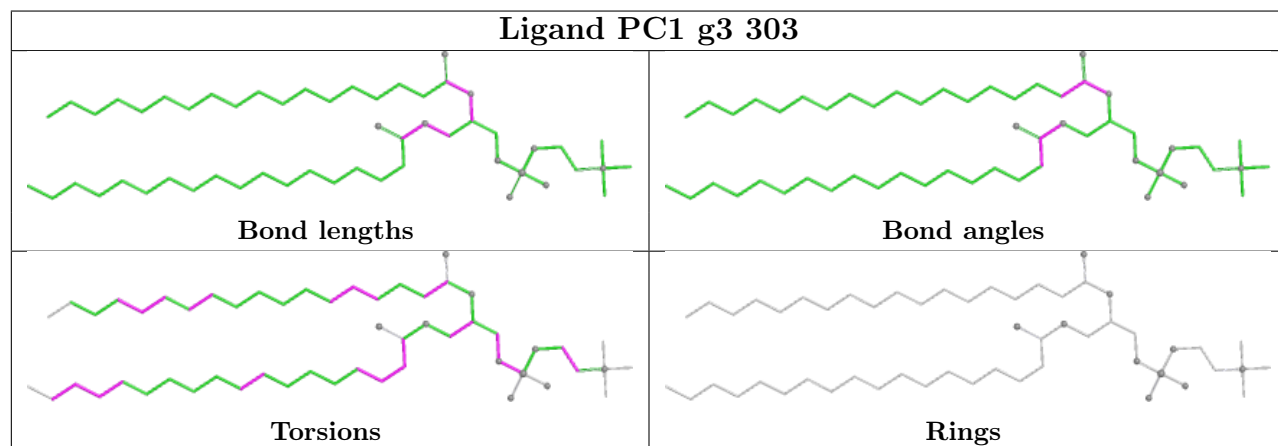
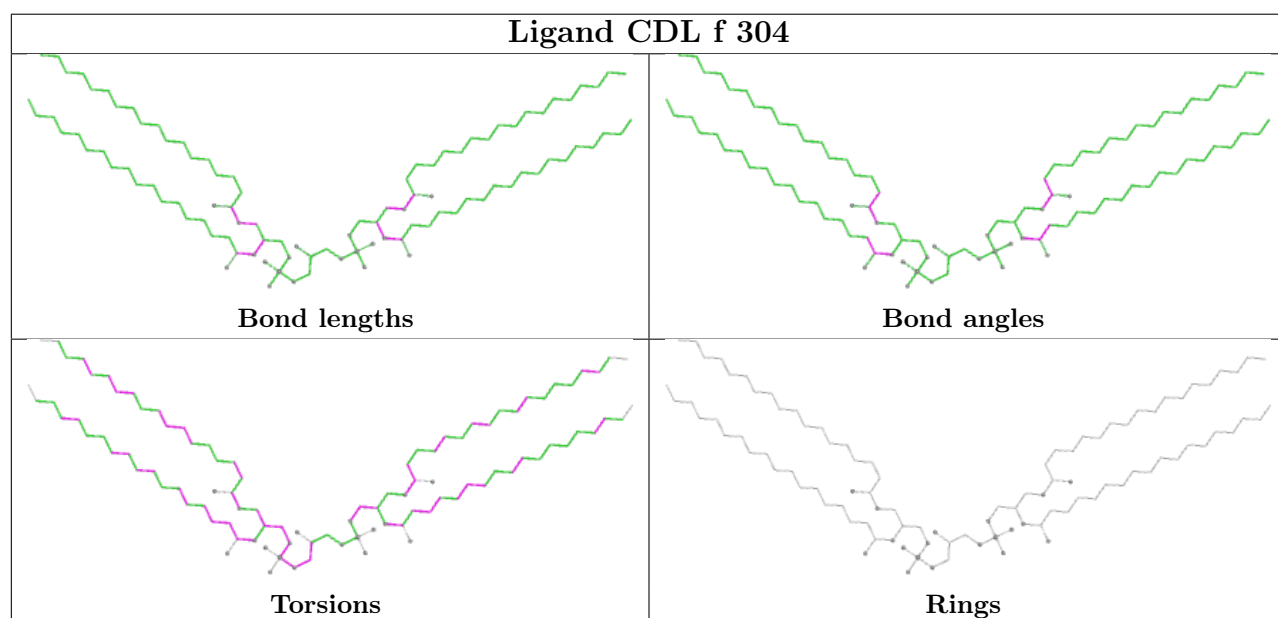
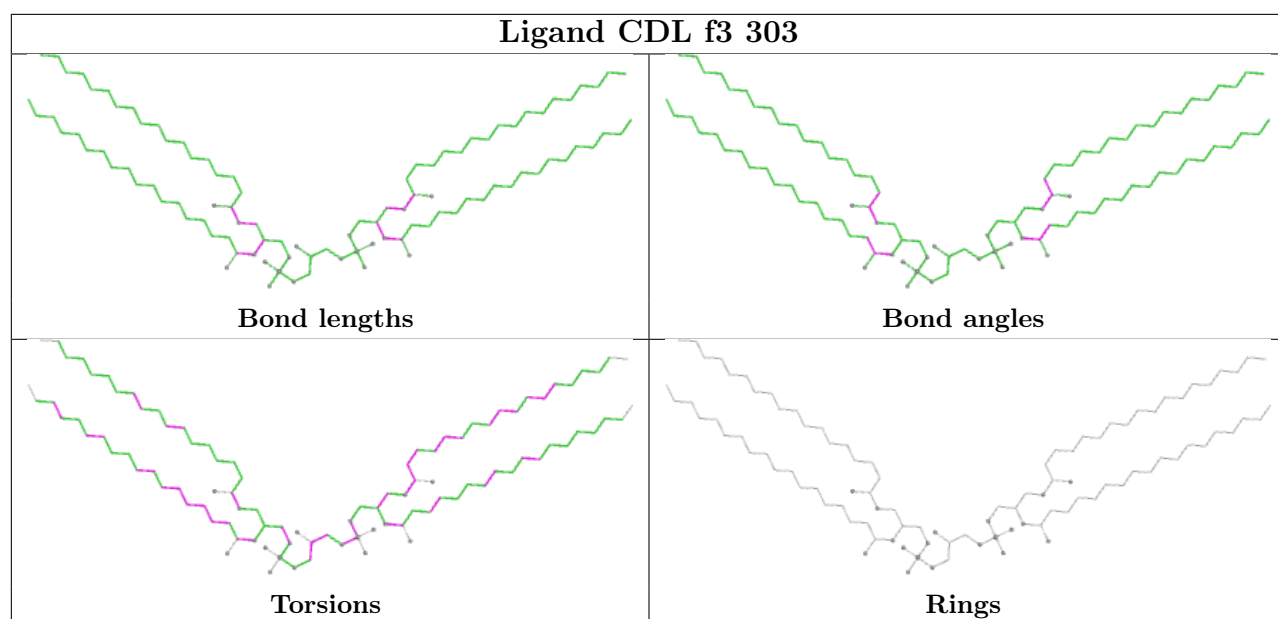
Ligand ADP D5 501

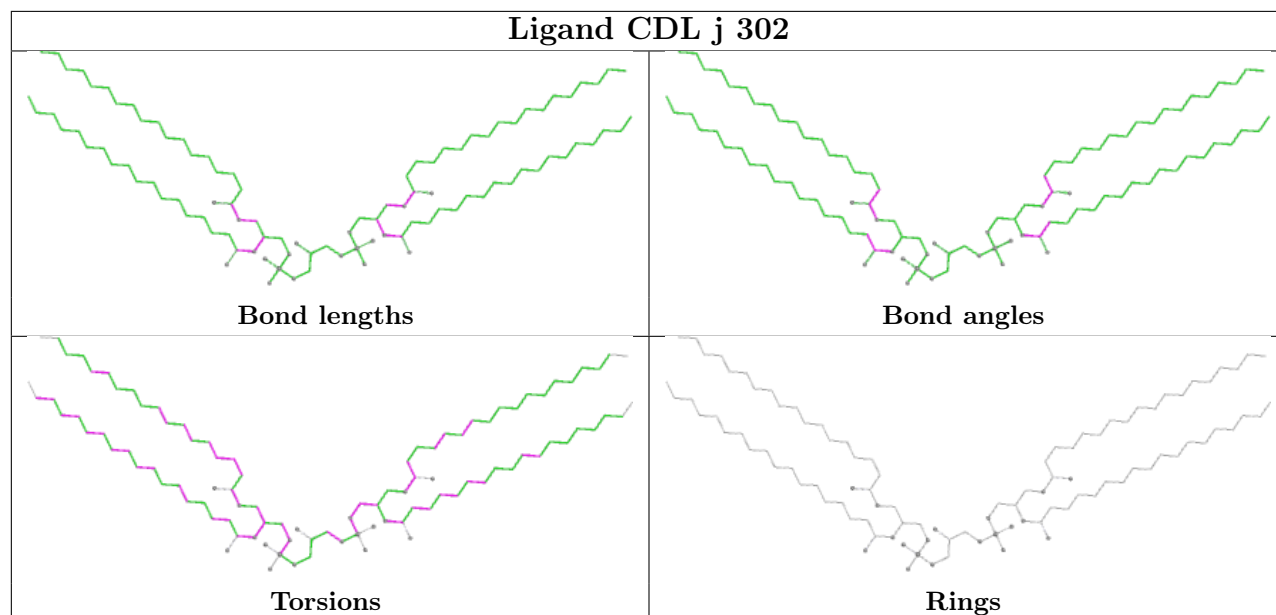
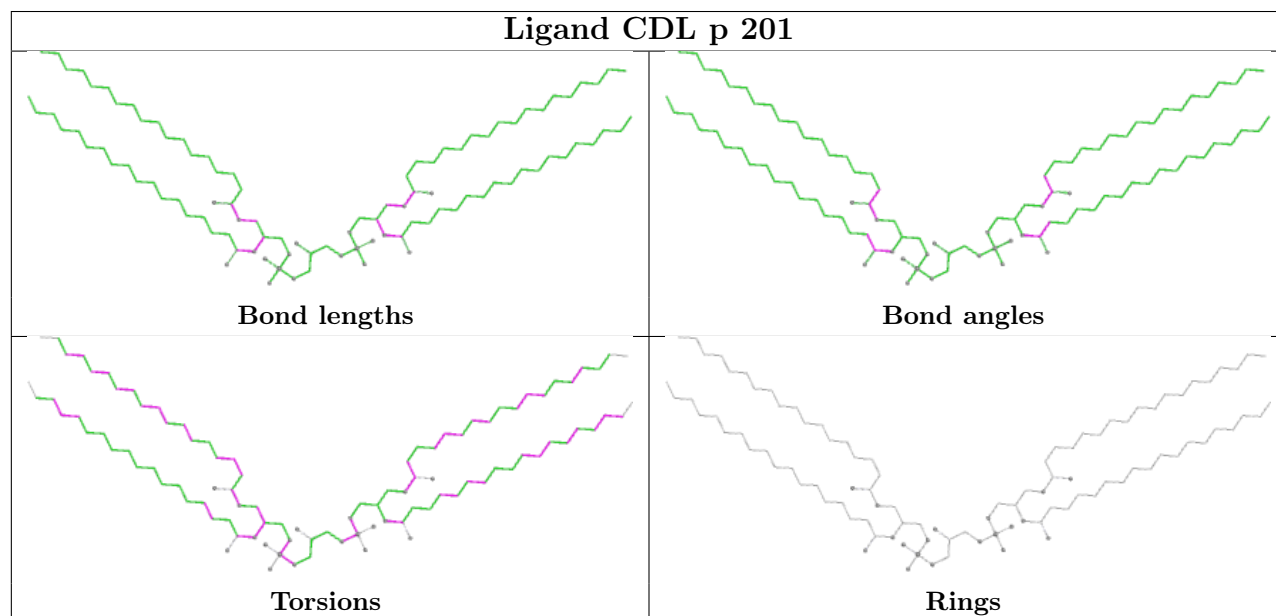
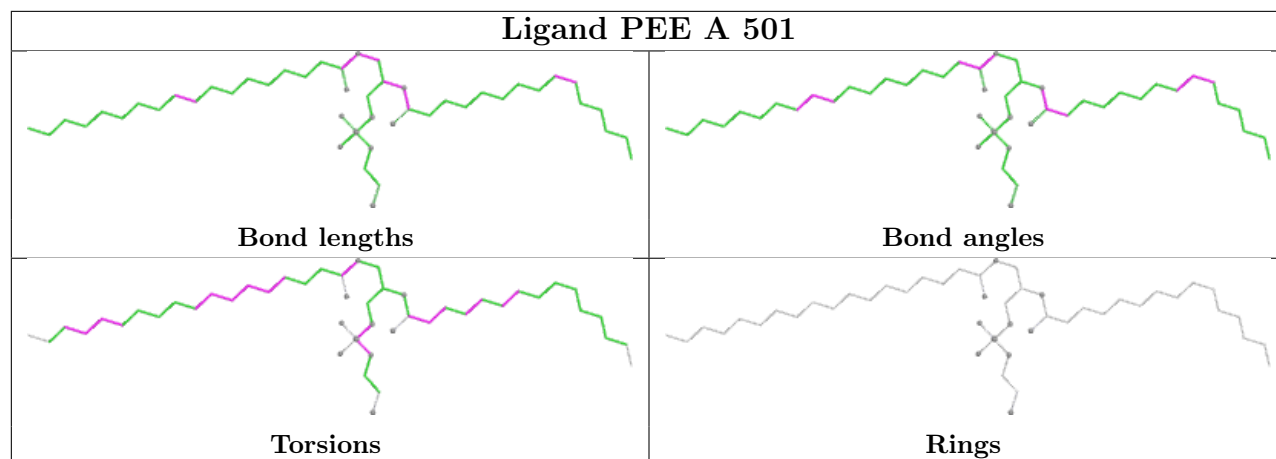


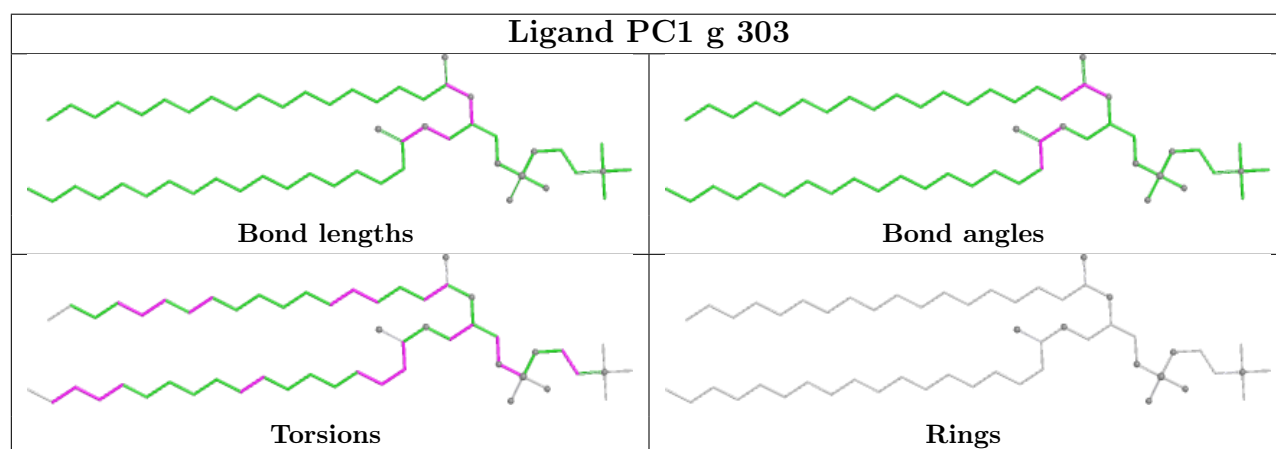
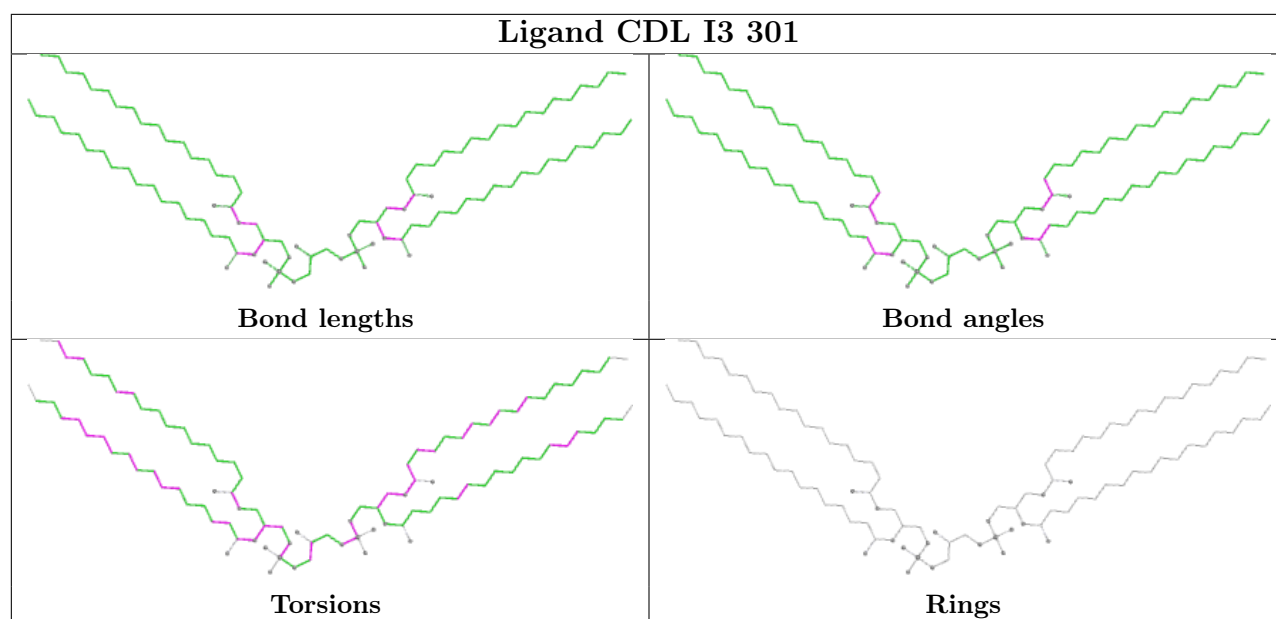


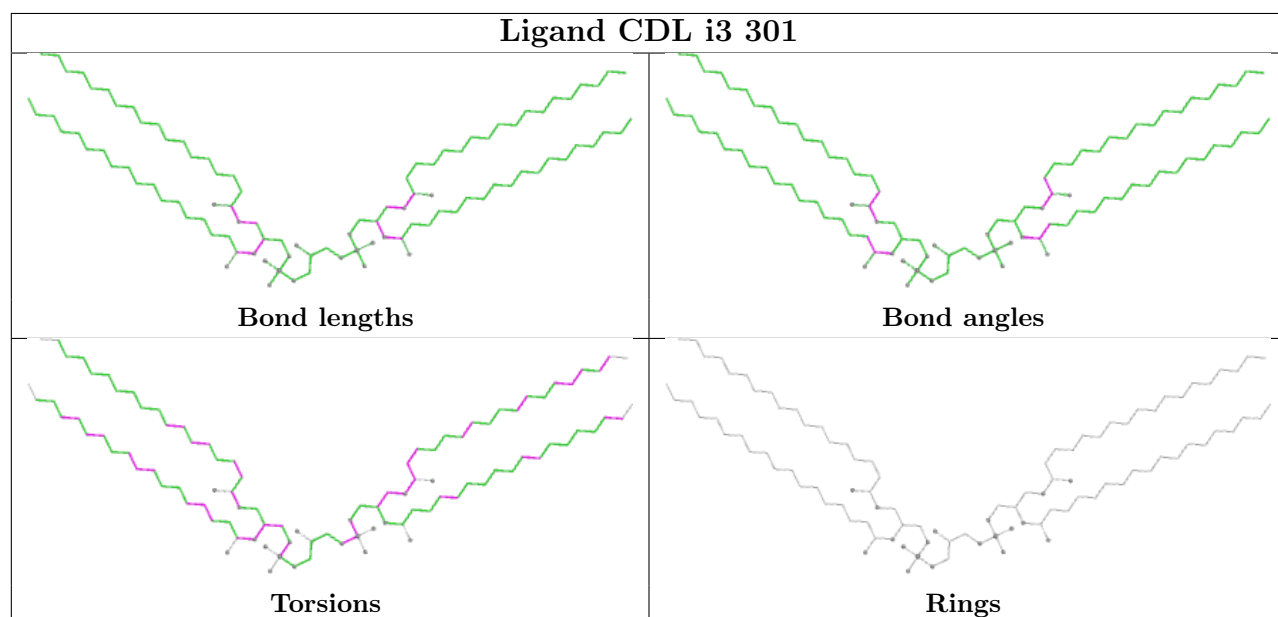
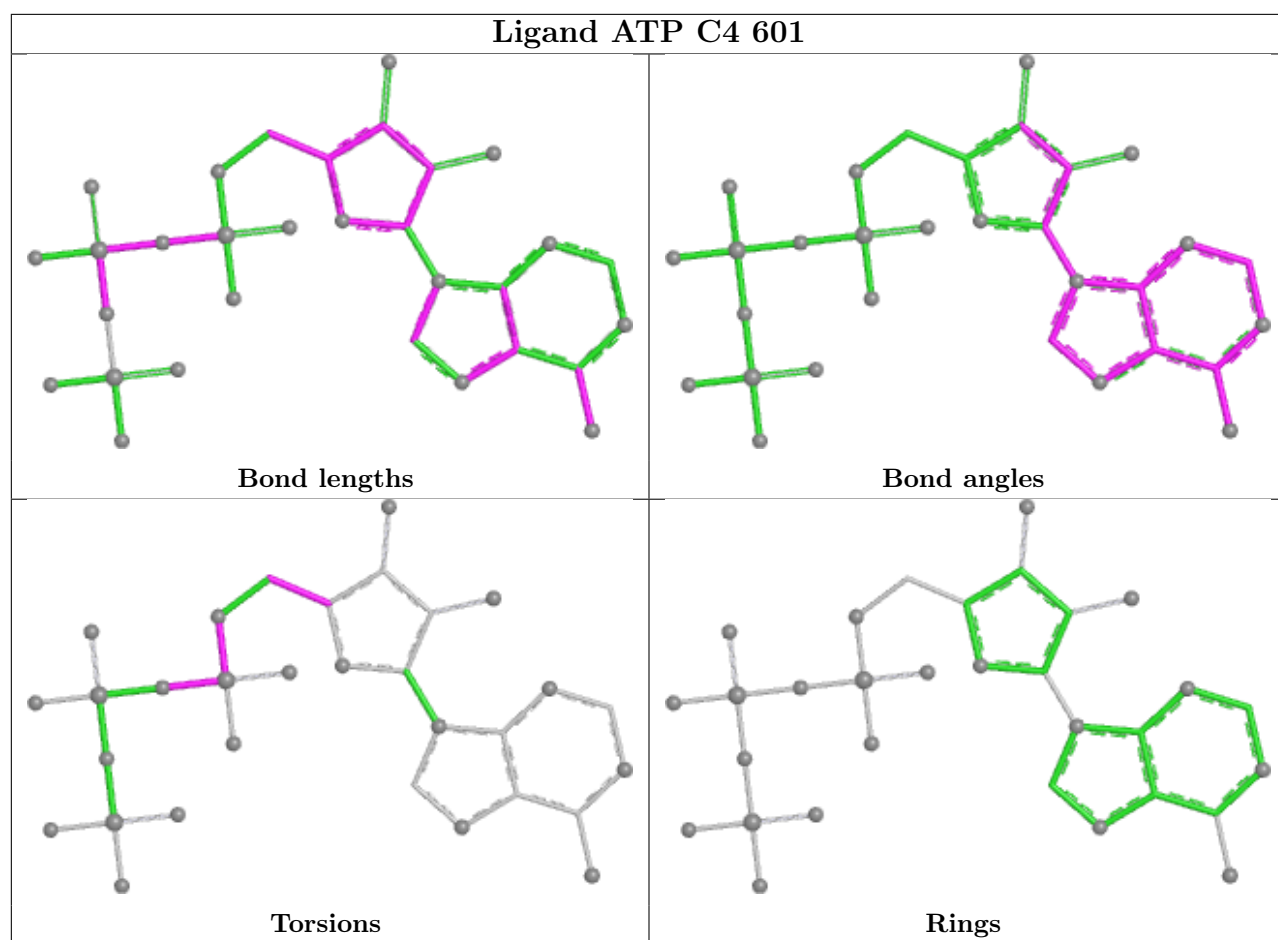


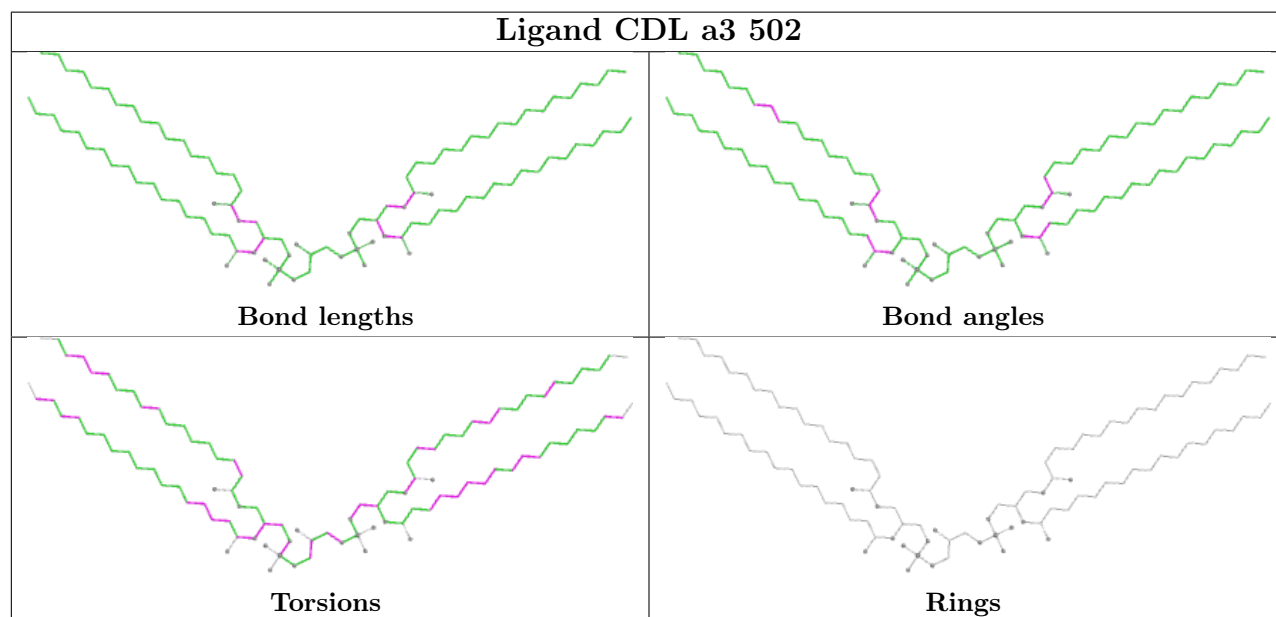
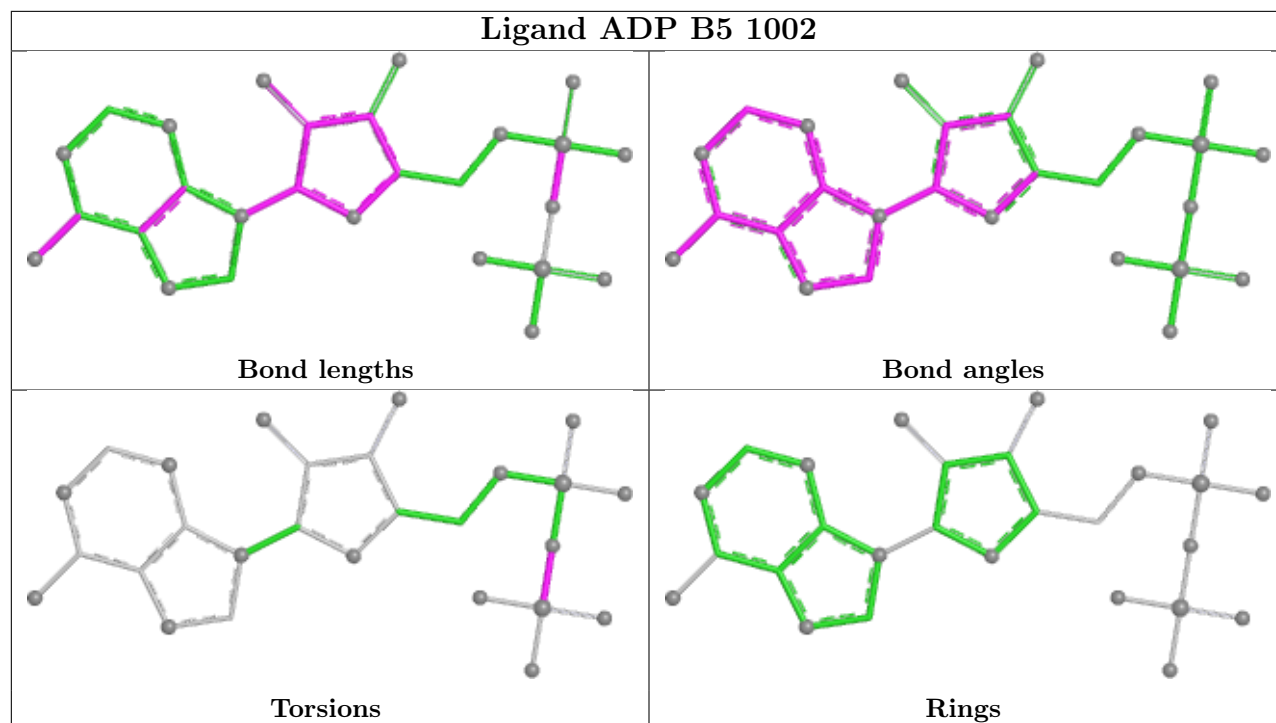


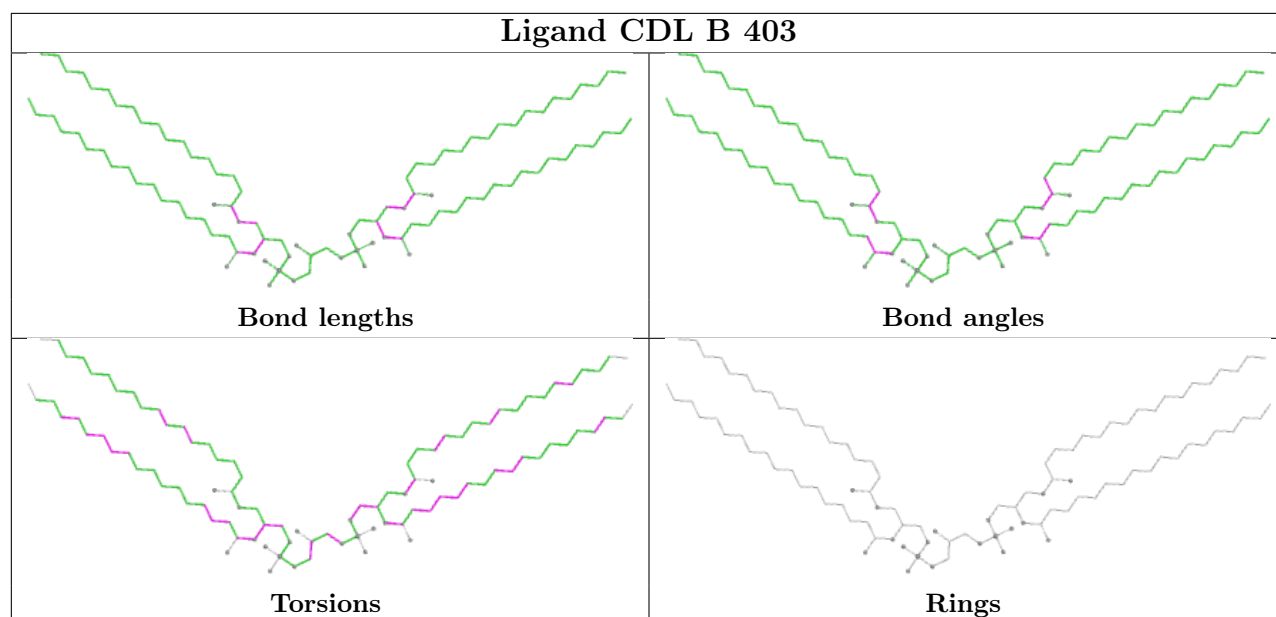
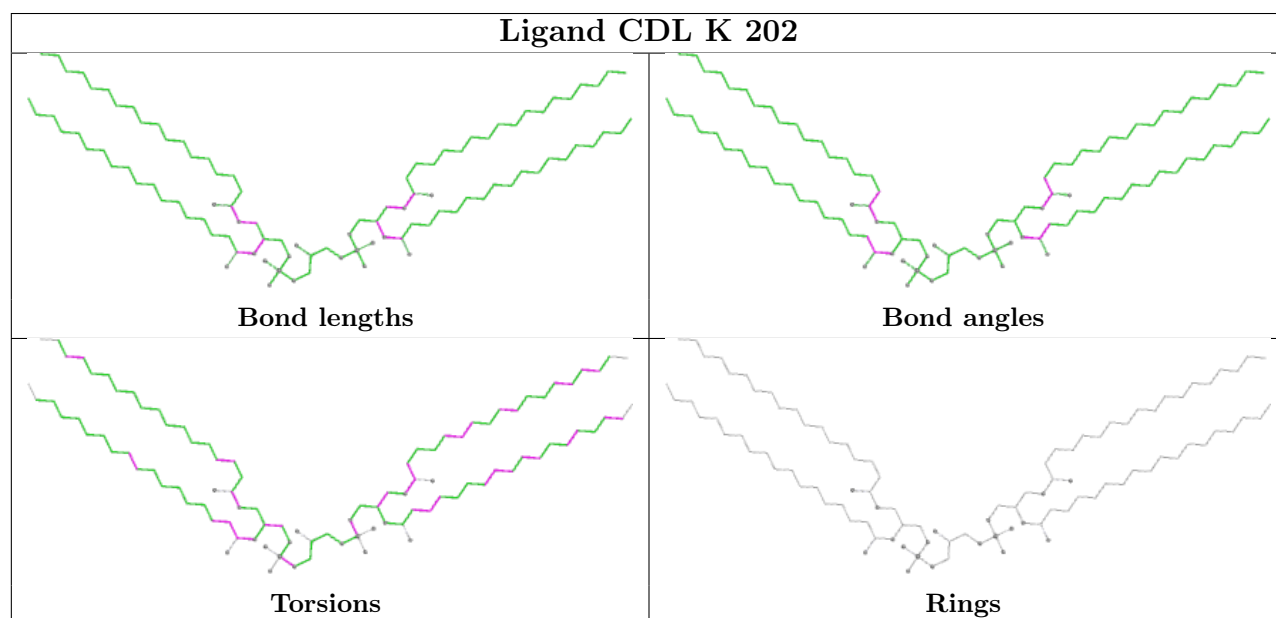
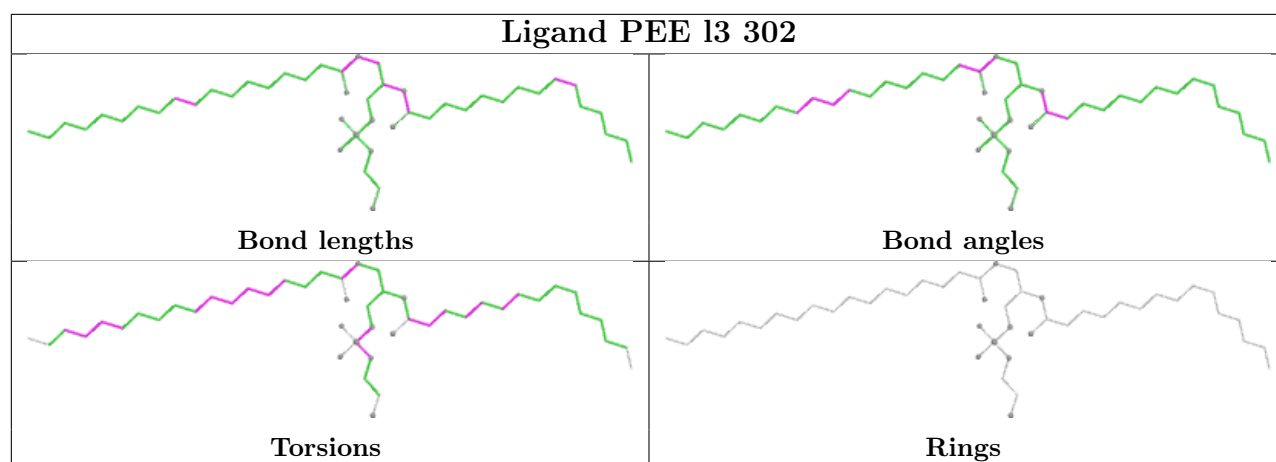


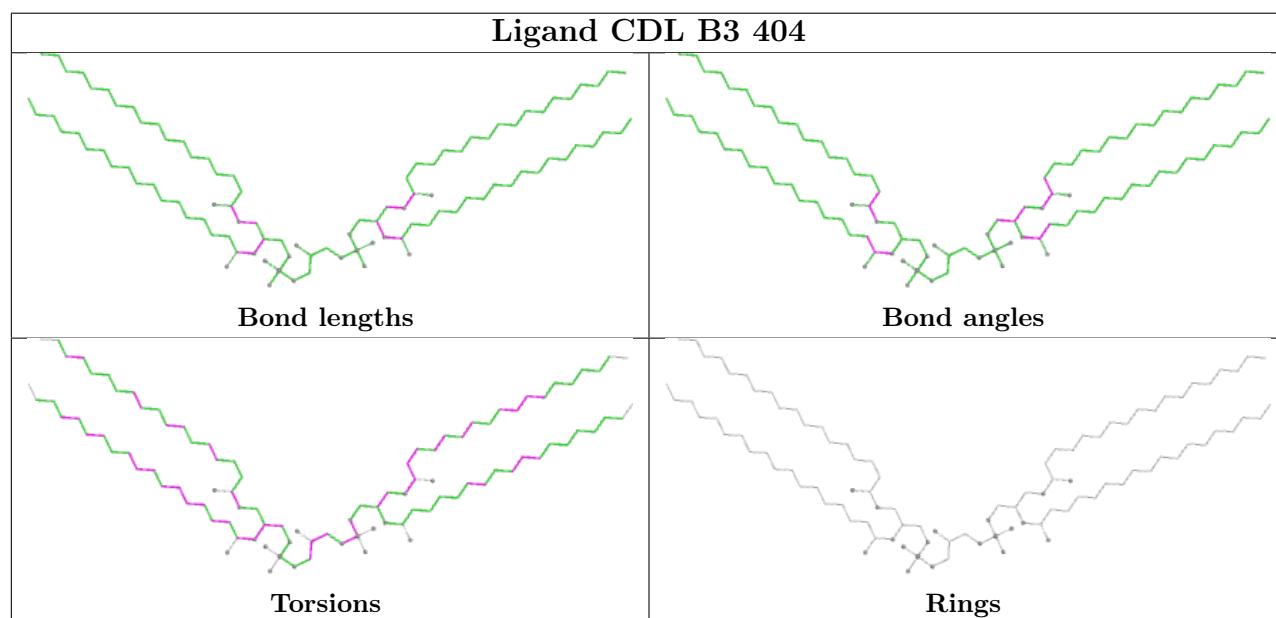
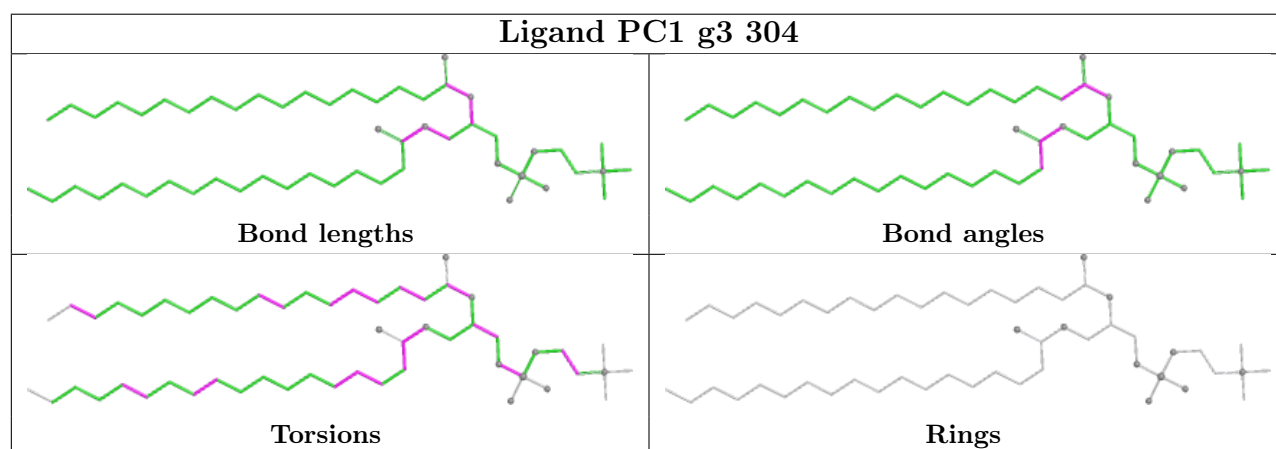
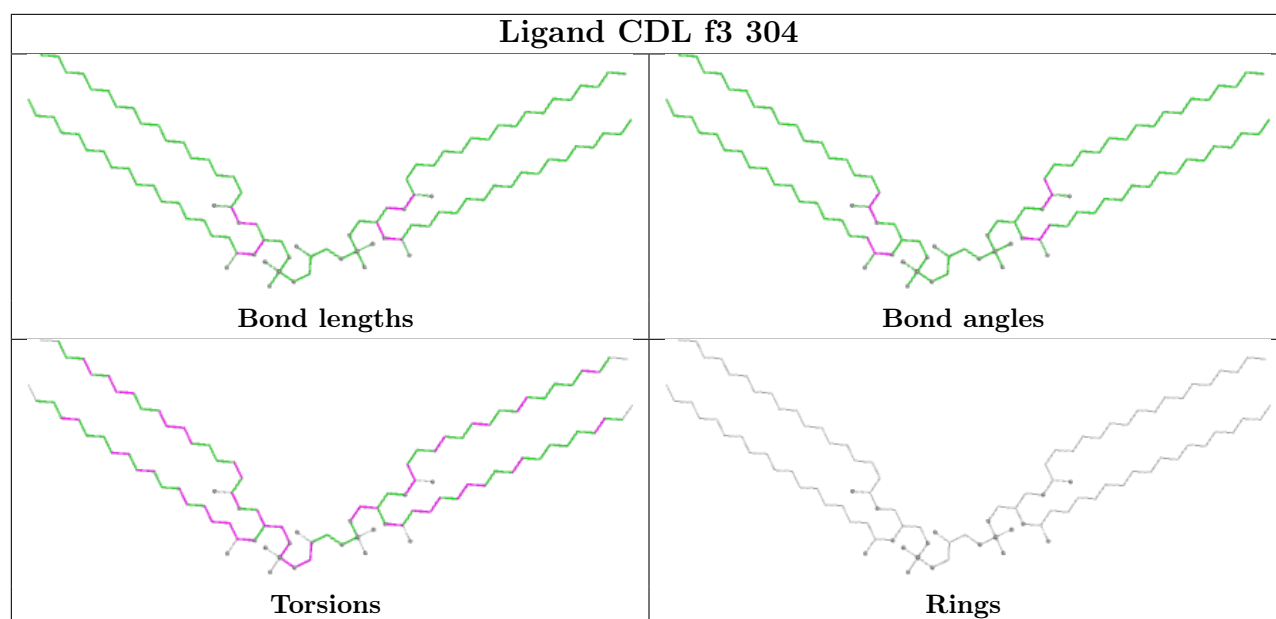




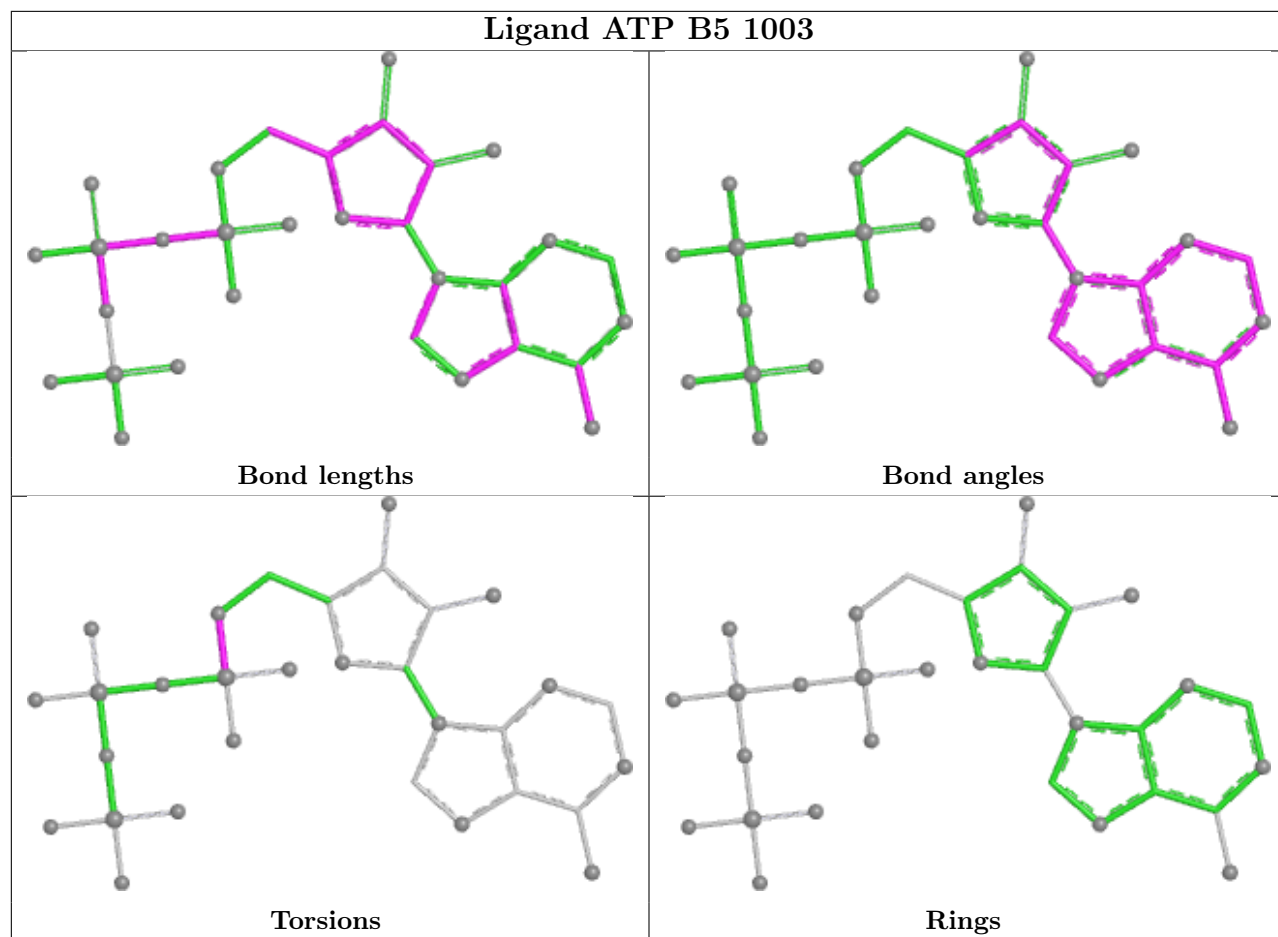




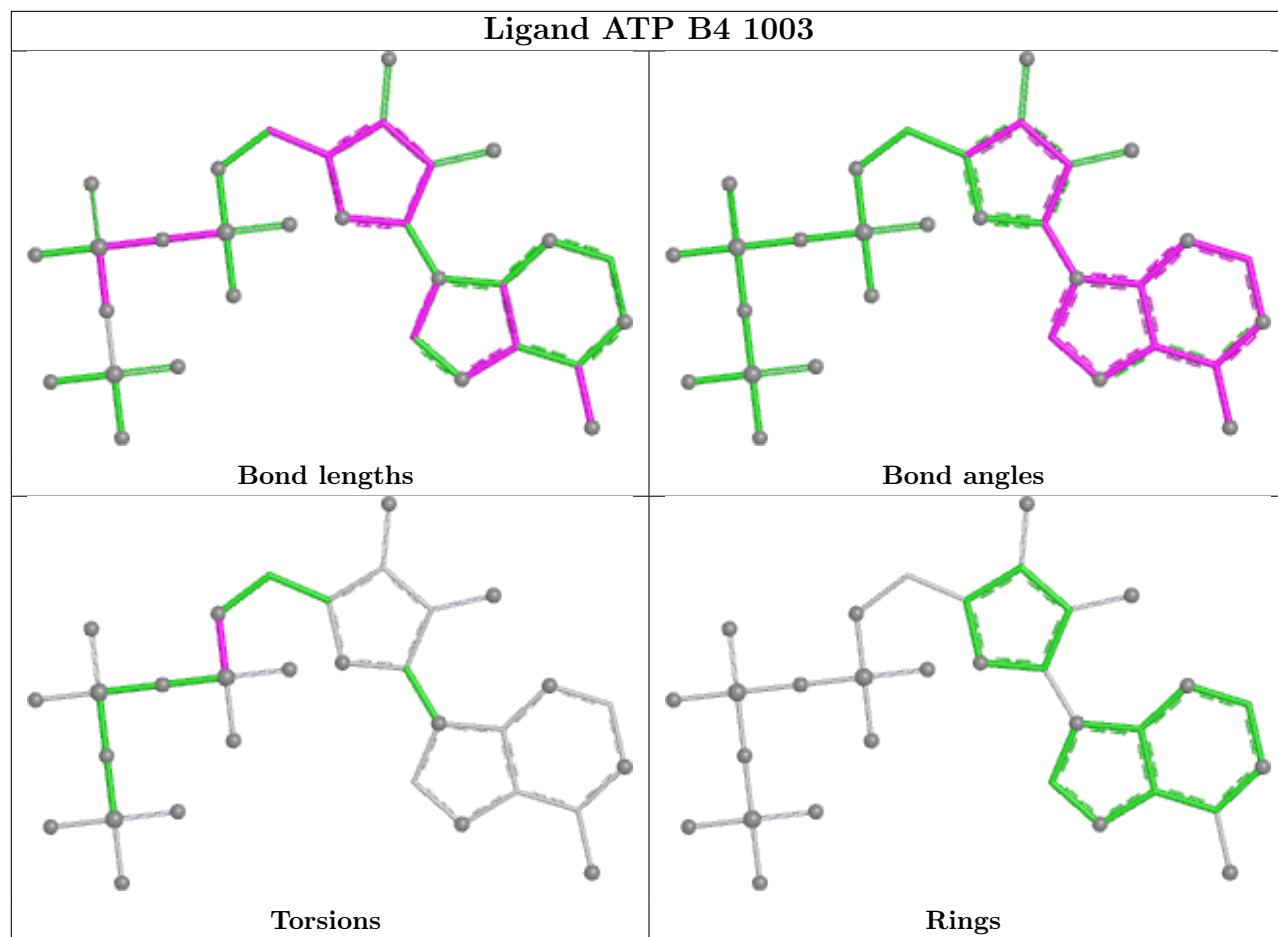




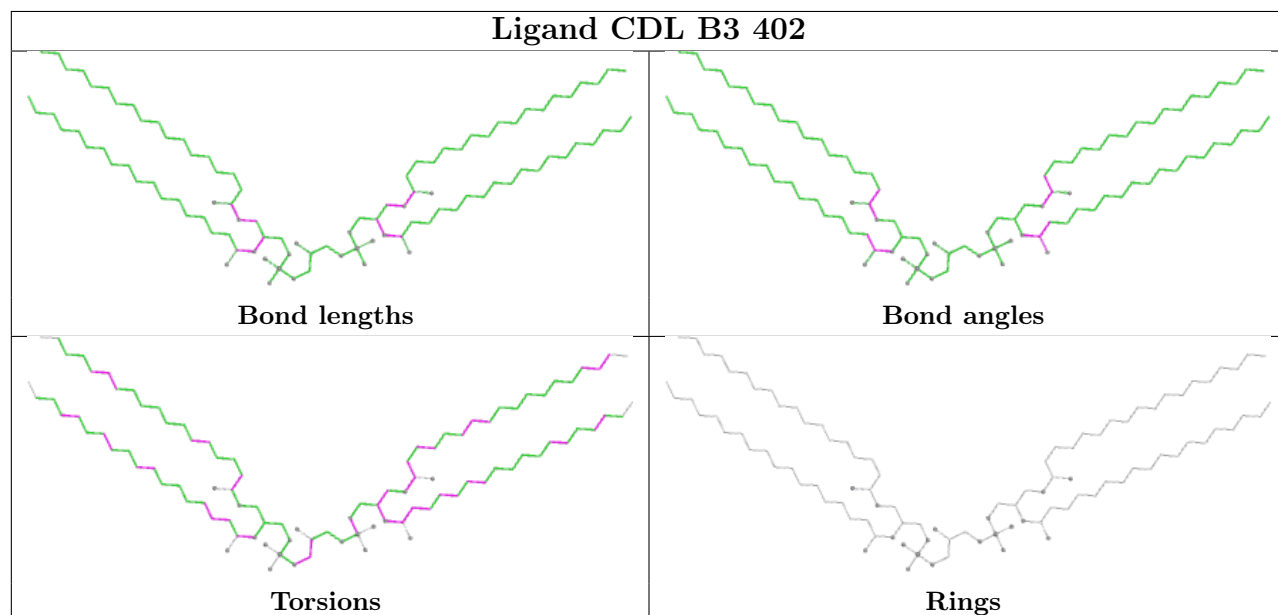
Ligand ATP B5 1003

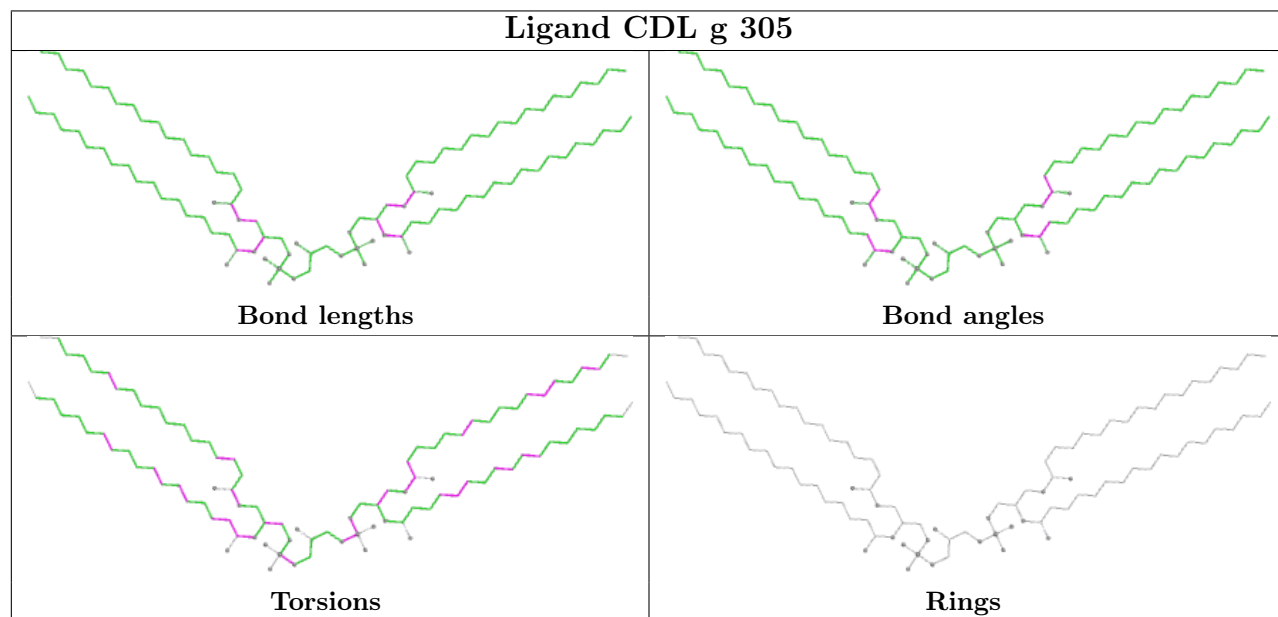
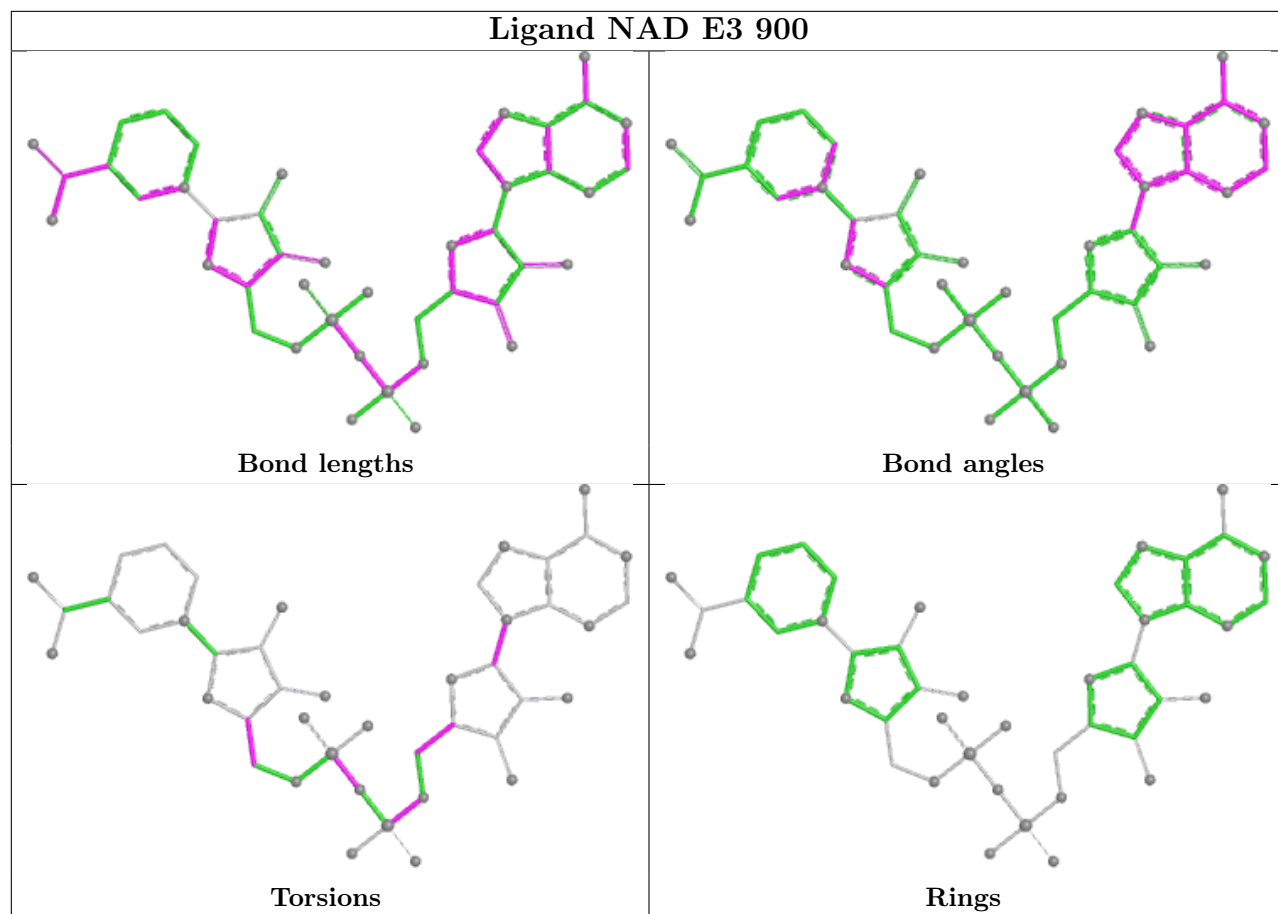


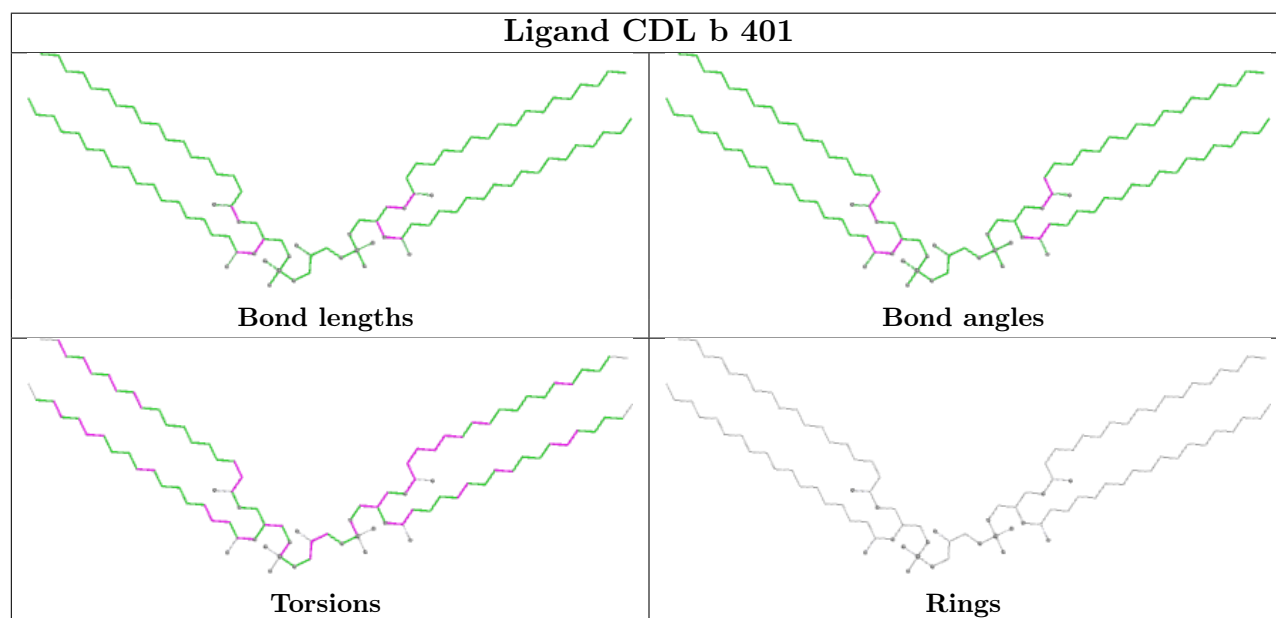
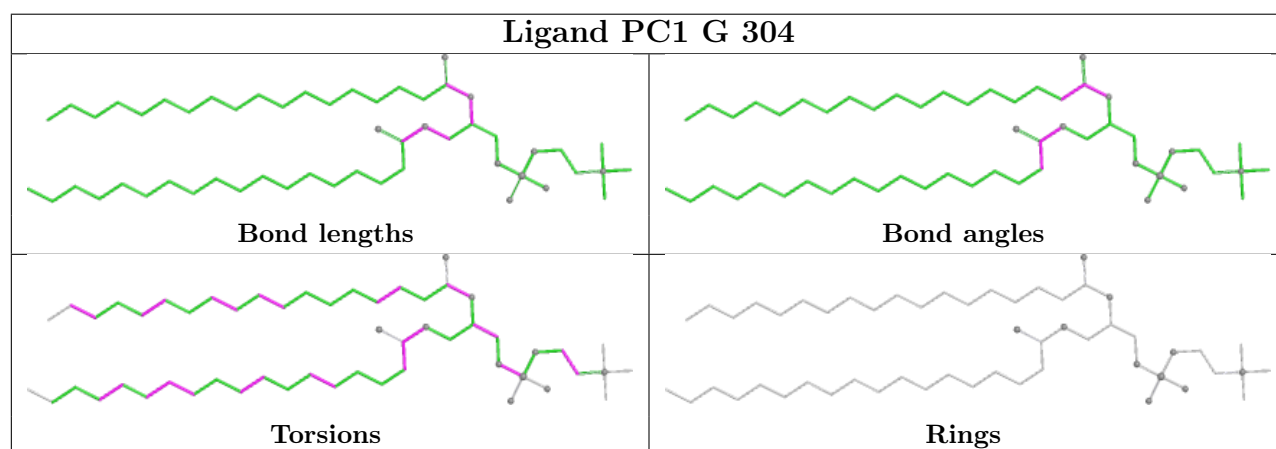
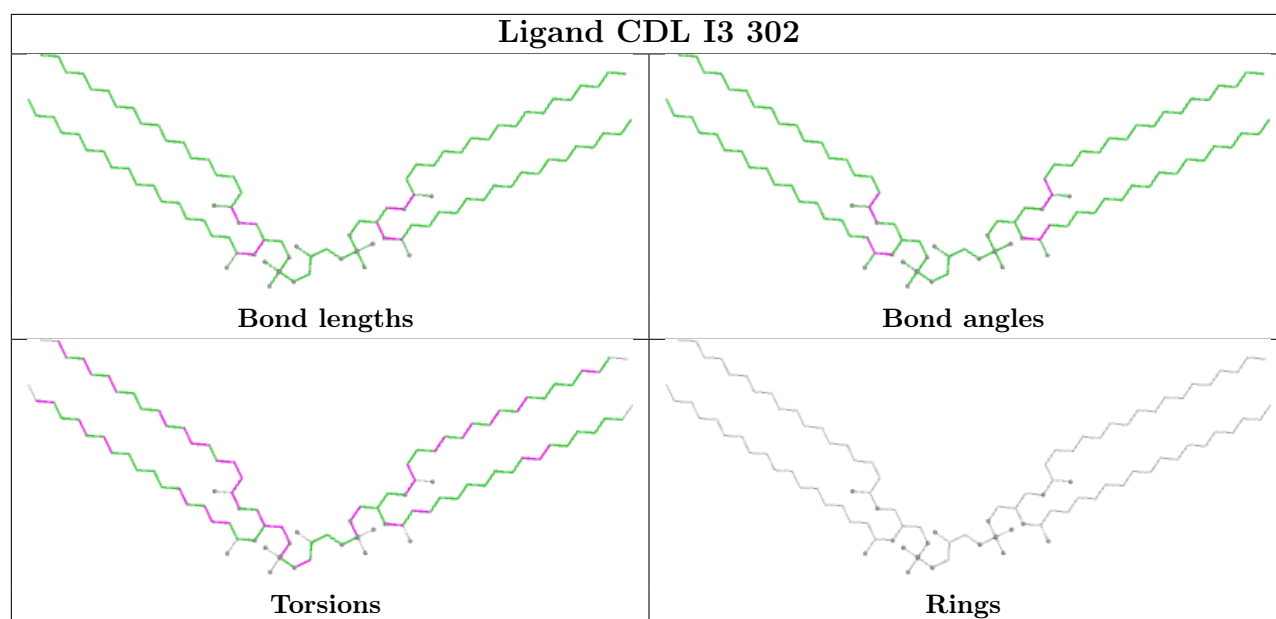
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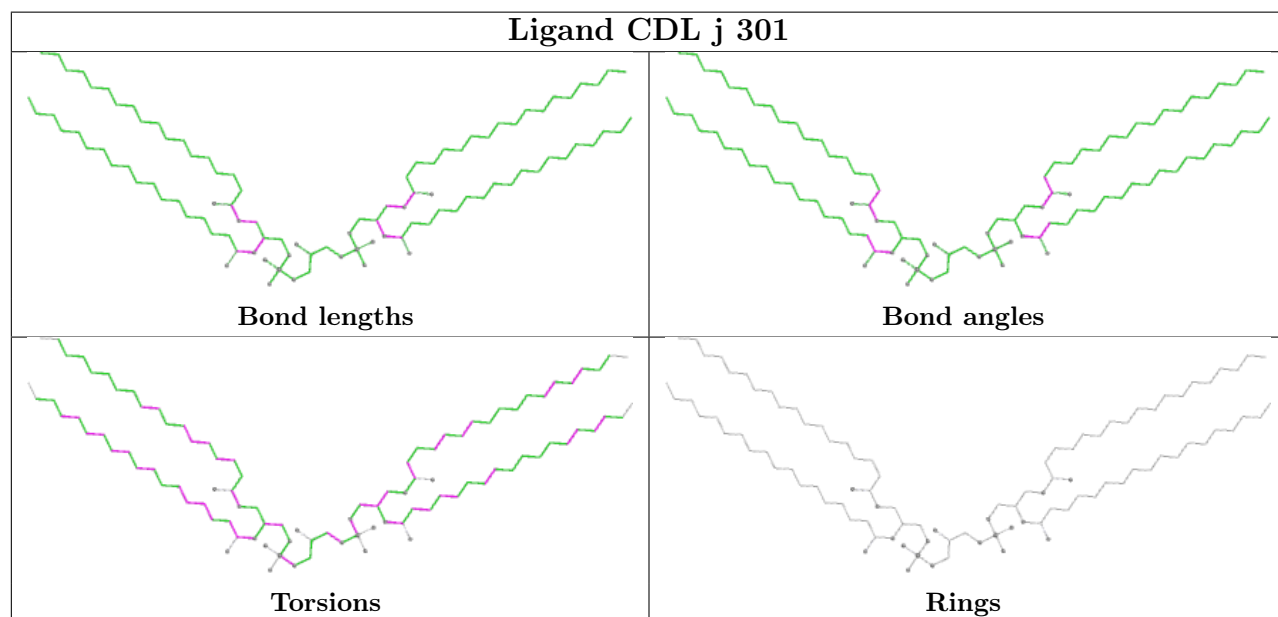
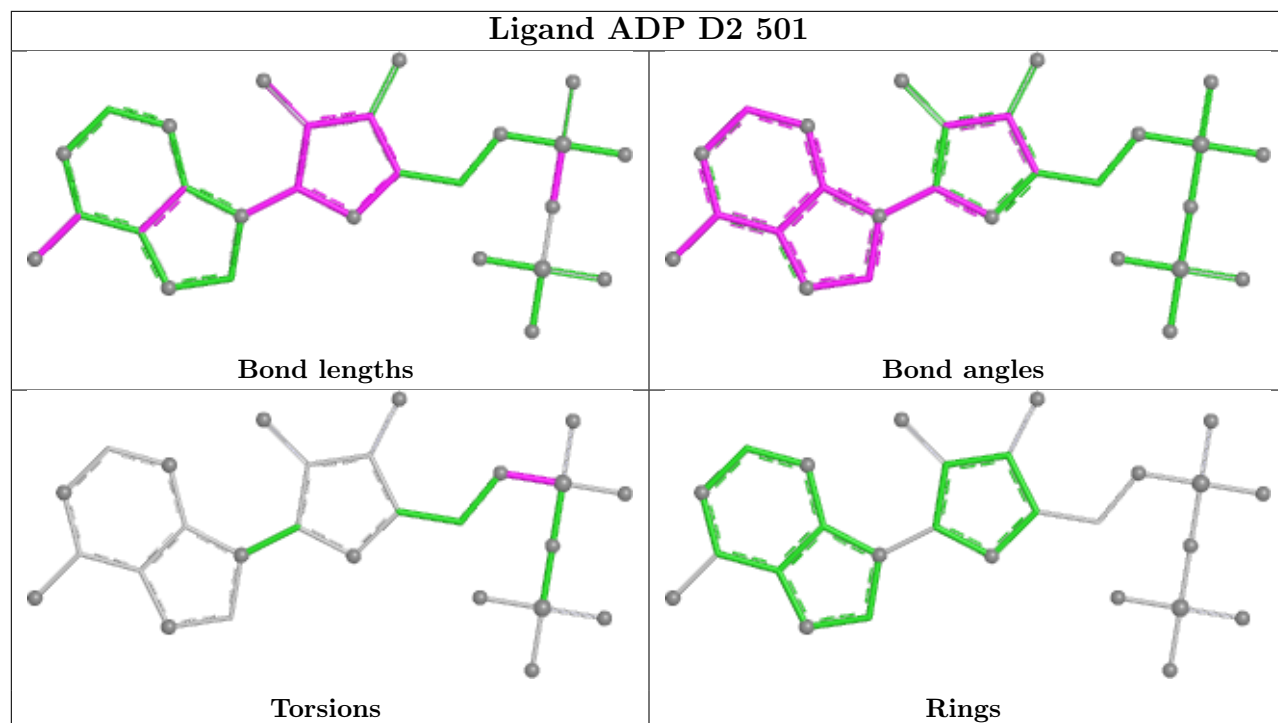


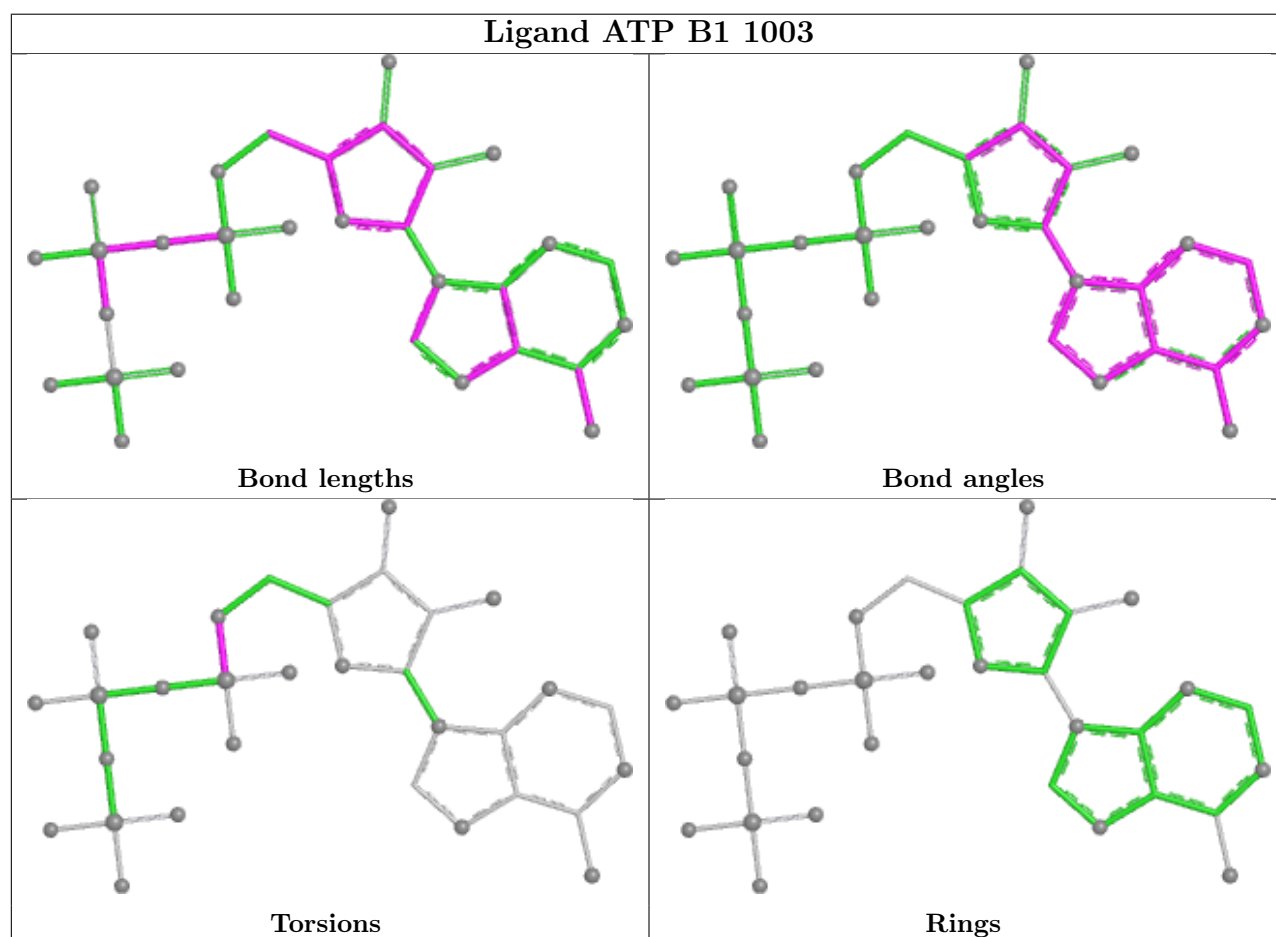
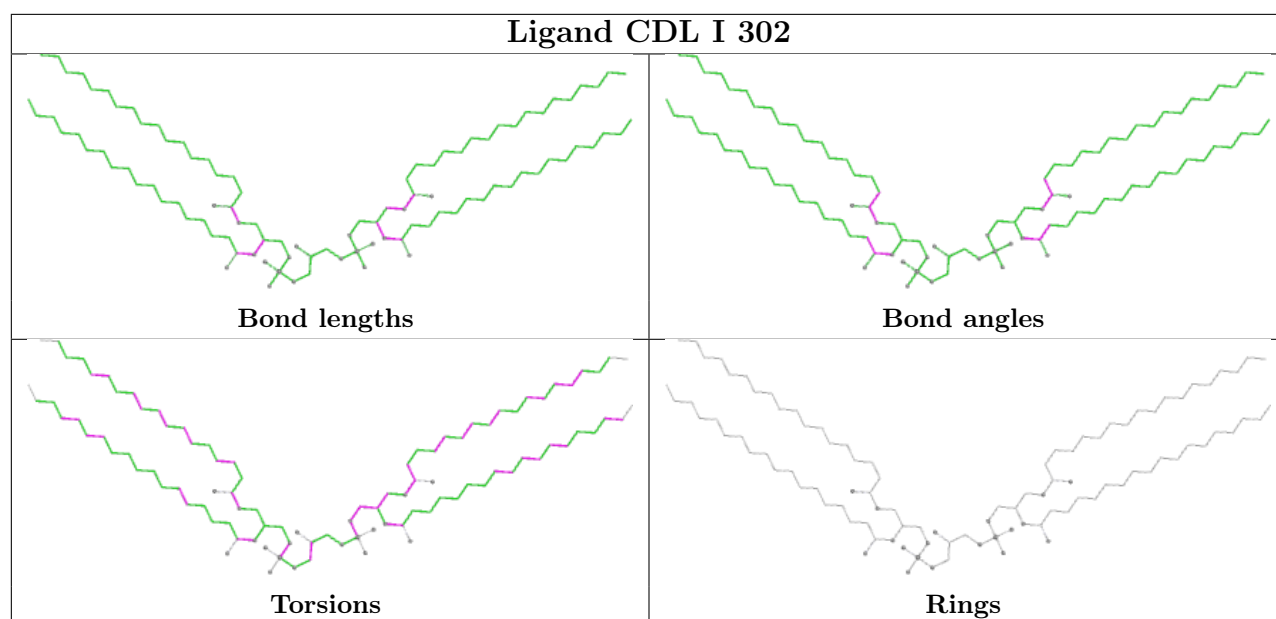
Ligand CDL B3 402

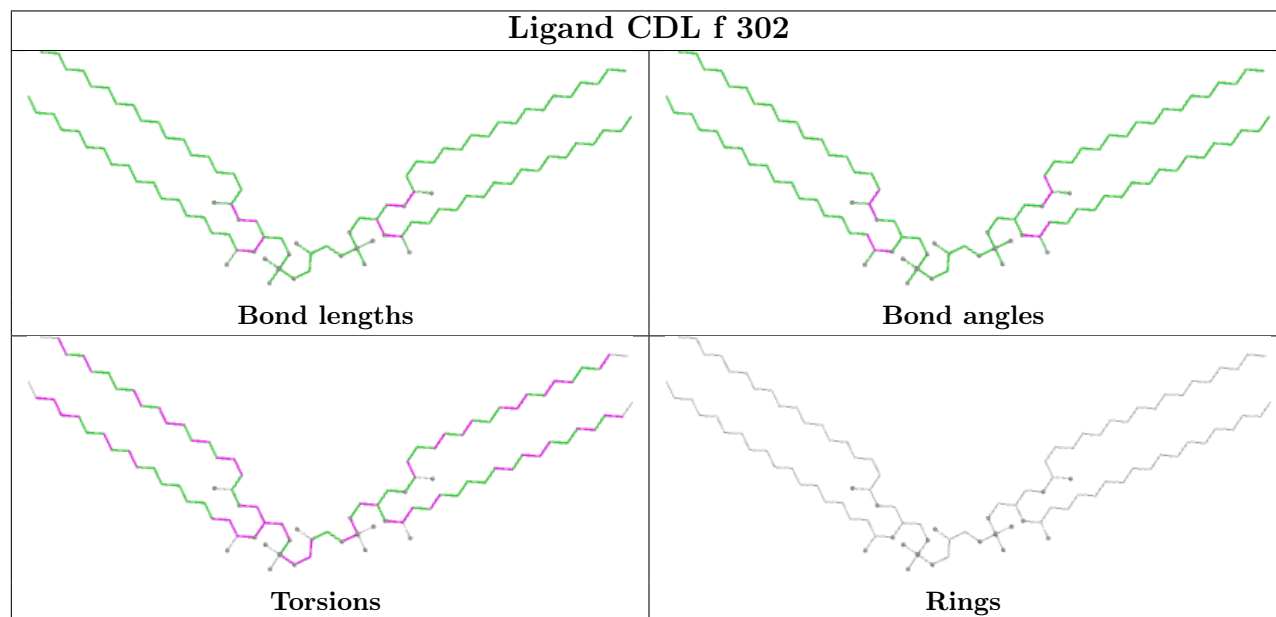
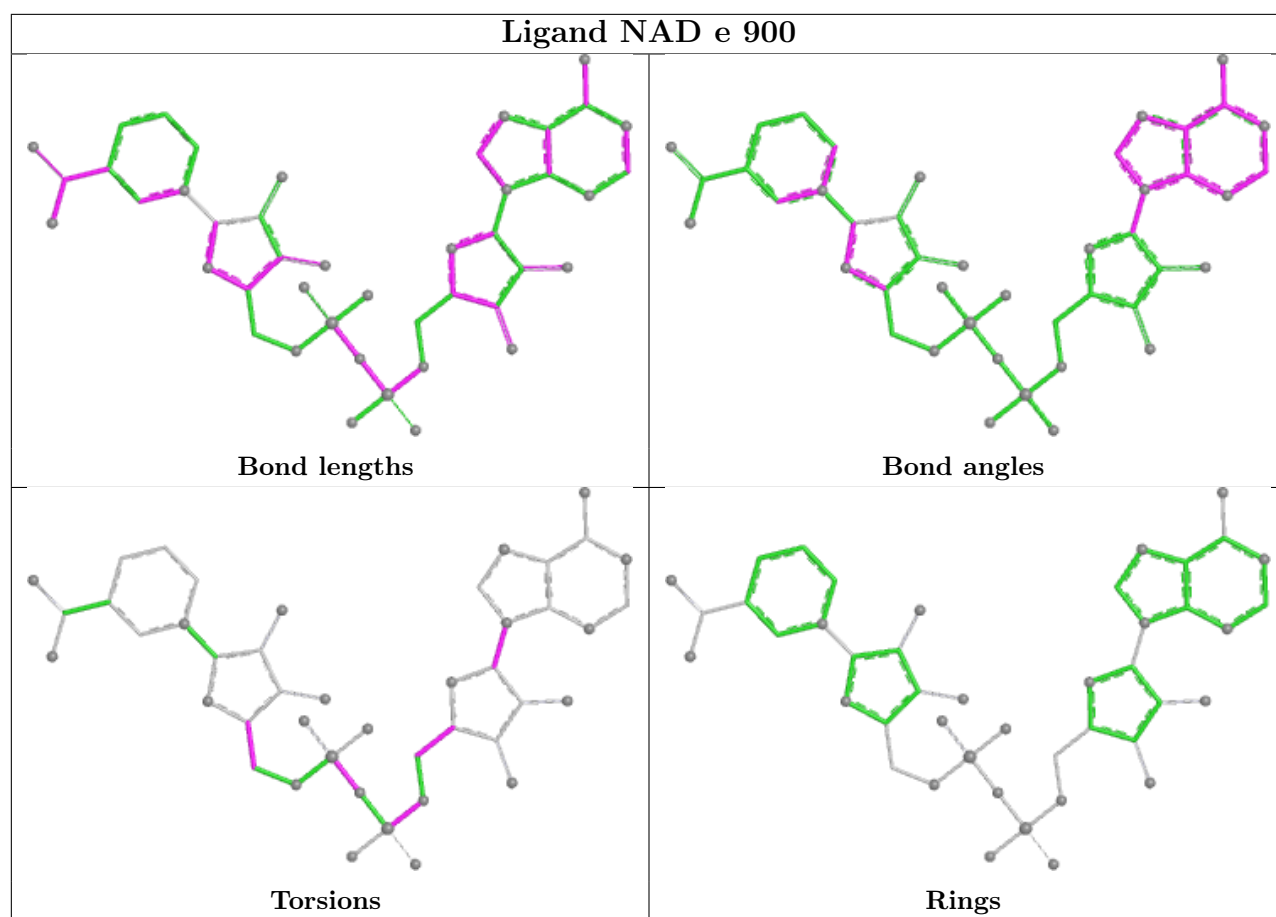


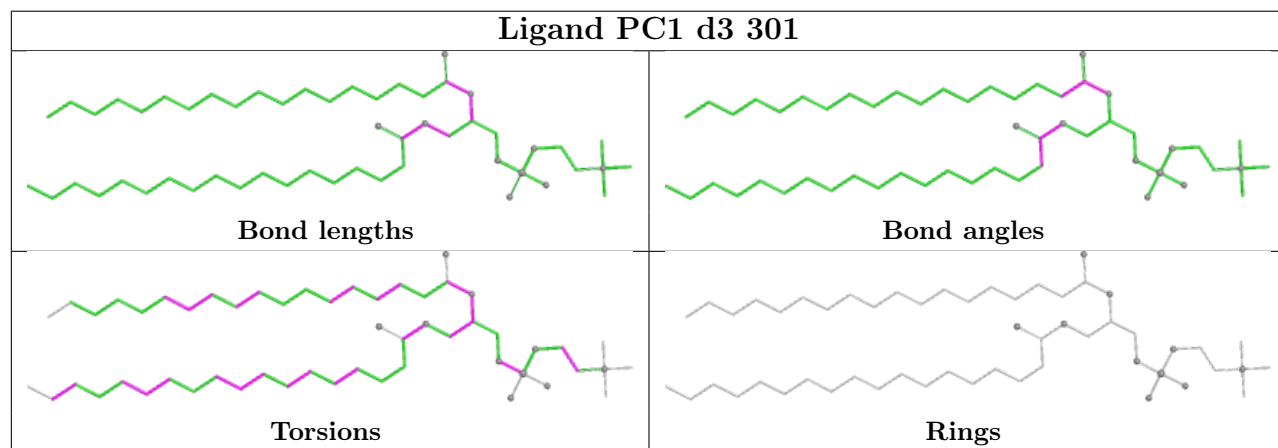
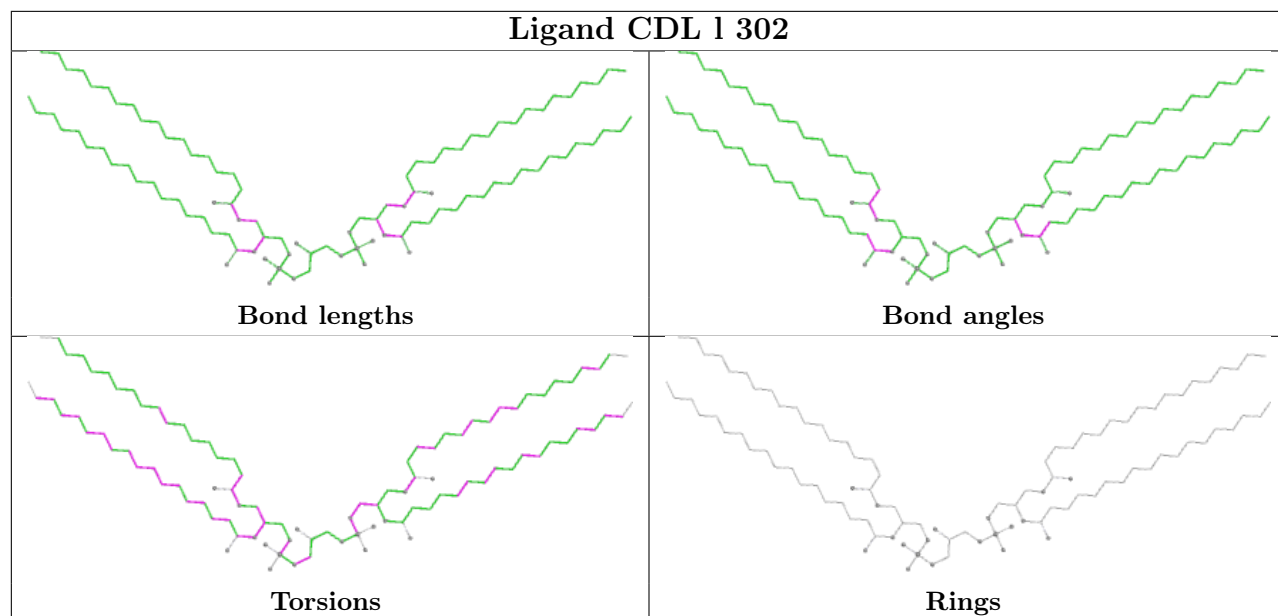


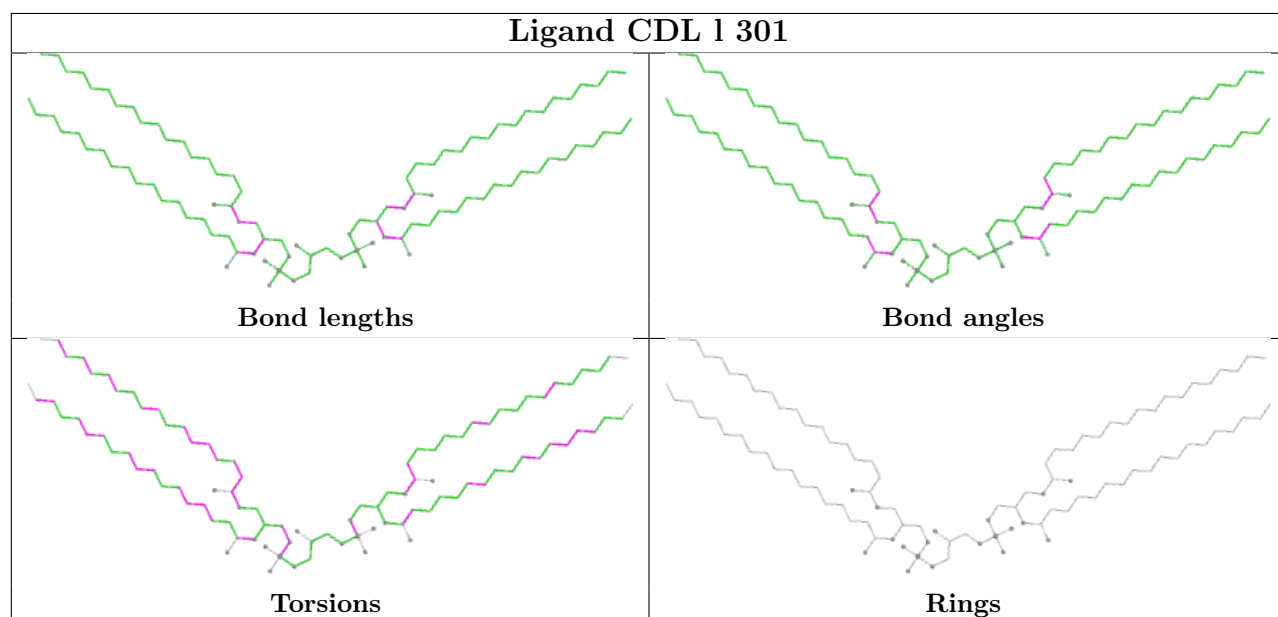
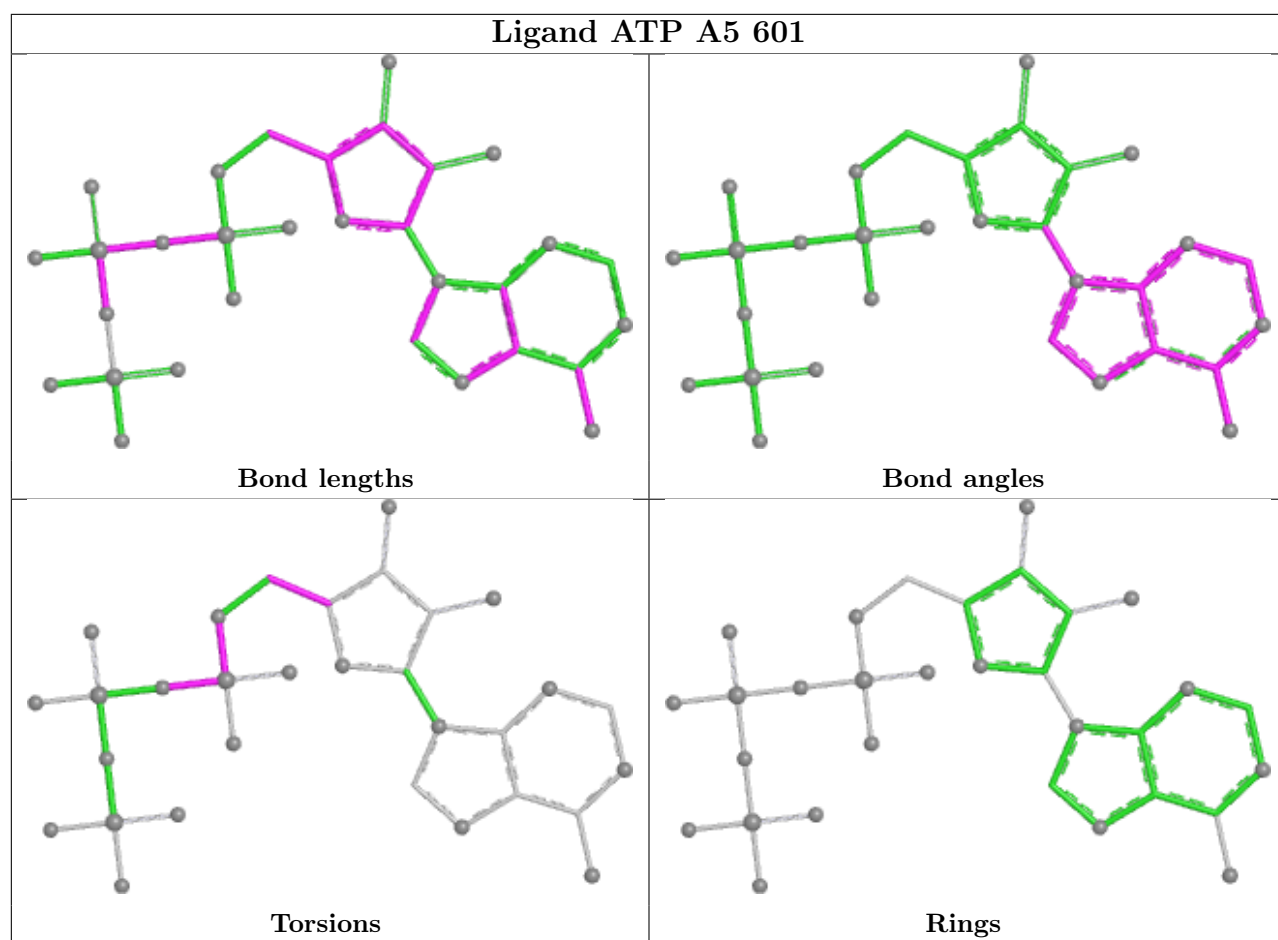


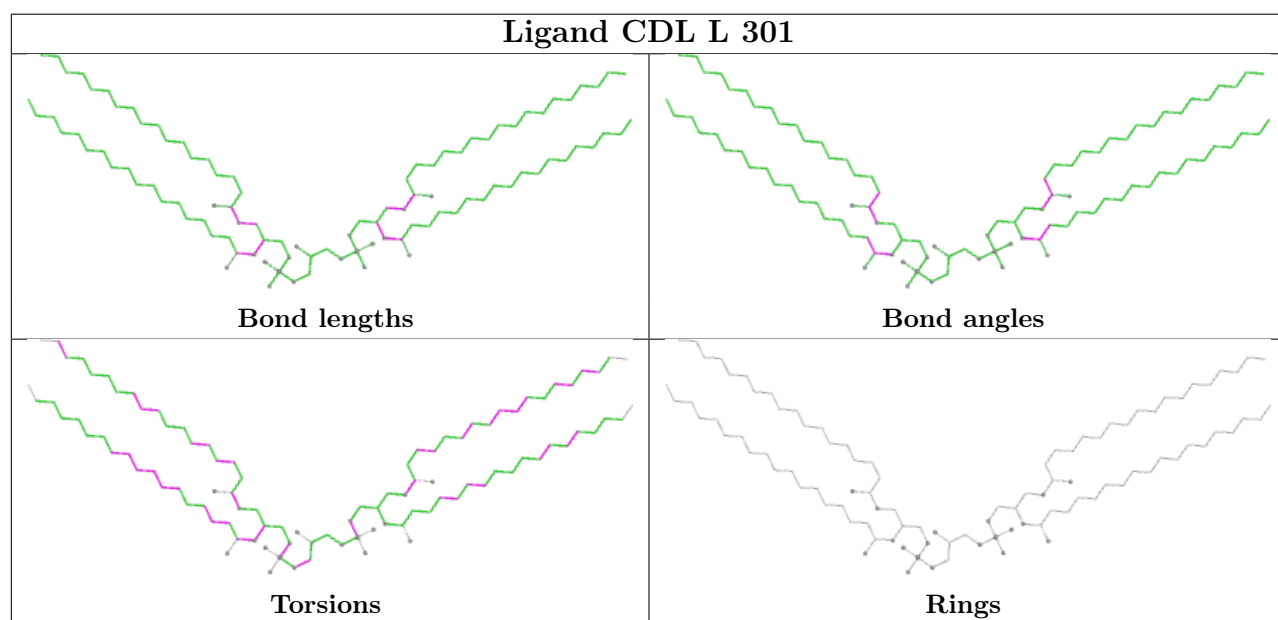
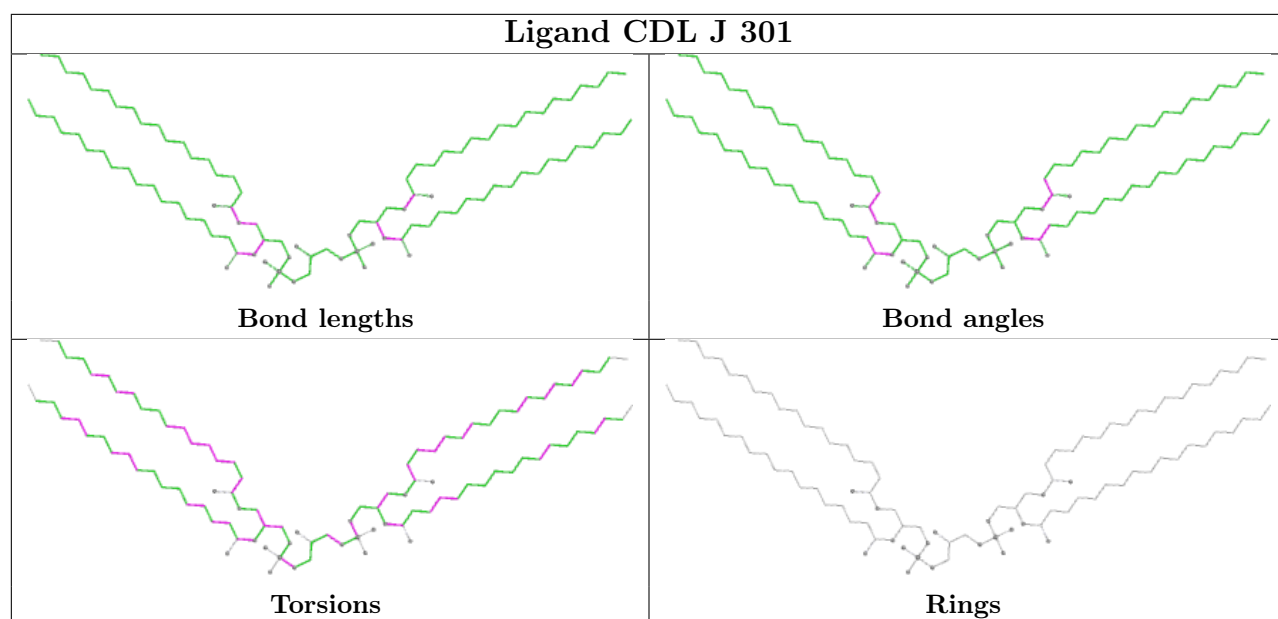




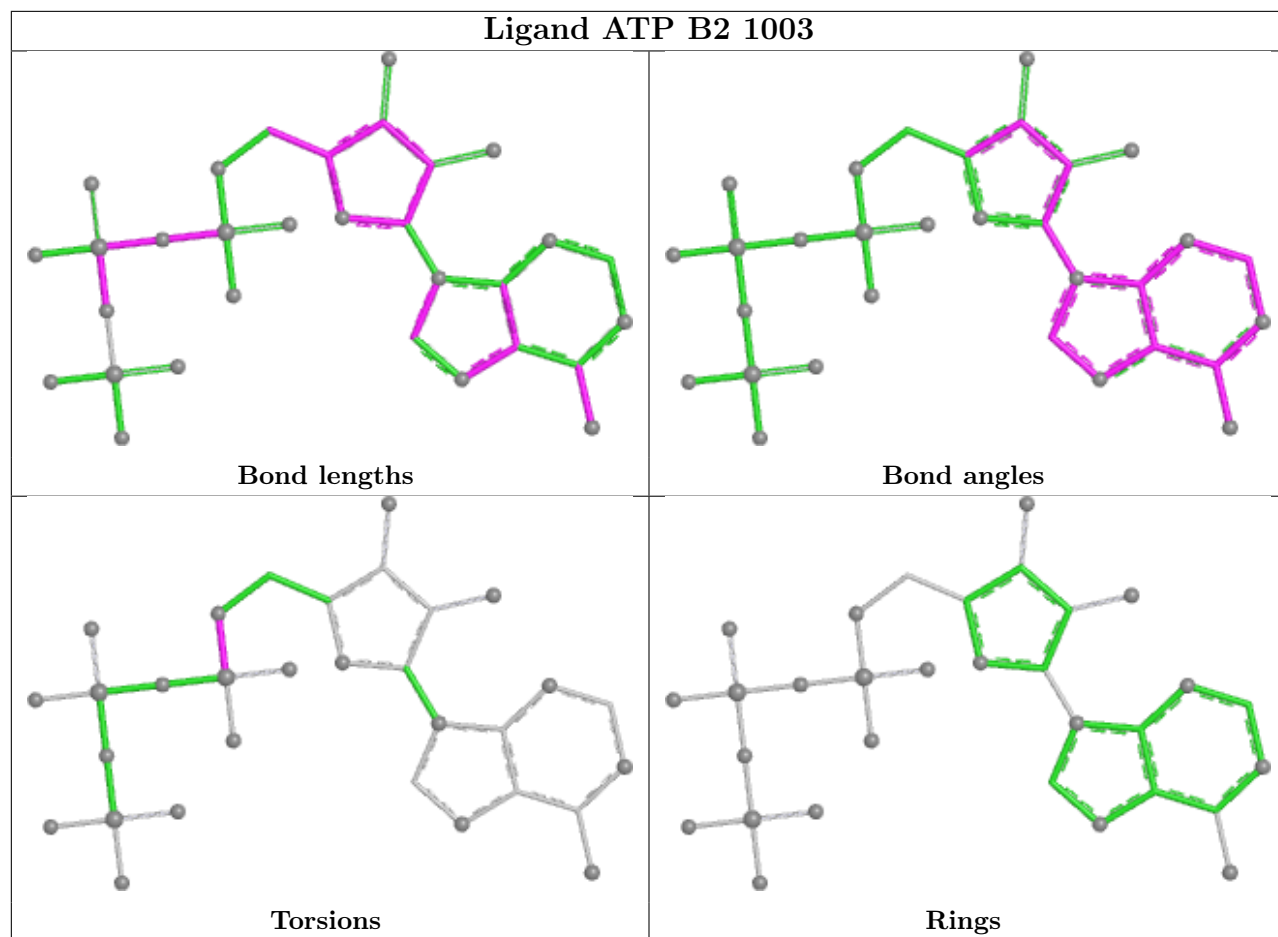




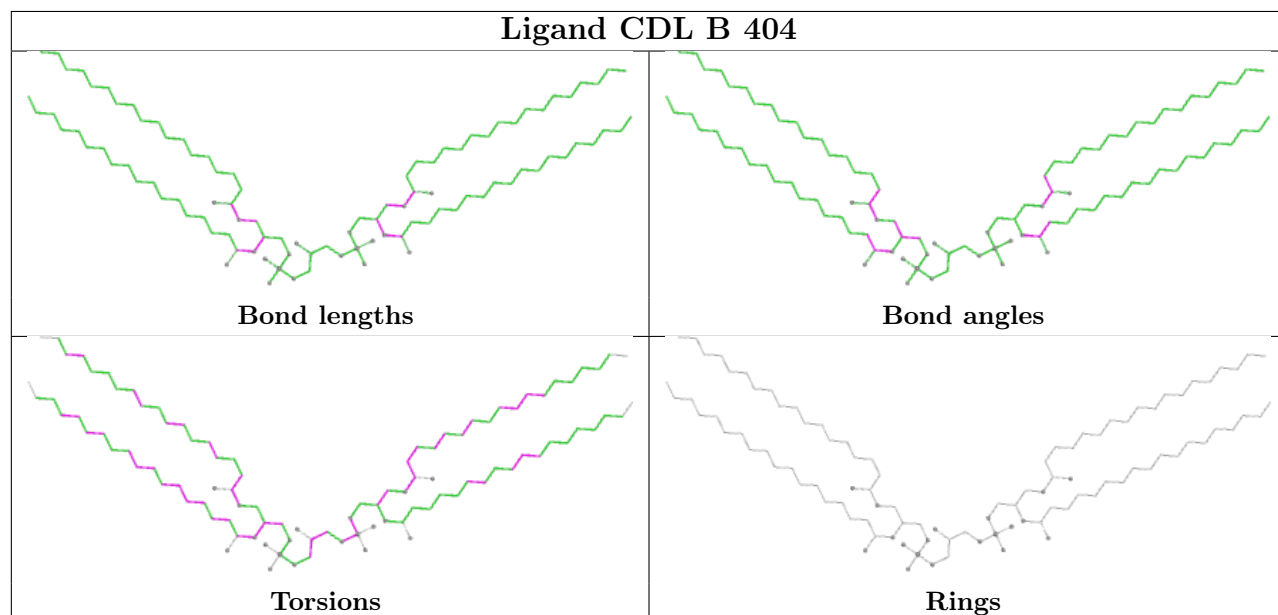


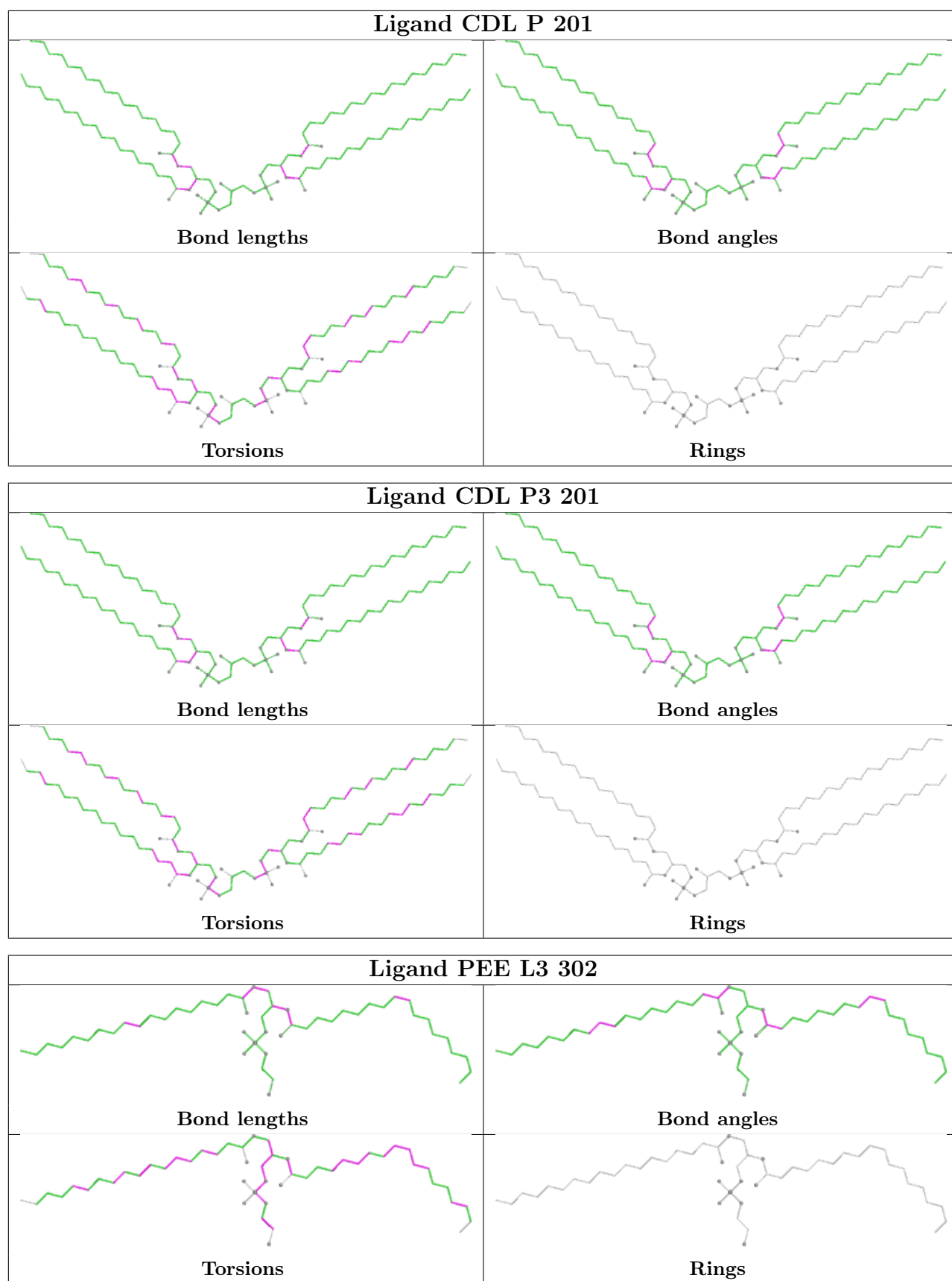


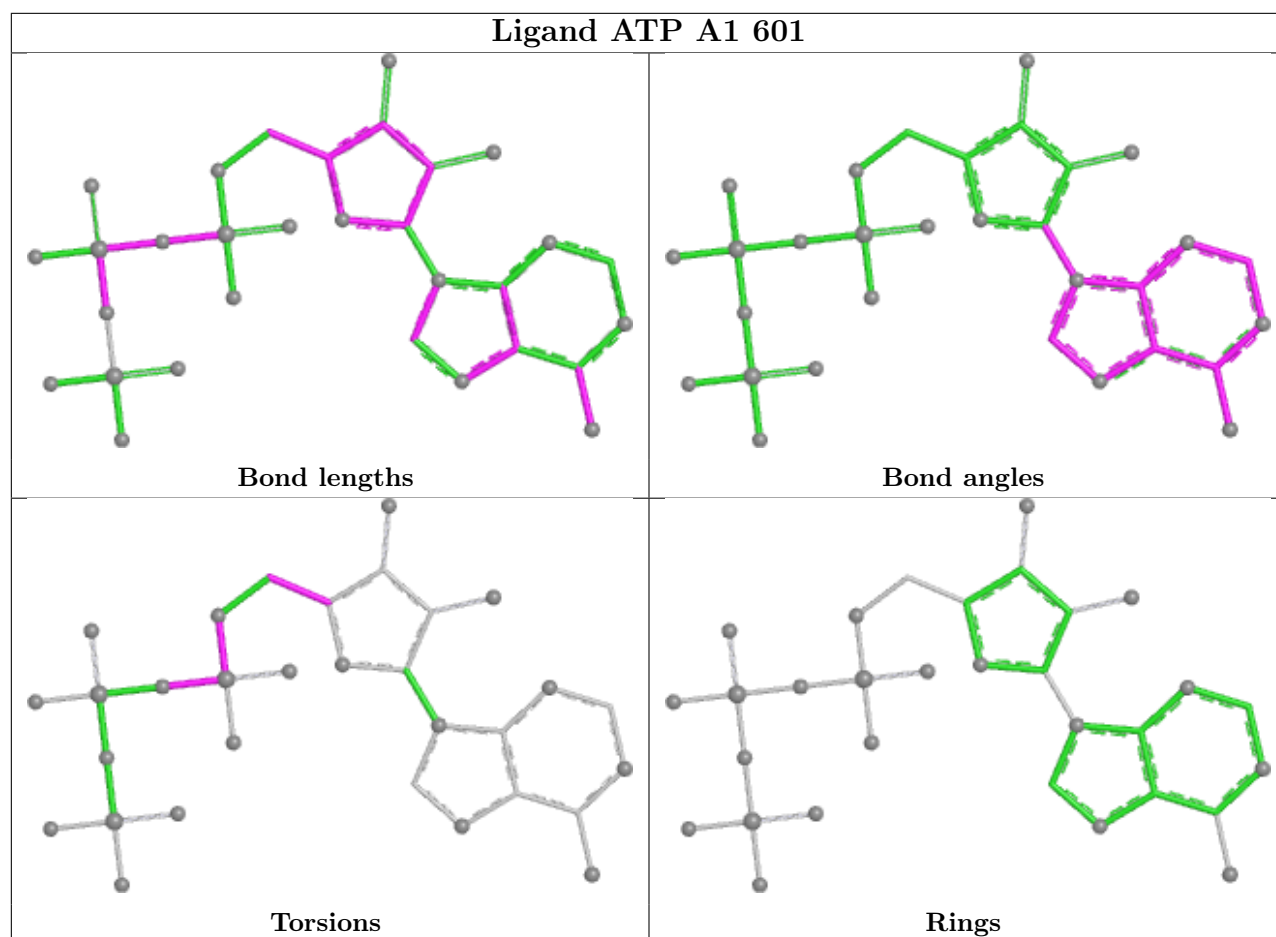
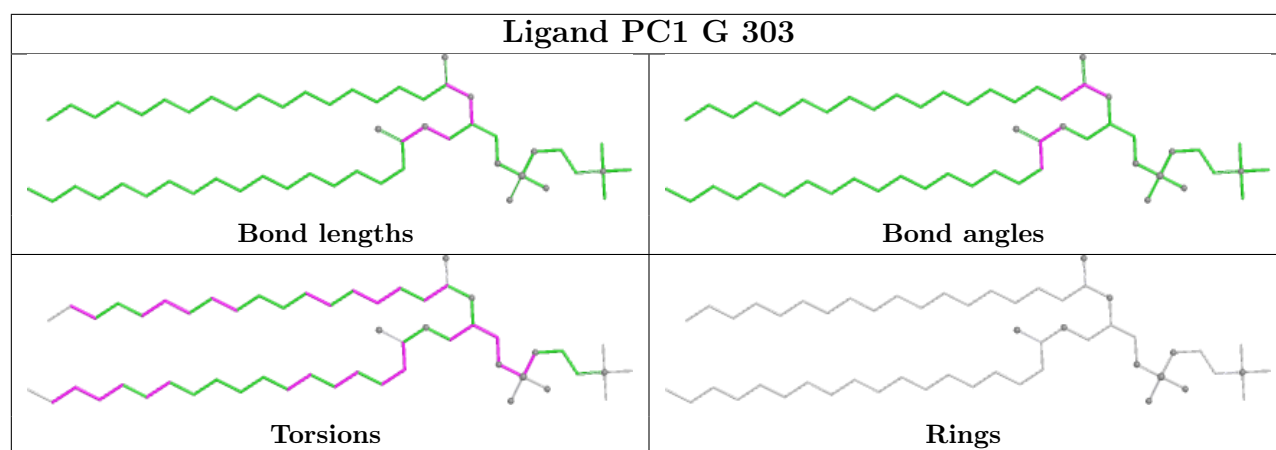
Ligand ATP B2 1003

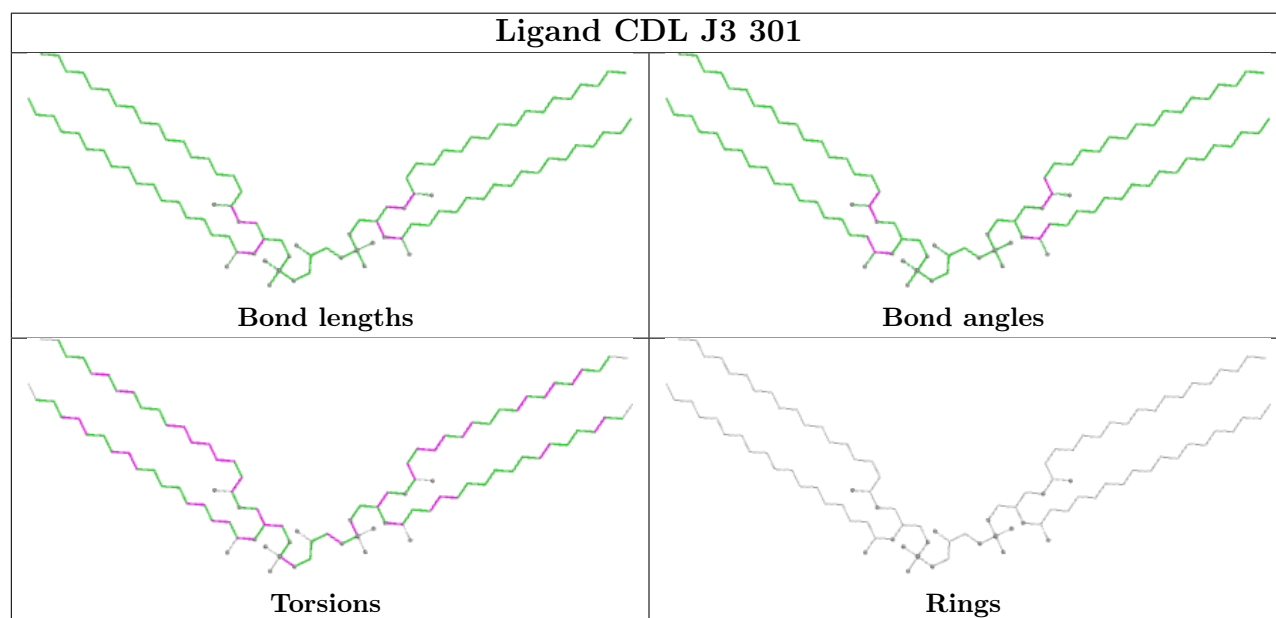
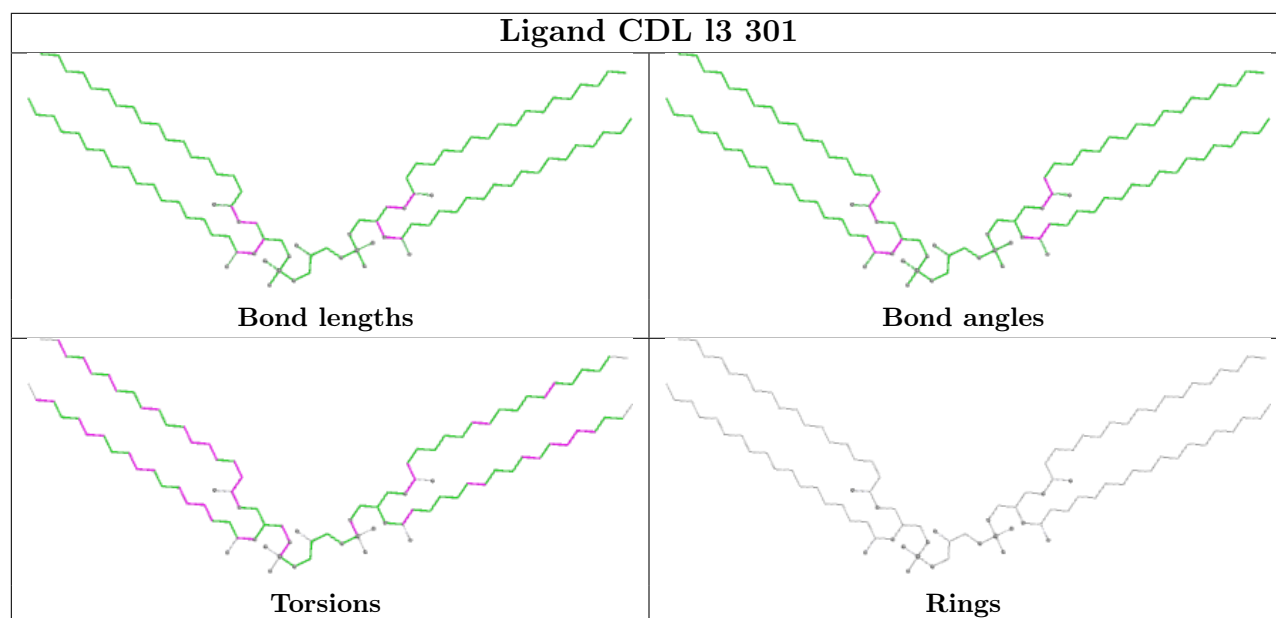
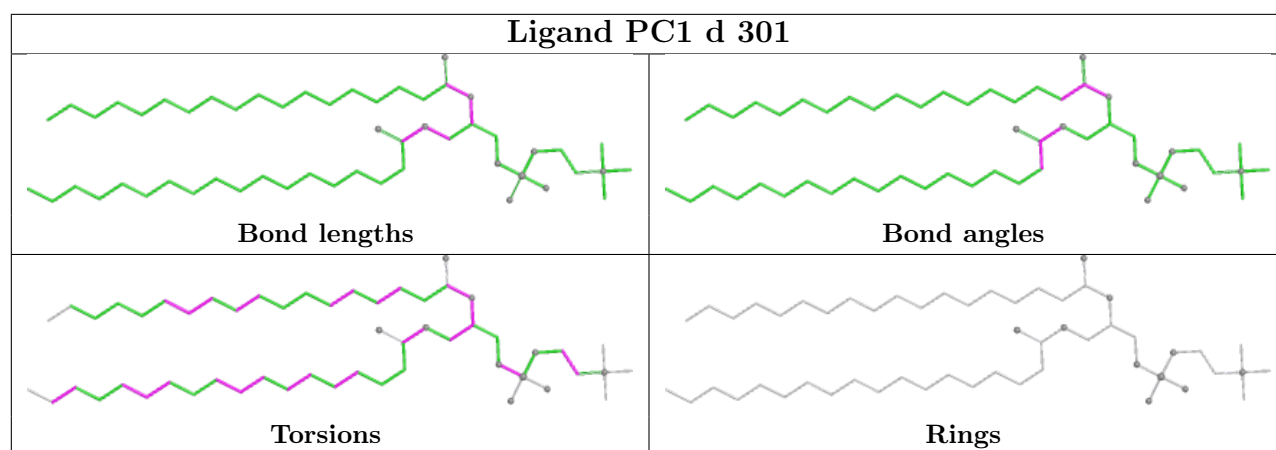


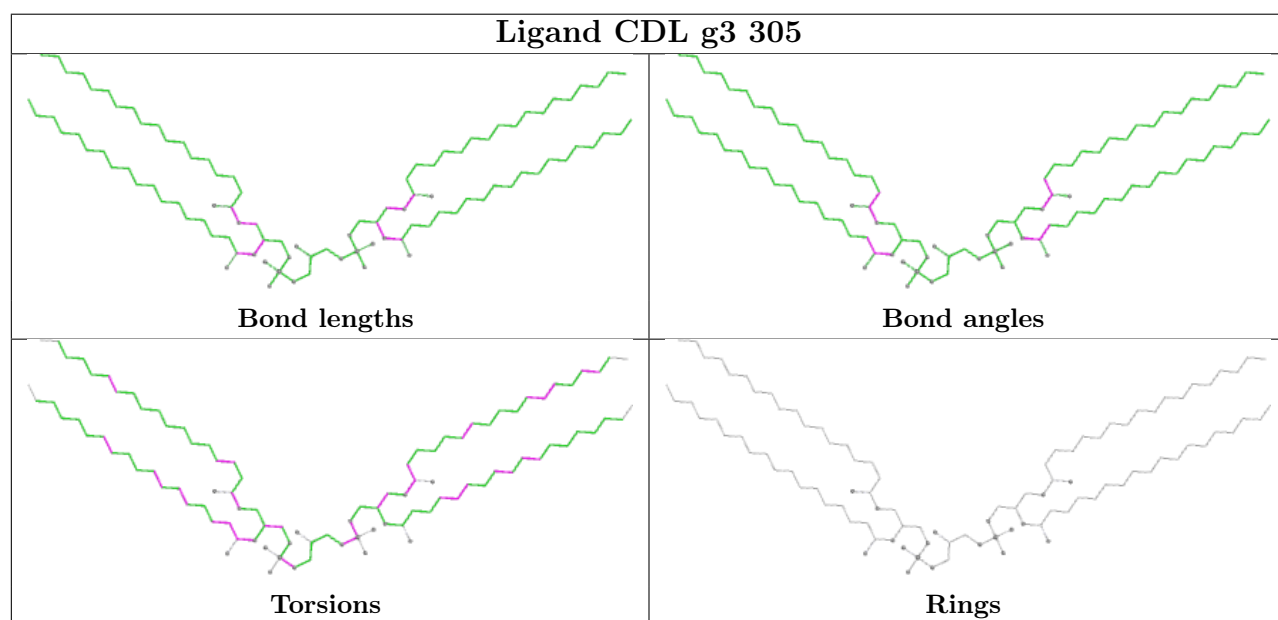
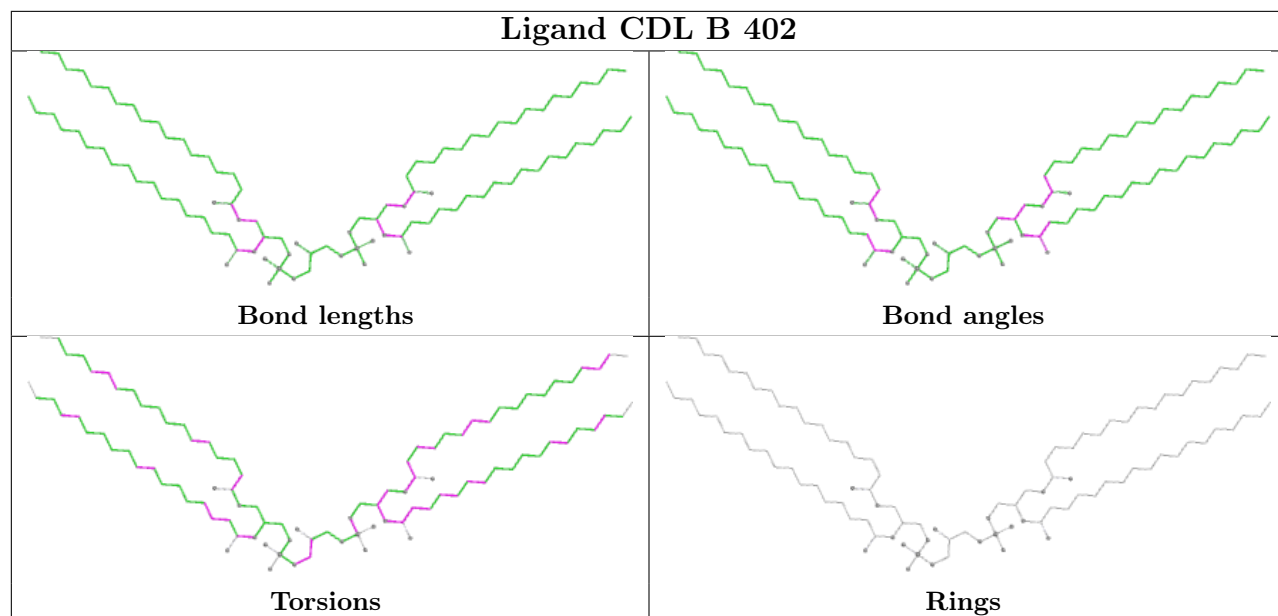
Ligand CDL B 404

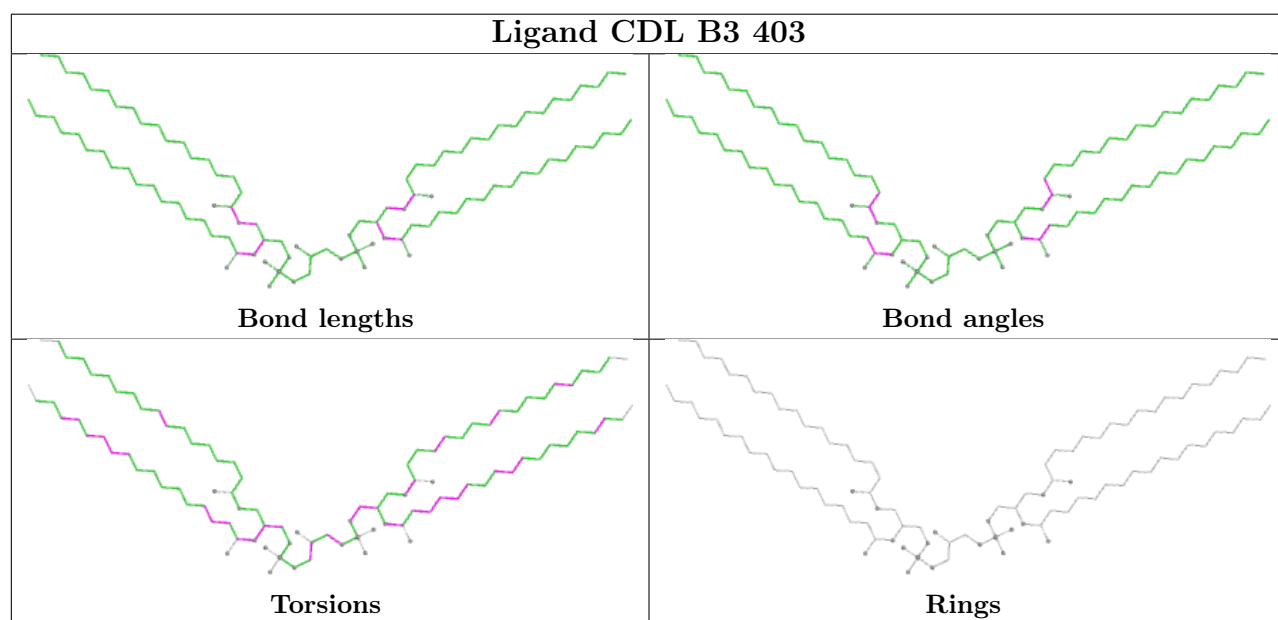
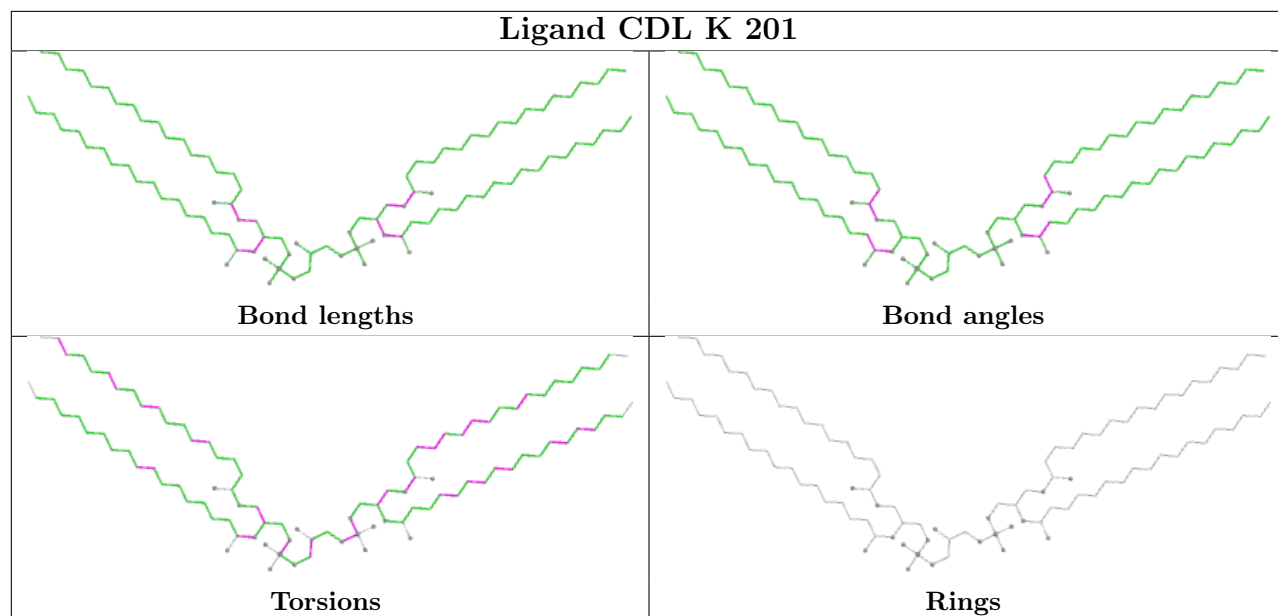


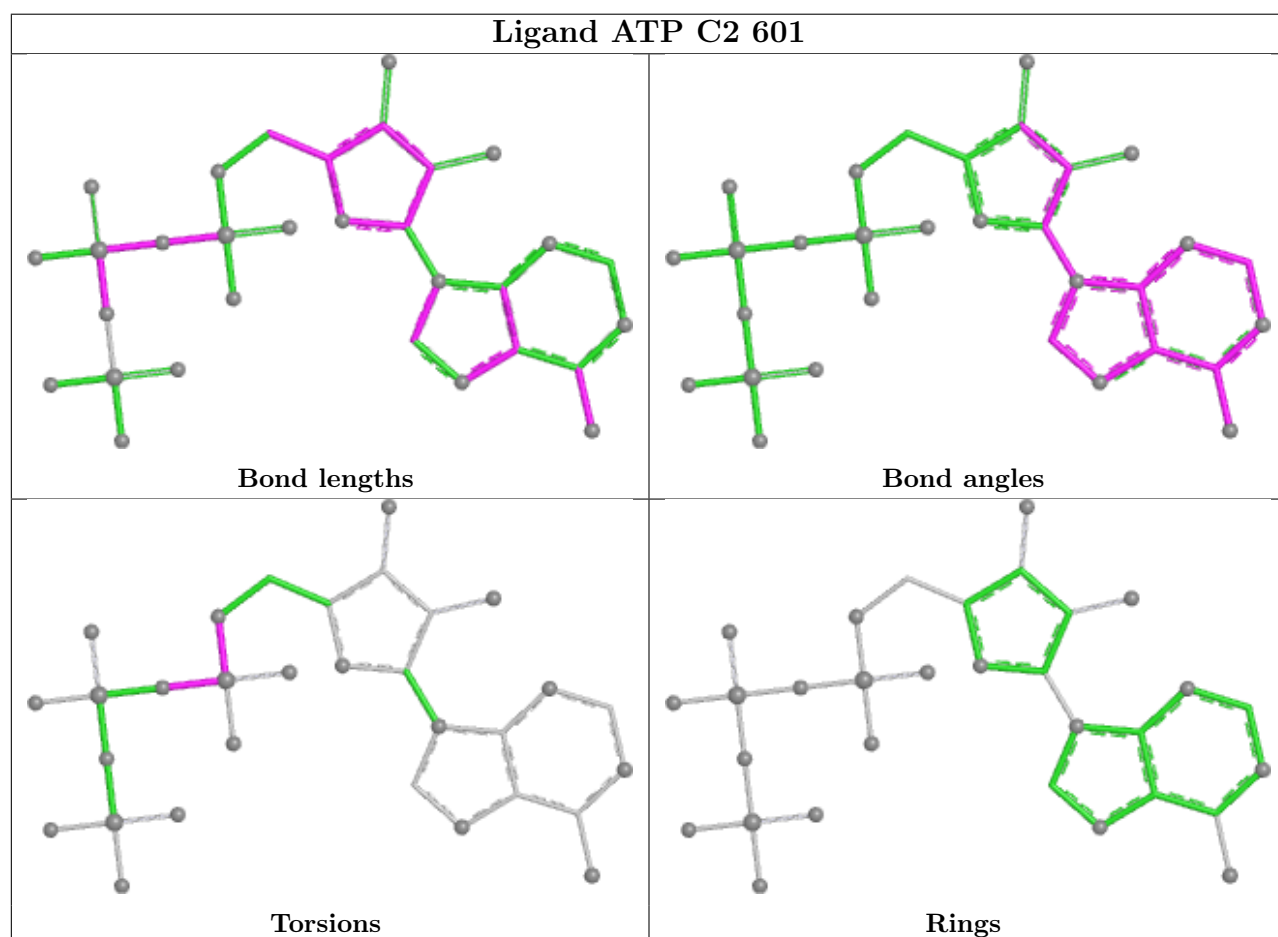
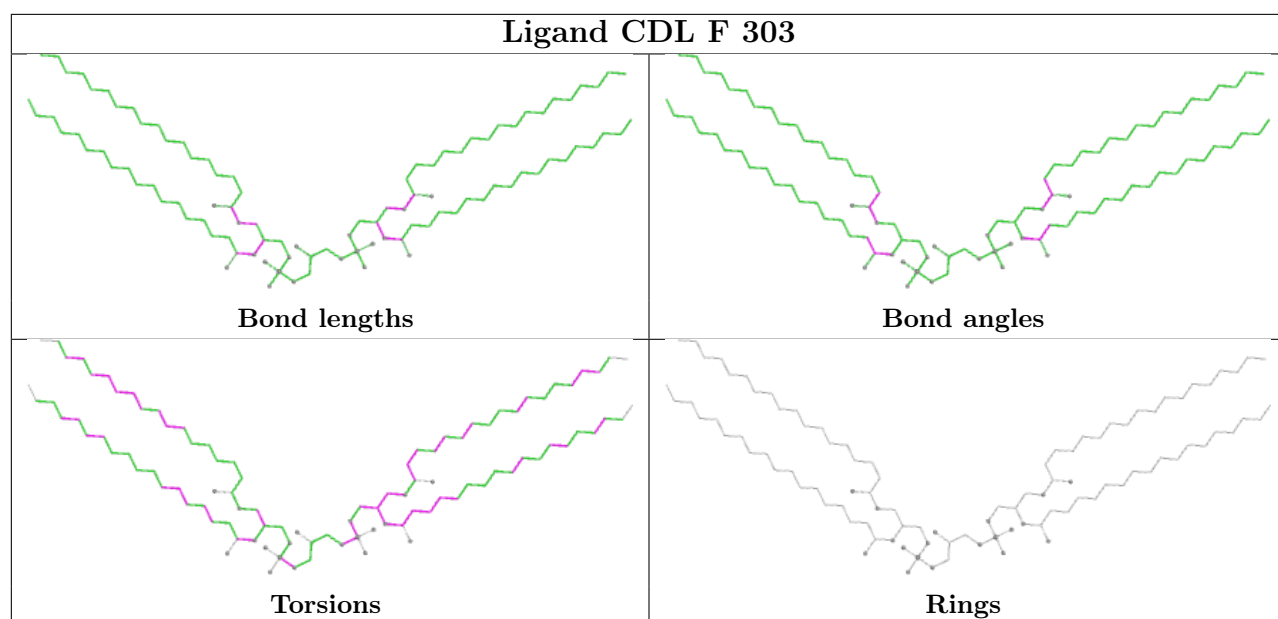


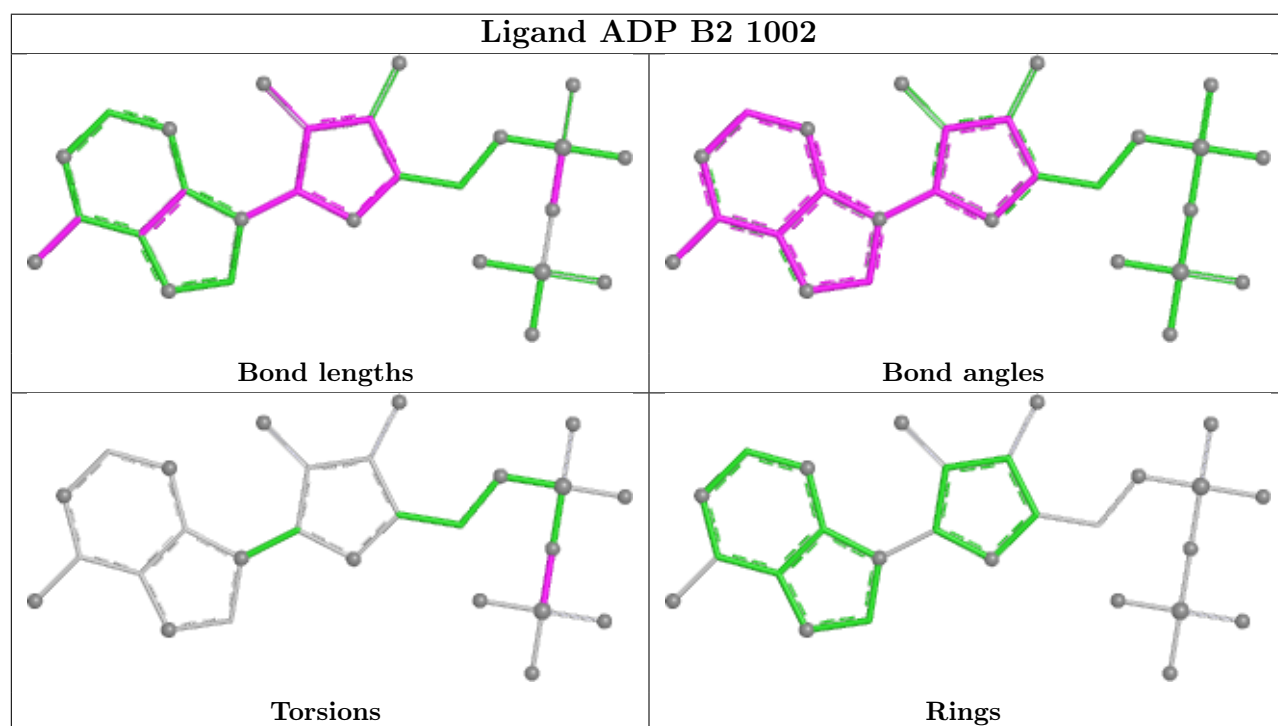
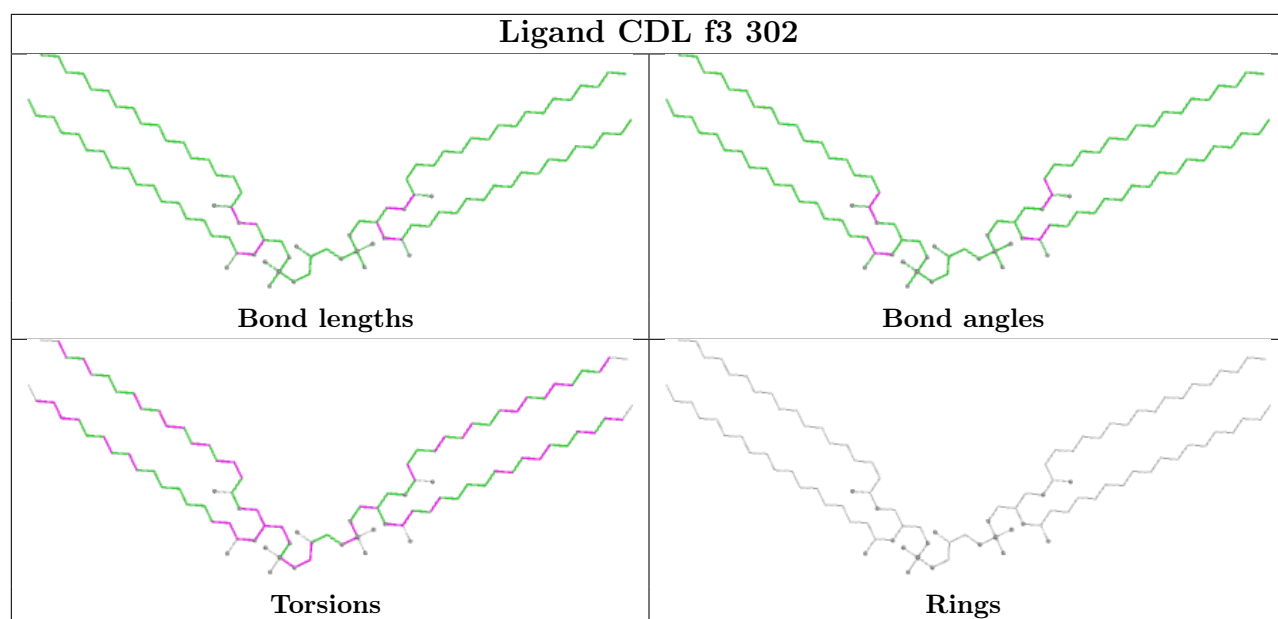


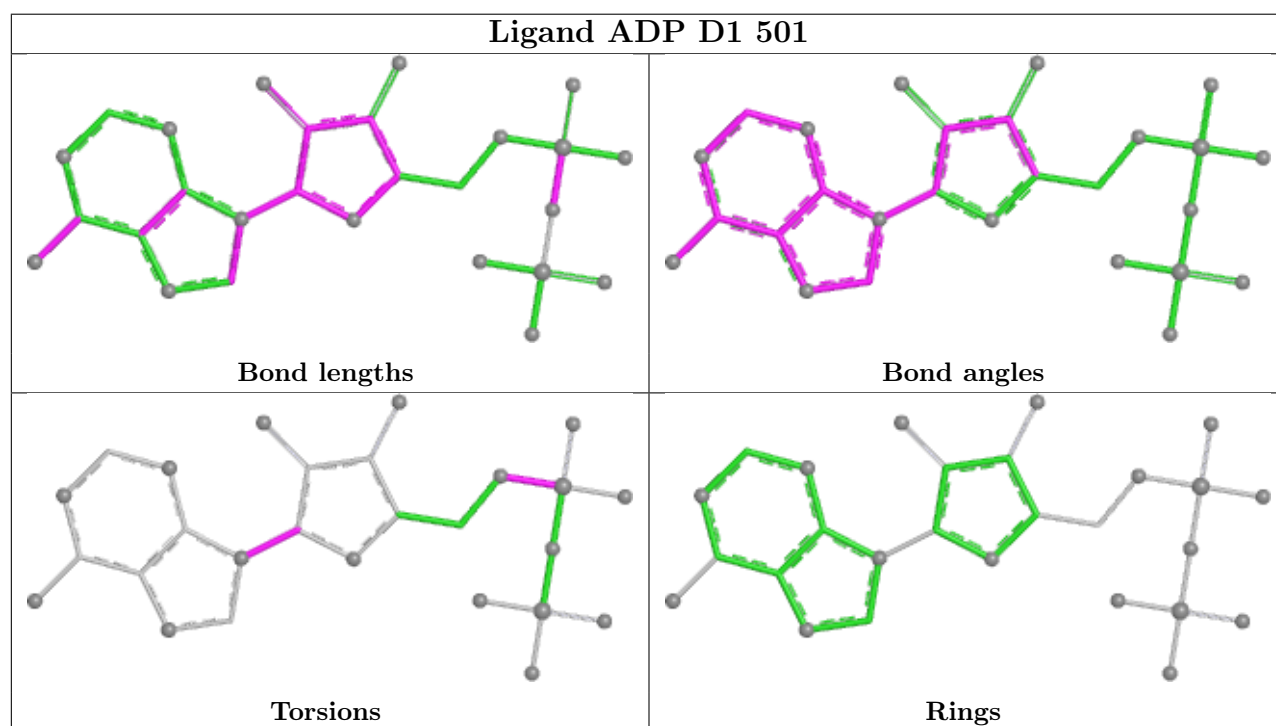
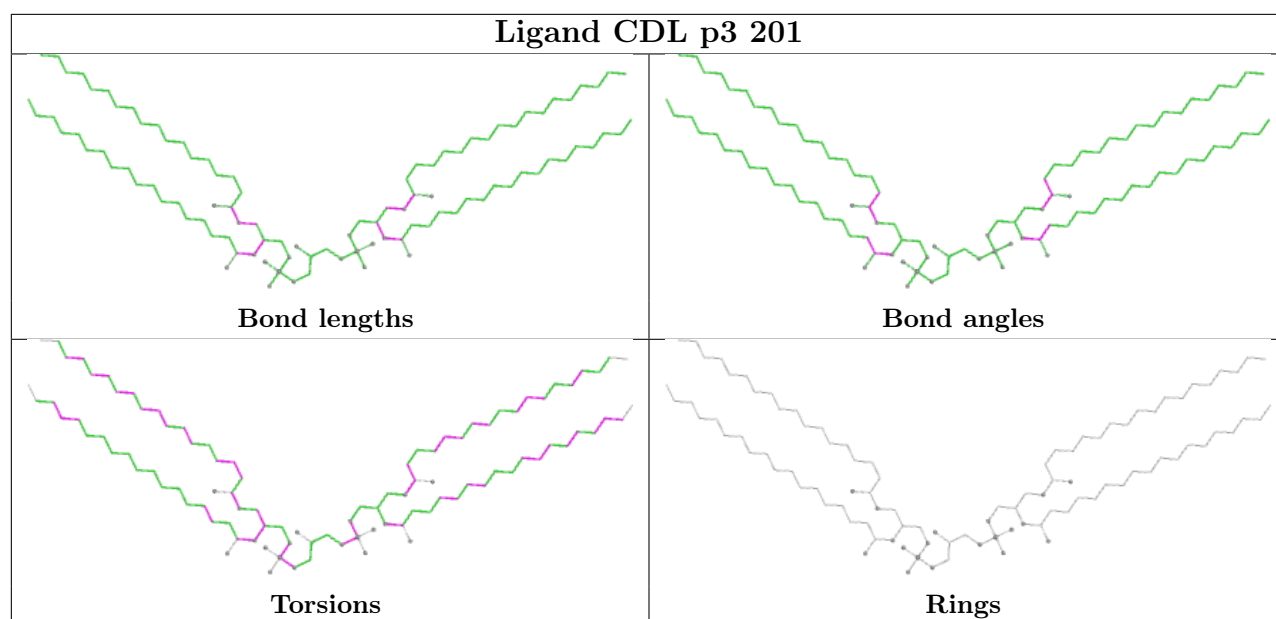


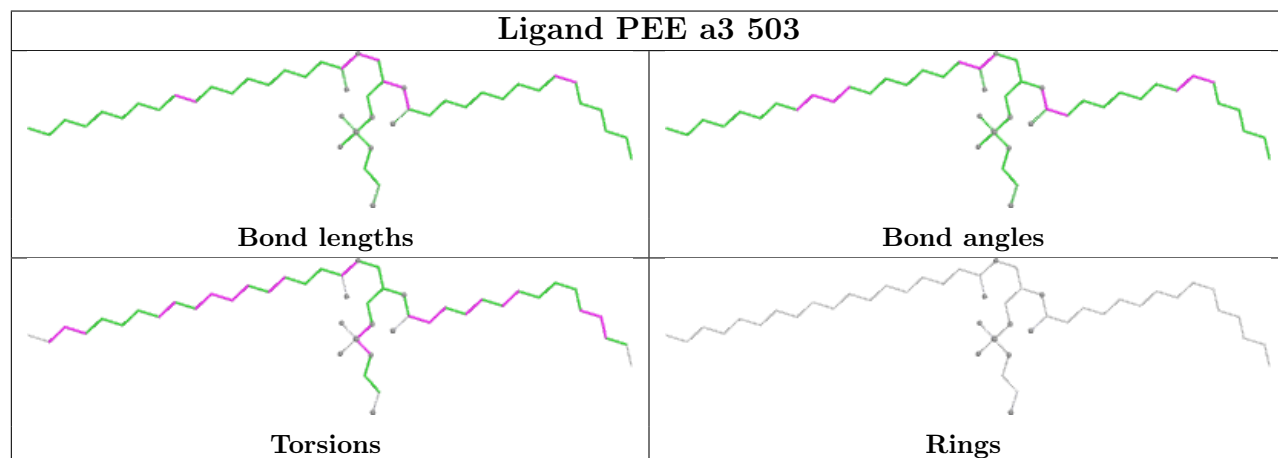
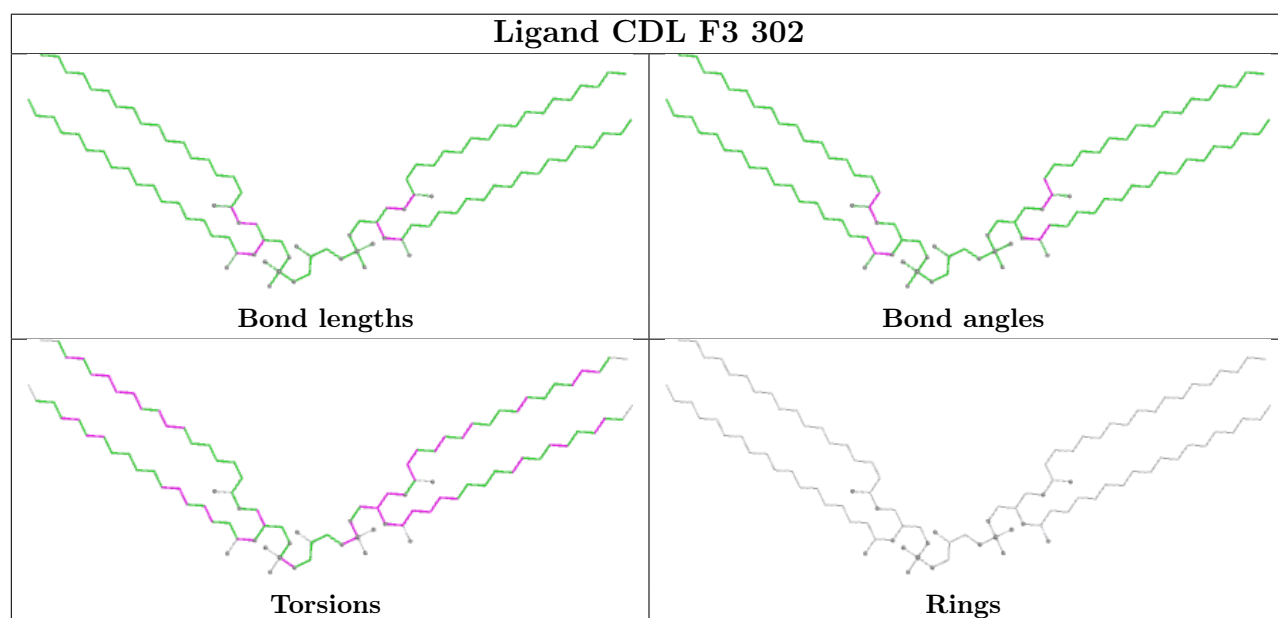
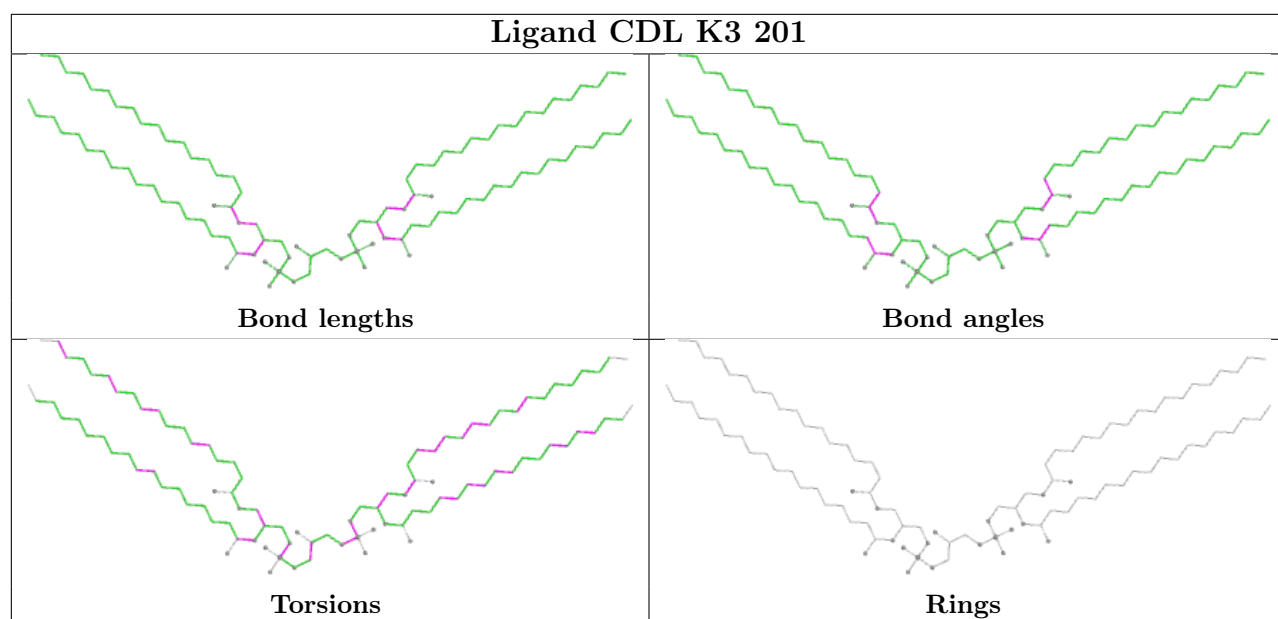


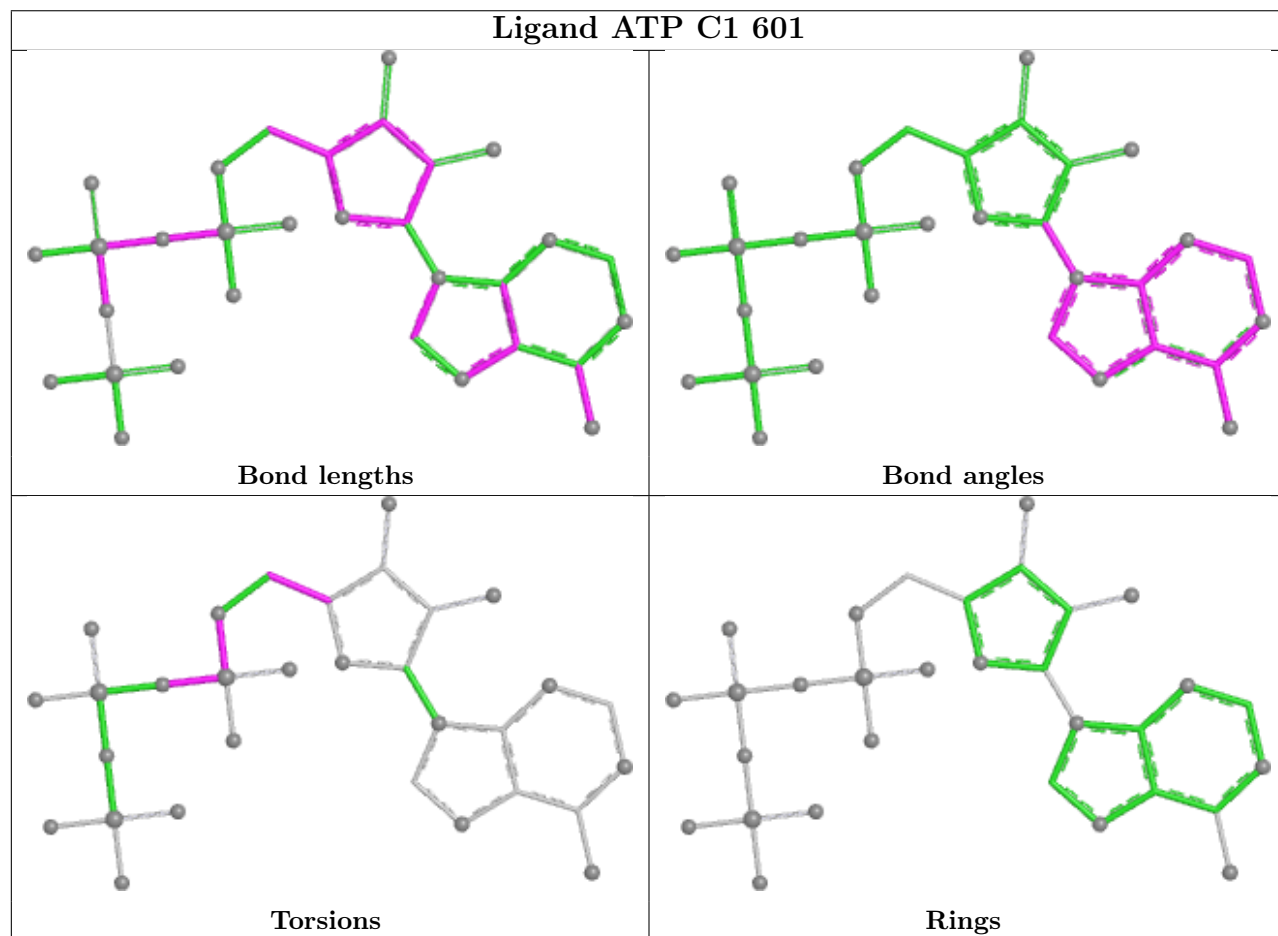
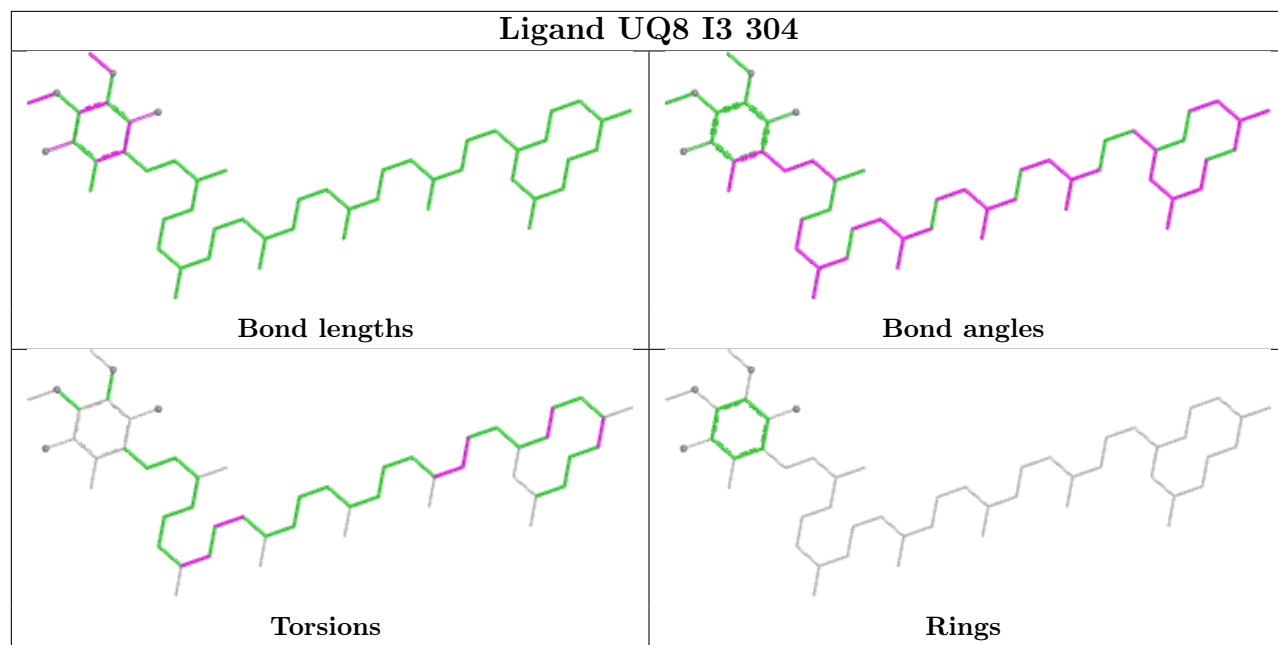


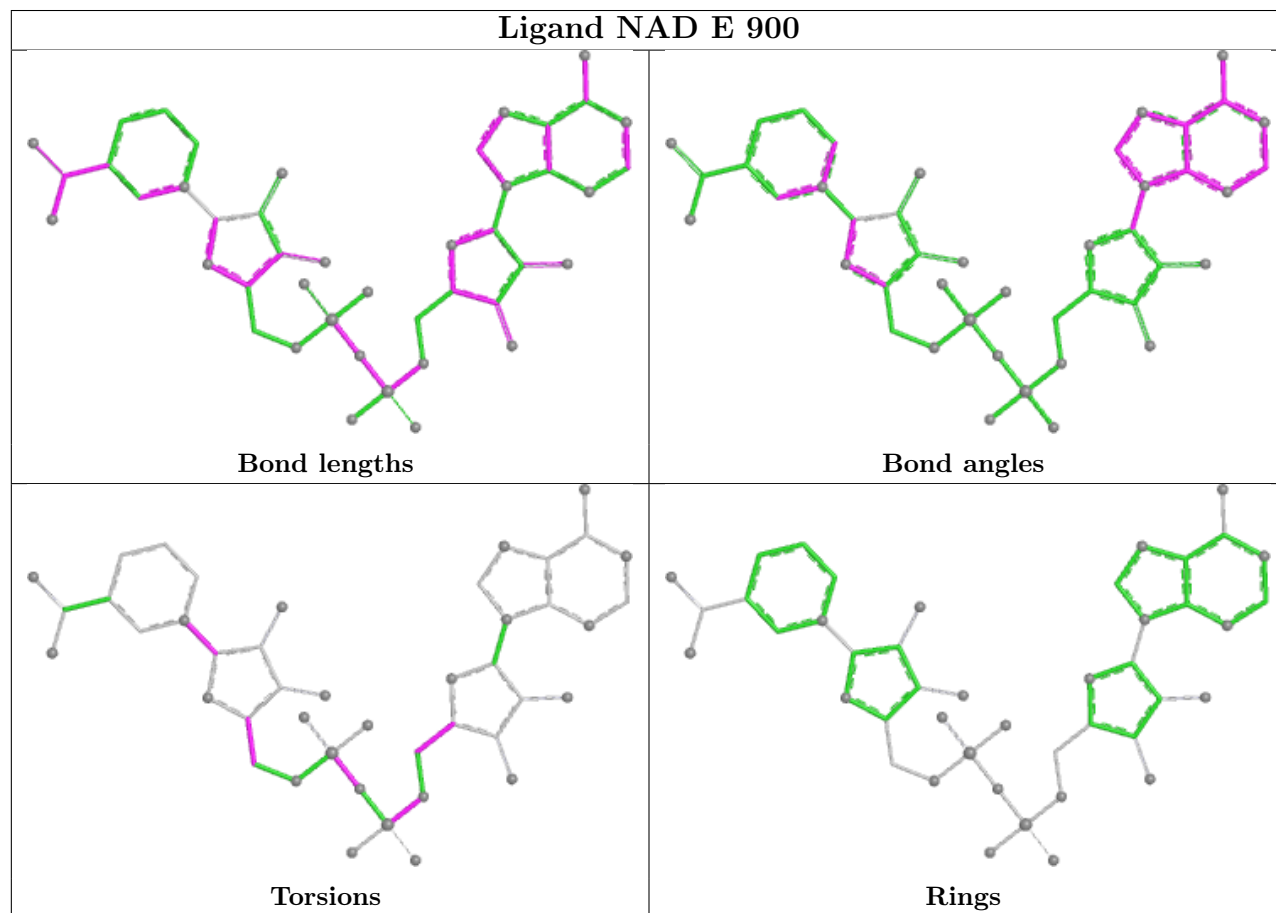
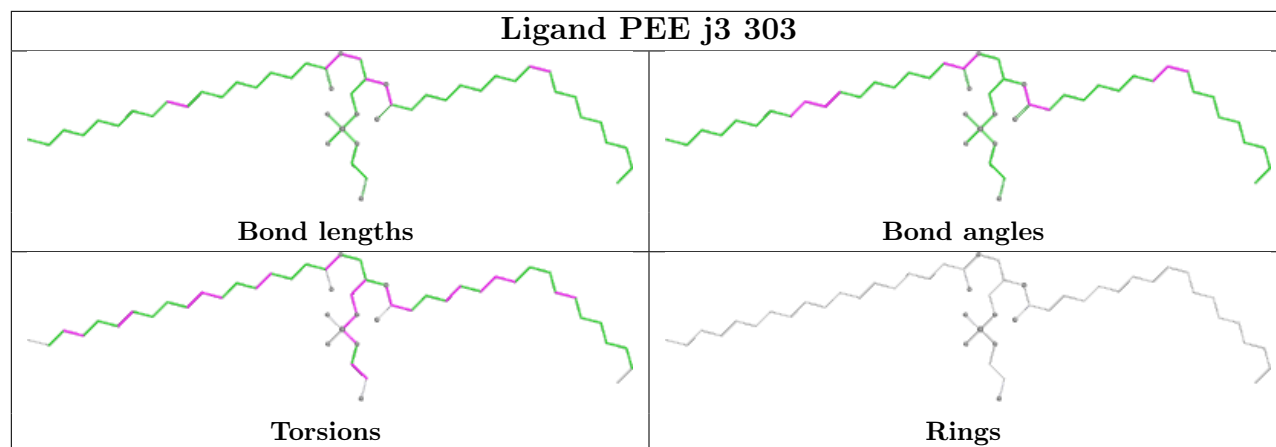


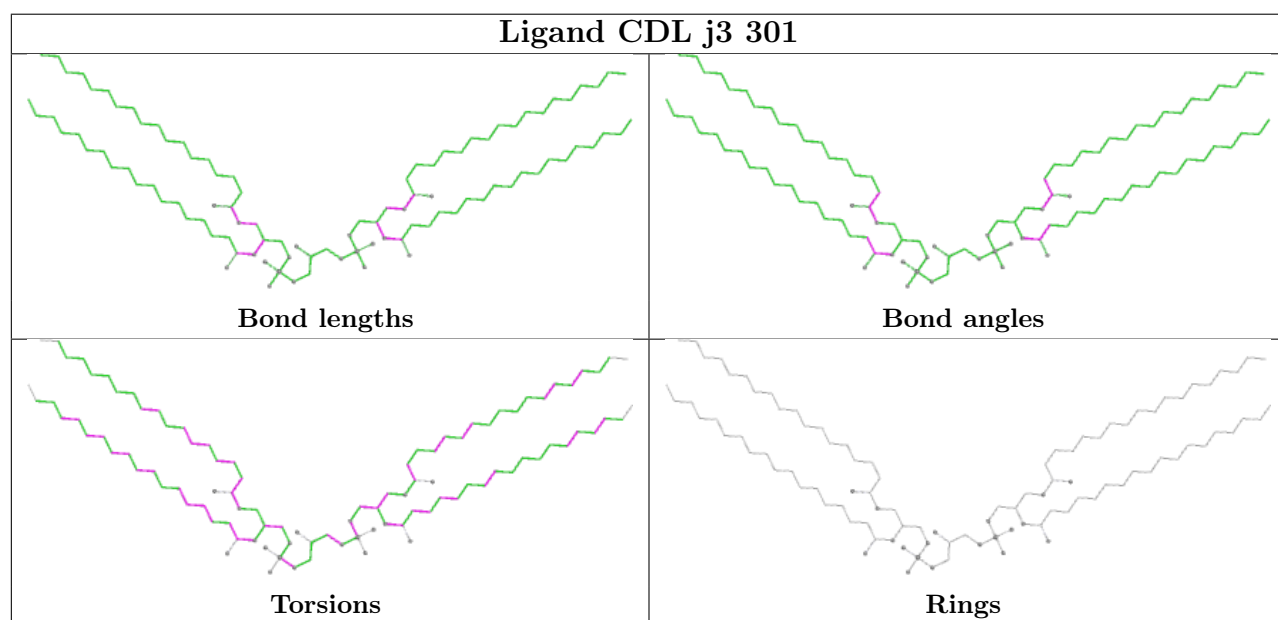
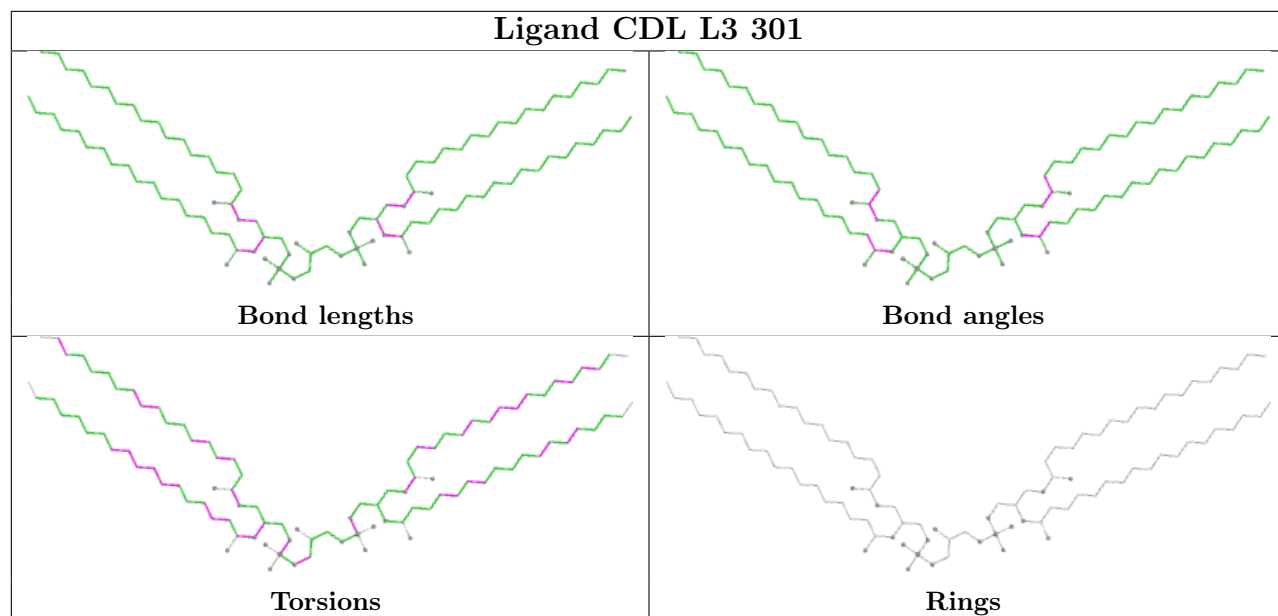




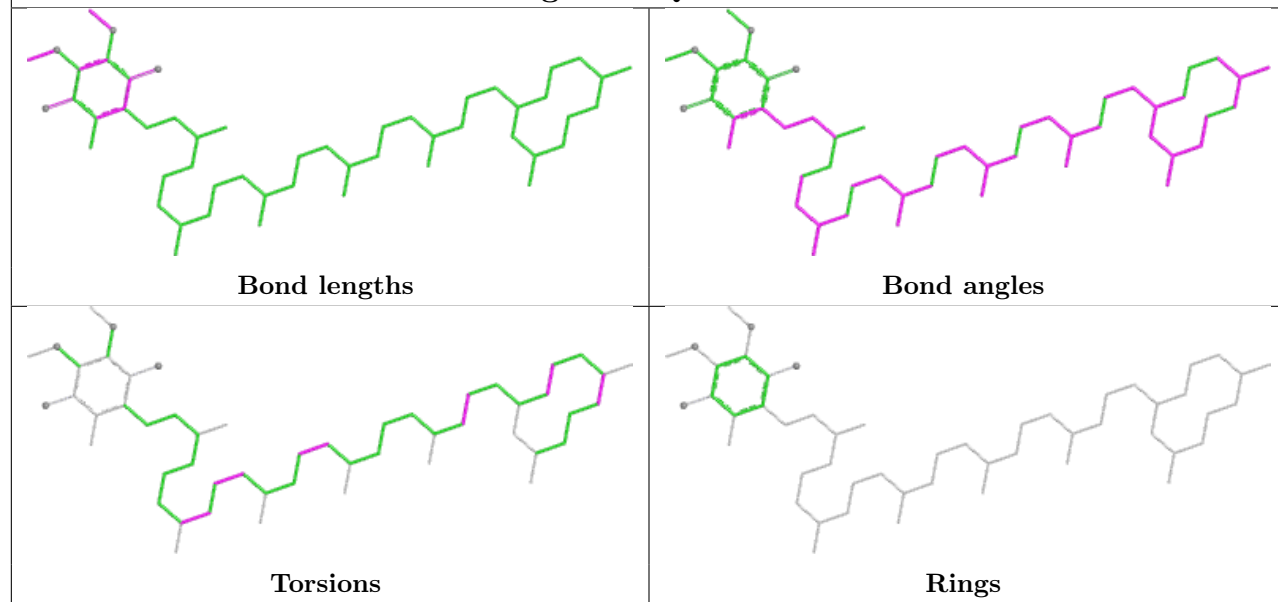




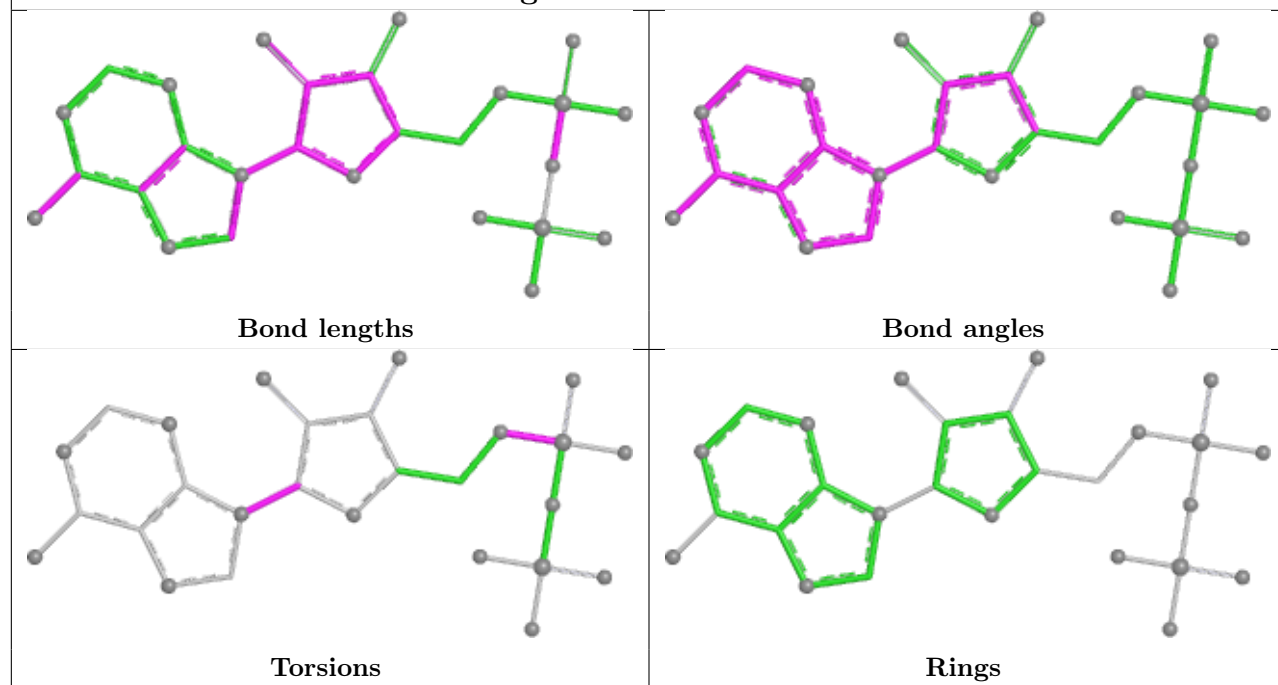


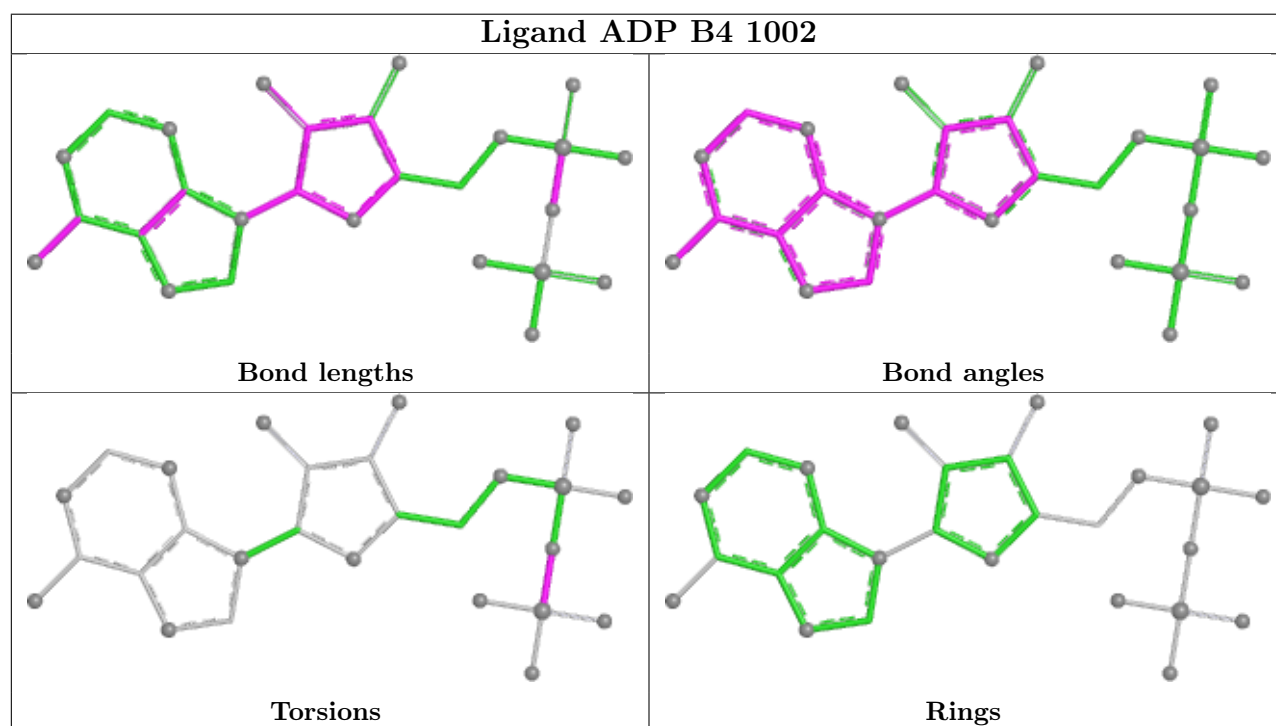
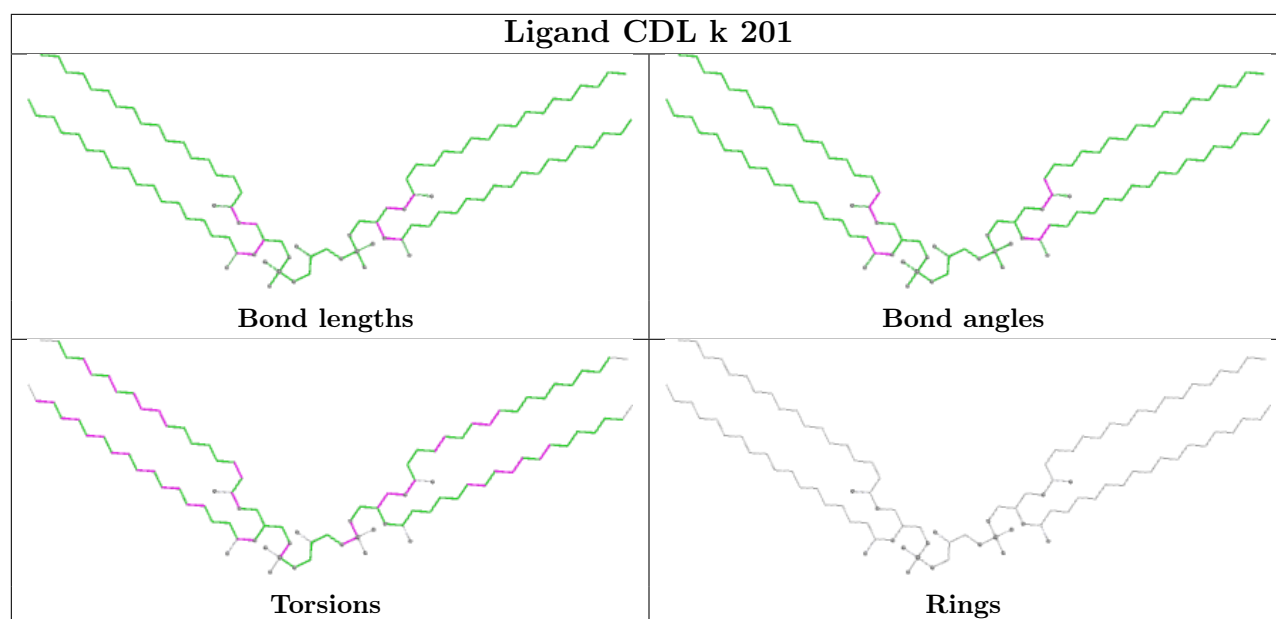


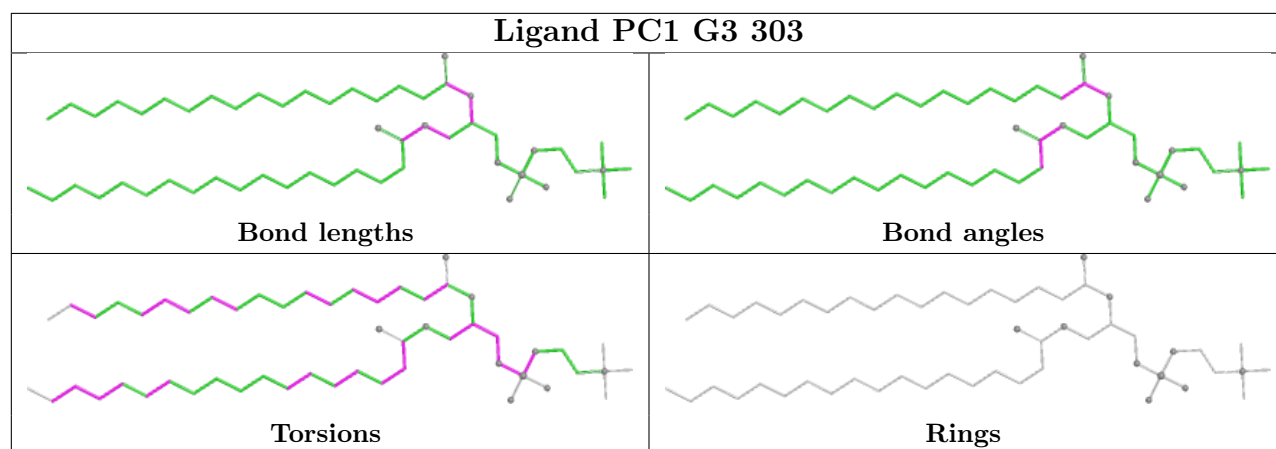
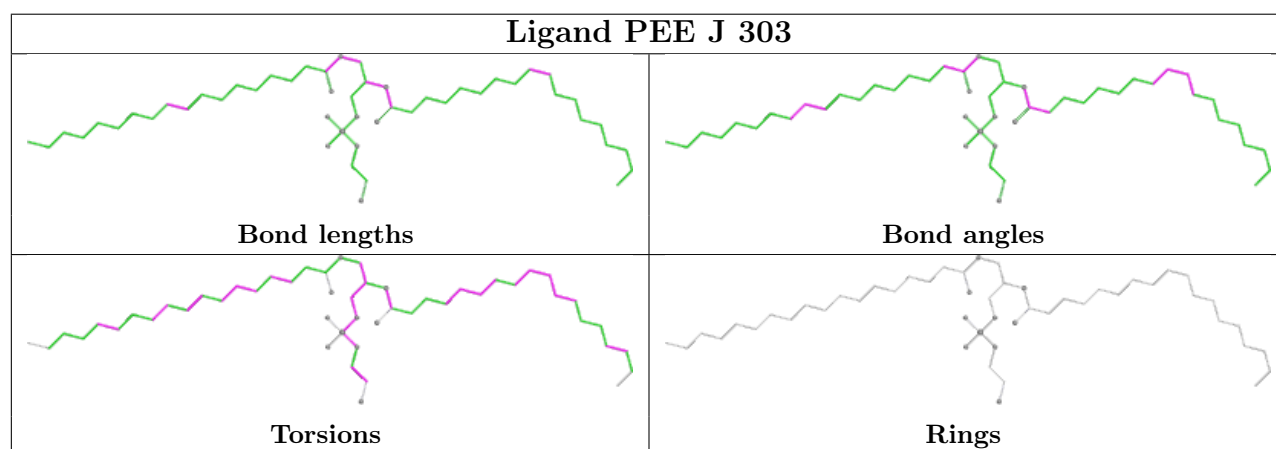
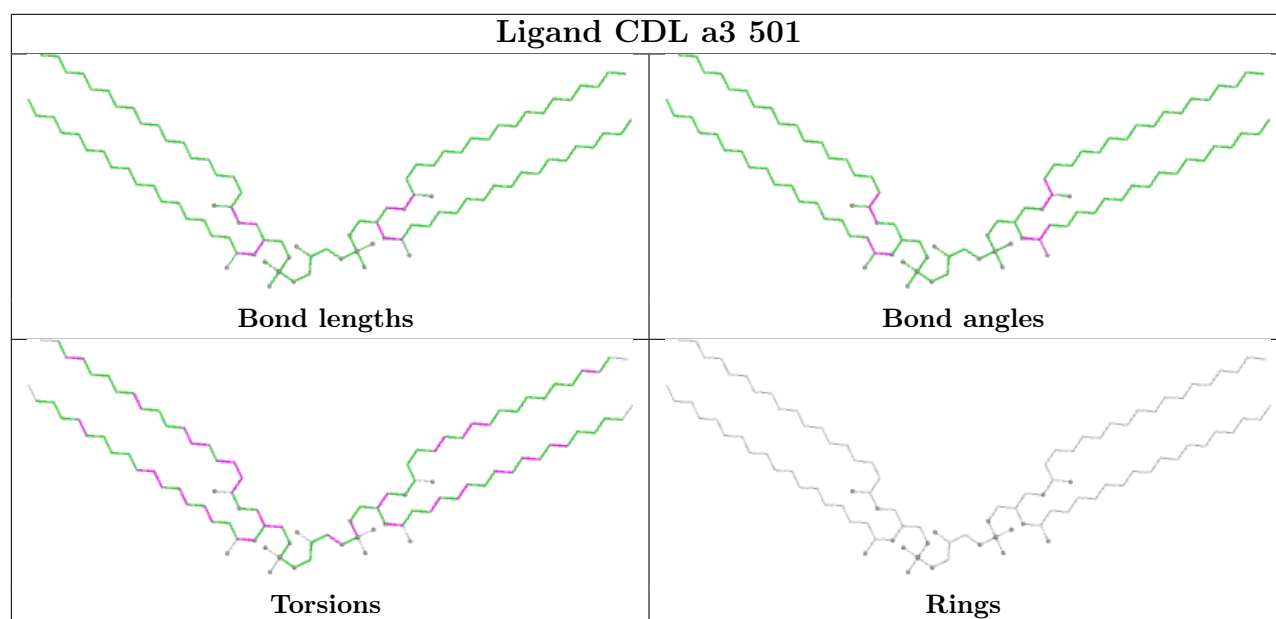
Ligand UQ8 i 302

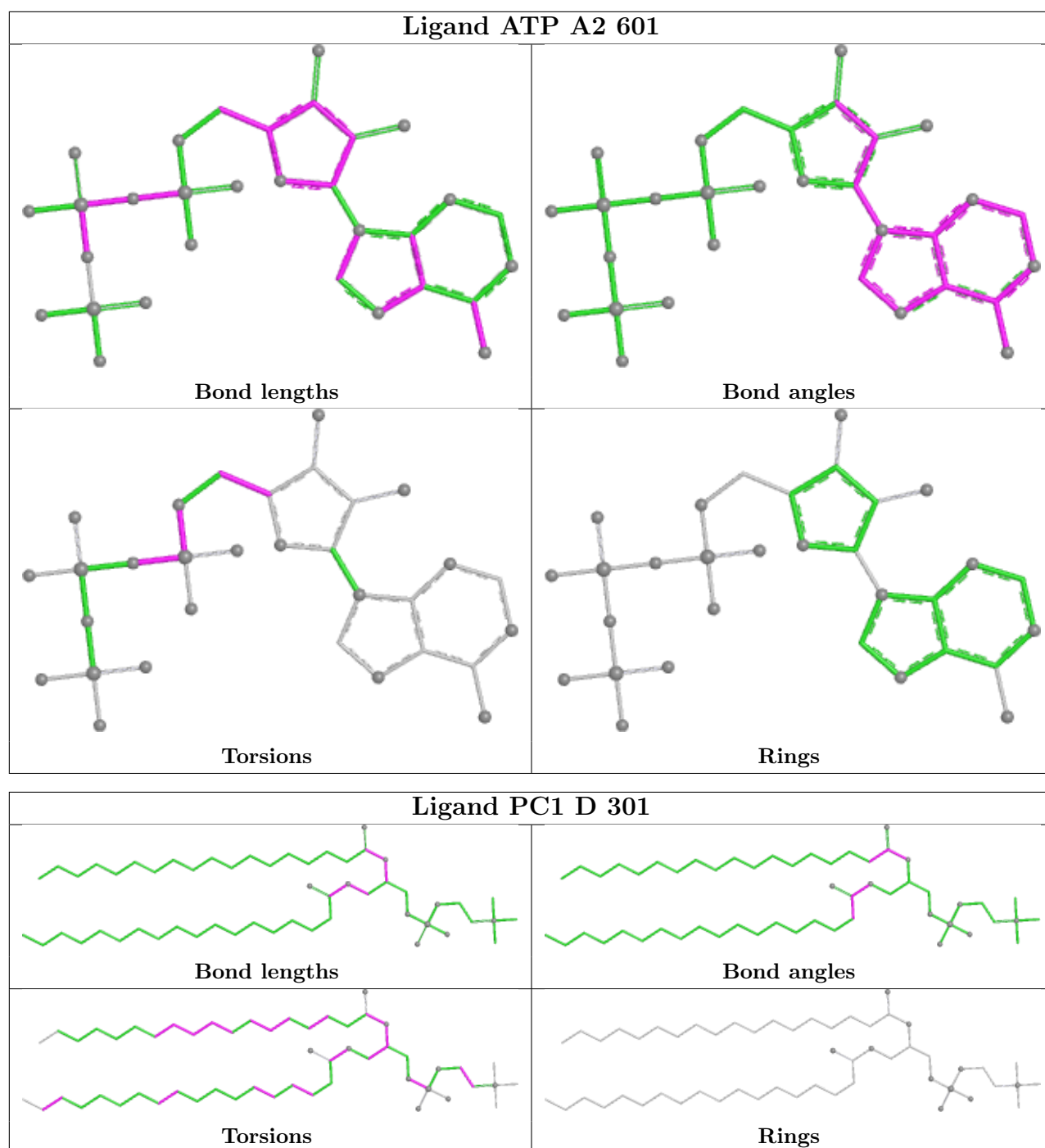


Ligand ADP D4 501









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.

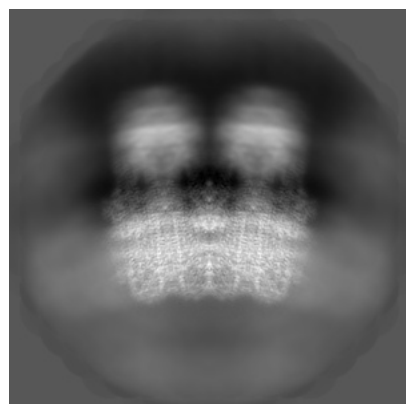
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10861. These allow visual inspection of the internal detail of the map and identification of artifacts.

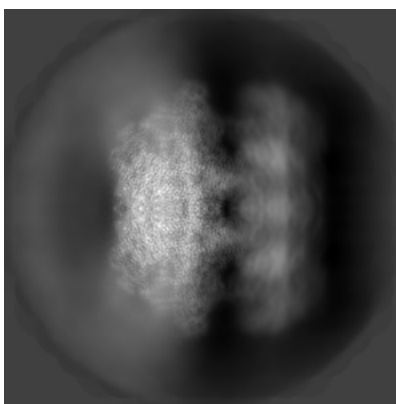
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

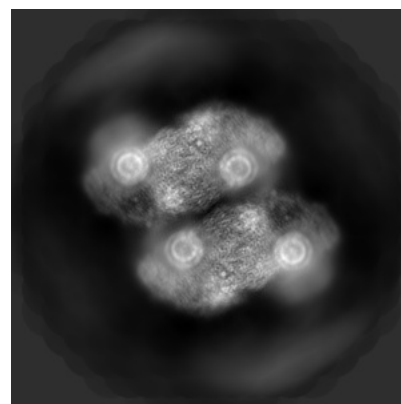
6.1.1 Primary map



X

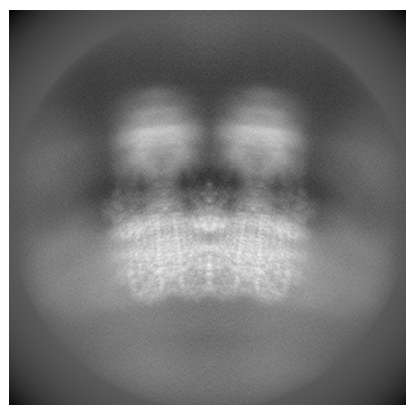


Y

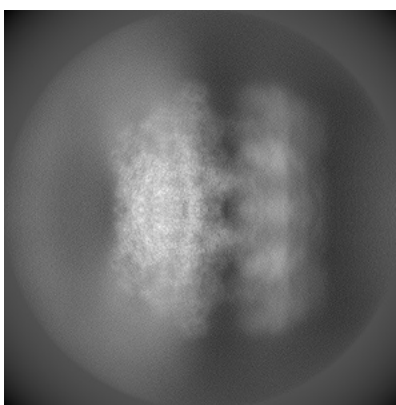


Z

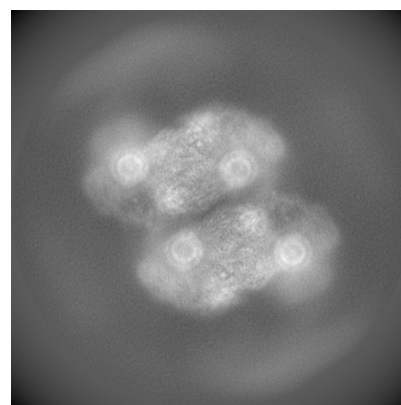
6.1.2 Raw map



X



Y

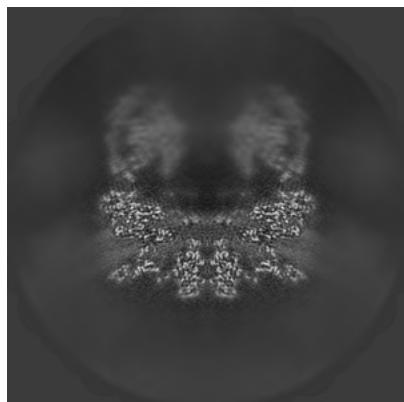


Z

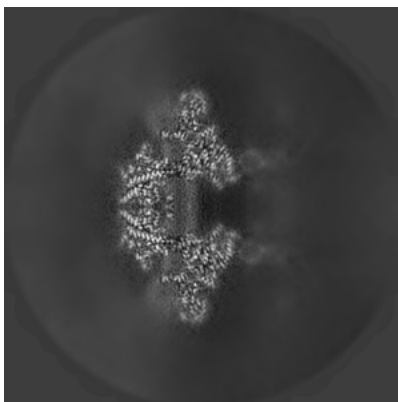
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

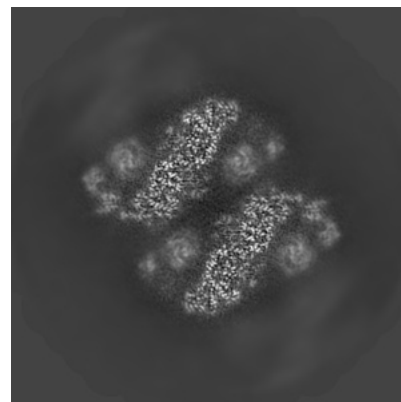
6.2.1 Primary map



X Index: 300

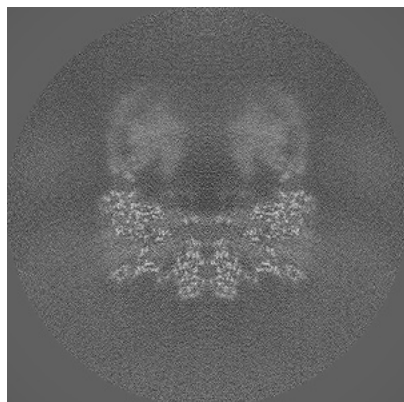


Y Index: 300

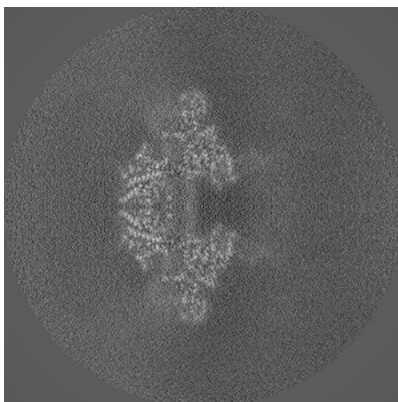


Z Index: 300

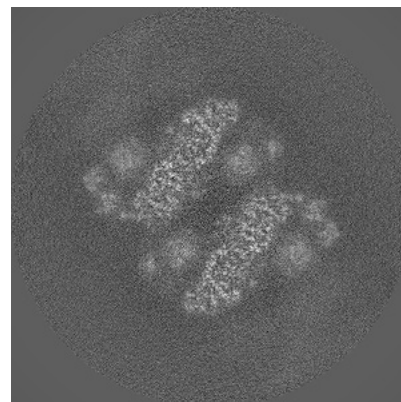
6.2.2 Raw map



X Index: 300



Y Index: 300

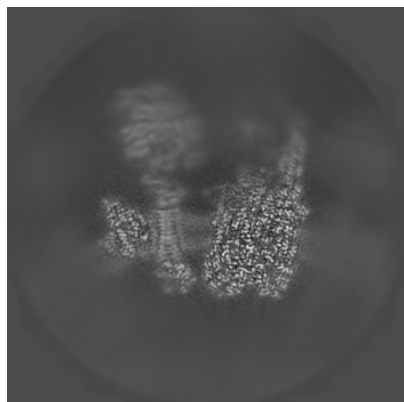


Z Index: 300

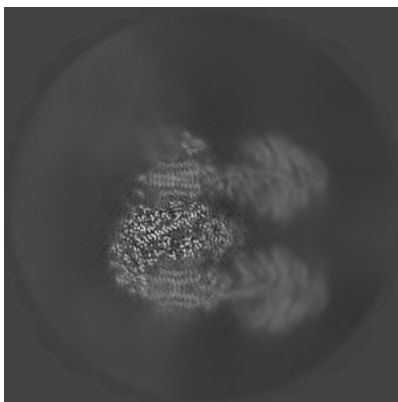
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

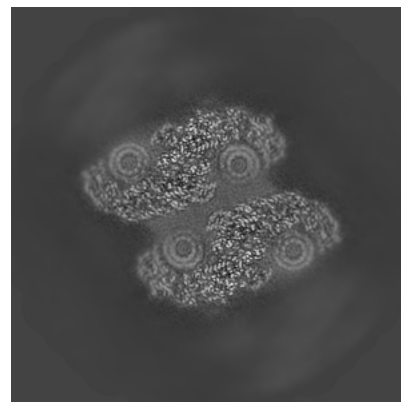
6.3.1 Primary map



X Index: 275

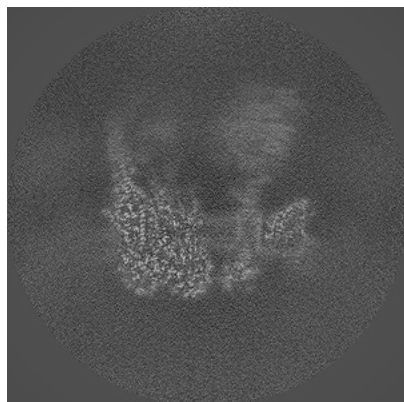


Y Index: 376

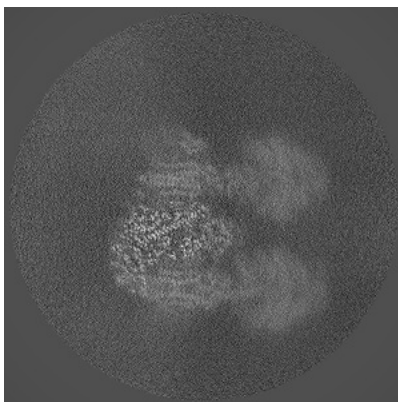


Z Index: 278

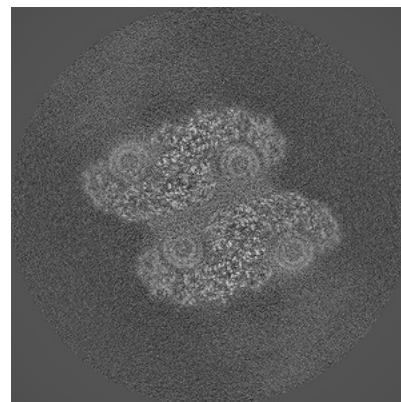
6.3.2 Raw map



X Index: 320



Y Index: 376

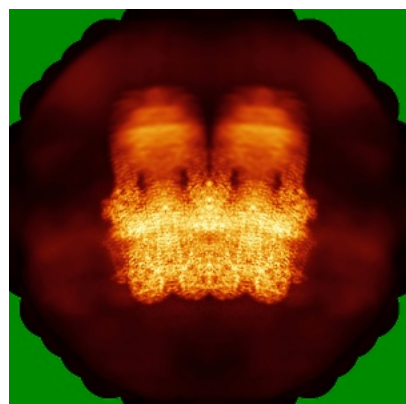


Z Index: 278

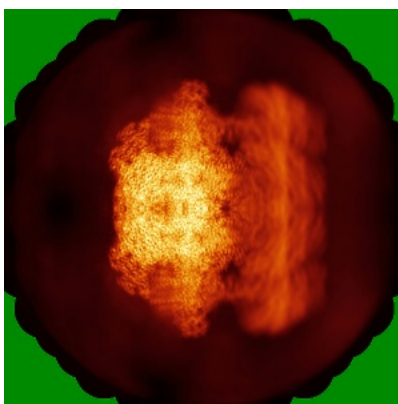
The images above show the largest variance slices of the map in three orthogonal directions.

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

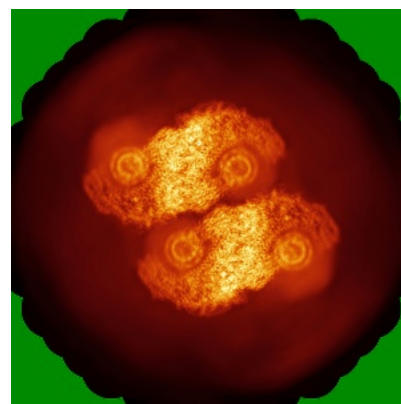
6.4.1 Primary map



X

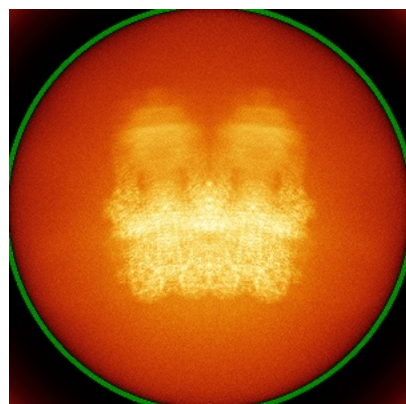


Y

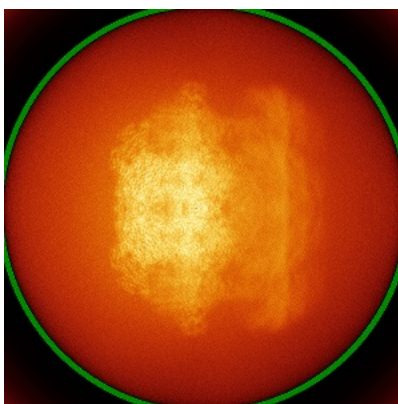


Z

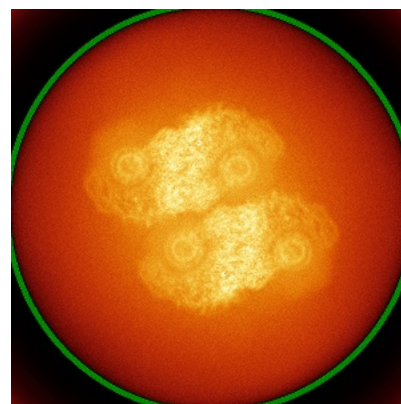
6.4.2 Raw map



X



Y



Z

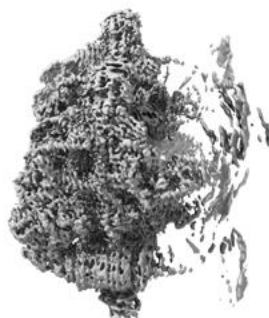
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

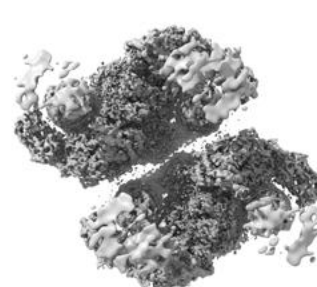
6.5.1 Primary map



X



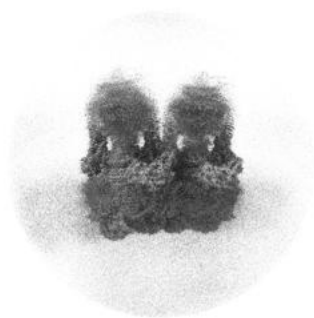
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

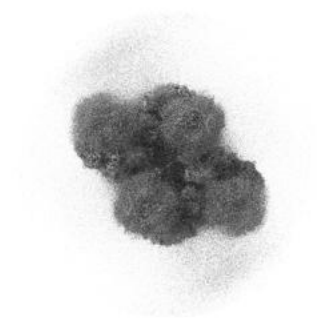
6.5.2 Raw map



X



Y



Z

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.

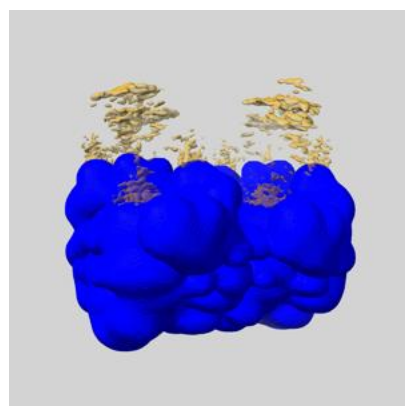
6.6 Mask visualisation [i](#)

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

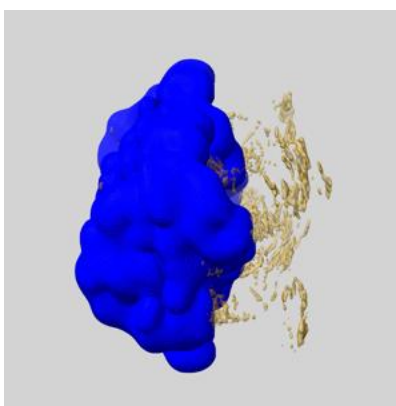
A mask typically either:

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

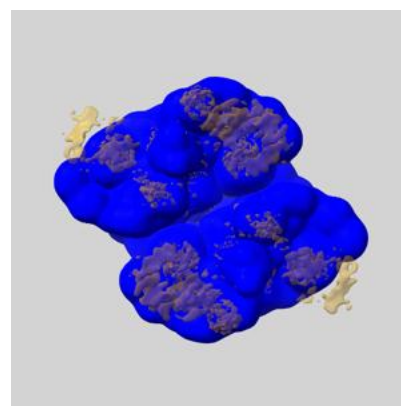
6.6.1 emd_10861_msk_1.map [i](#)



X



Y

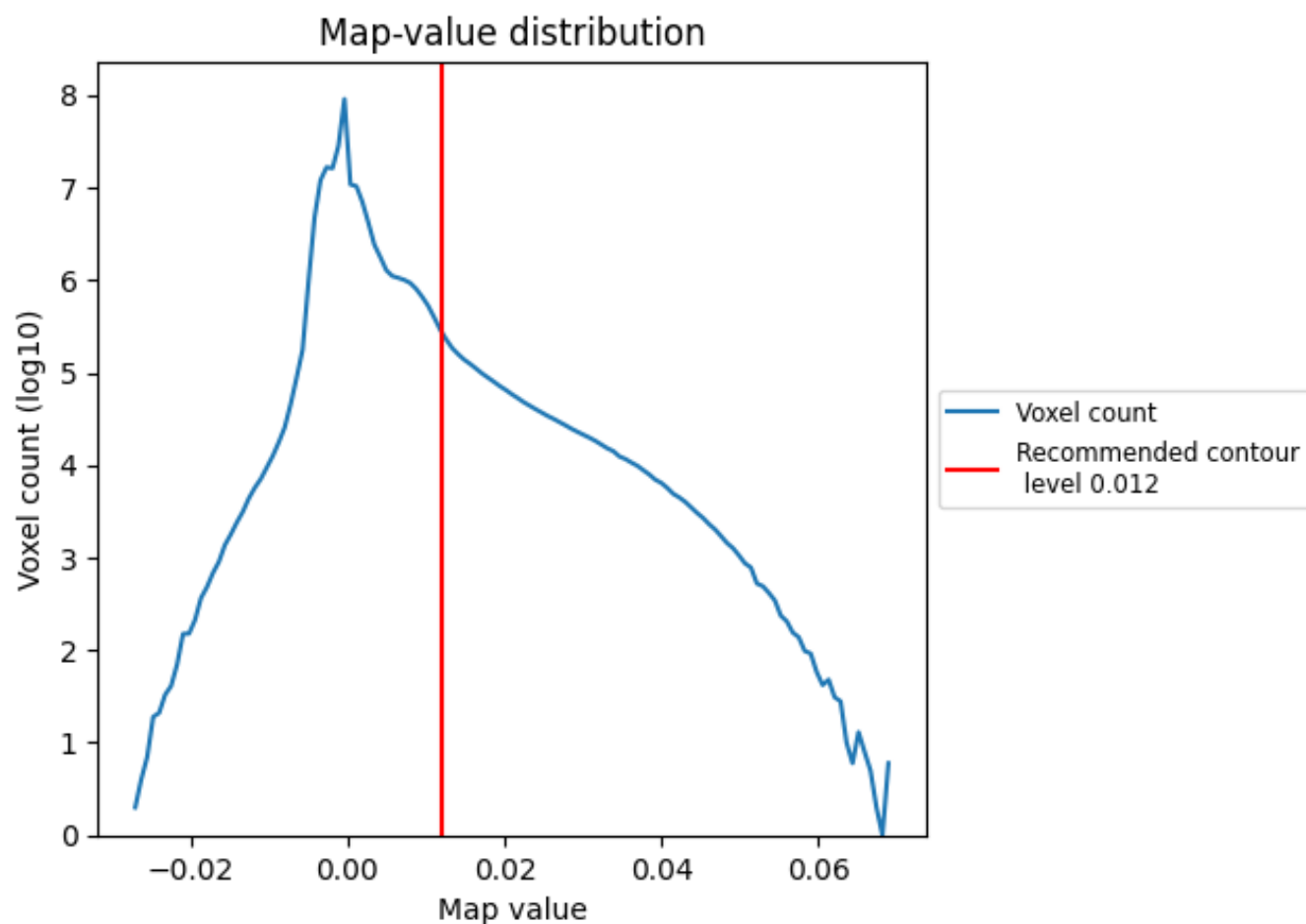


Z

7 Map analysis [i](#)

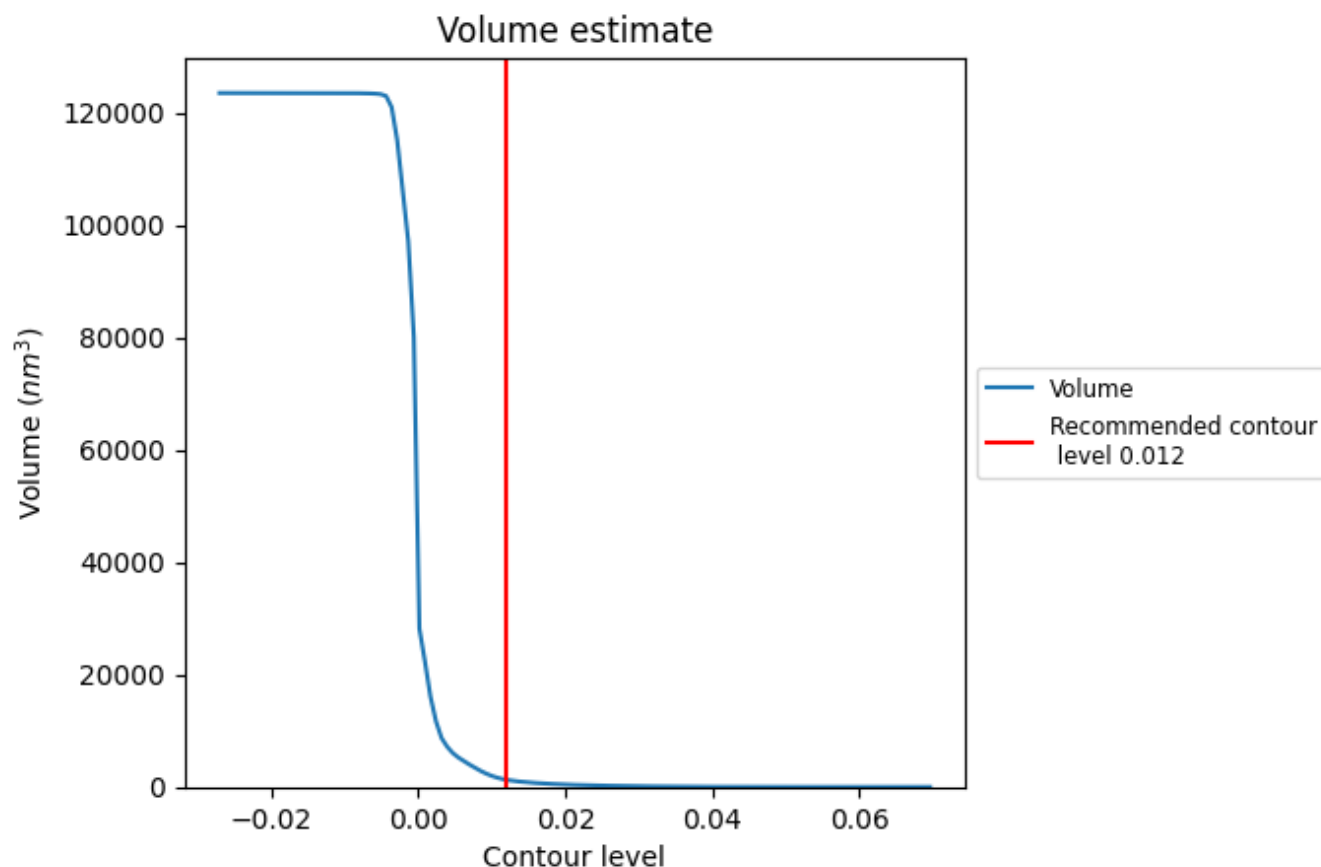
This section contains the results of statistical analysis of the map.

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.

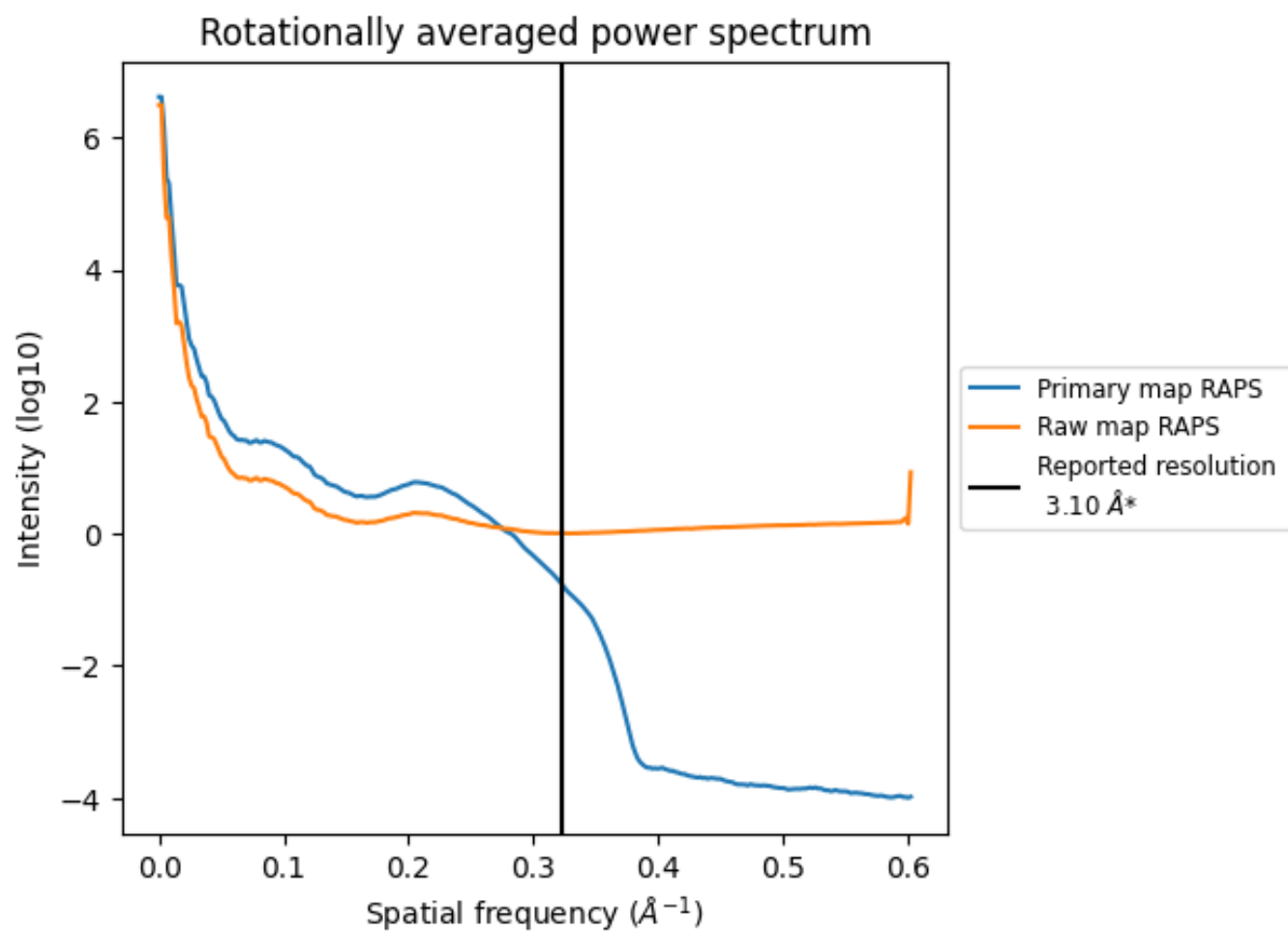
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1280 nm^3 ; this corresponds to an approximate mass of 1157 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

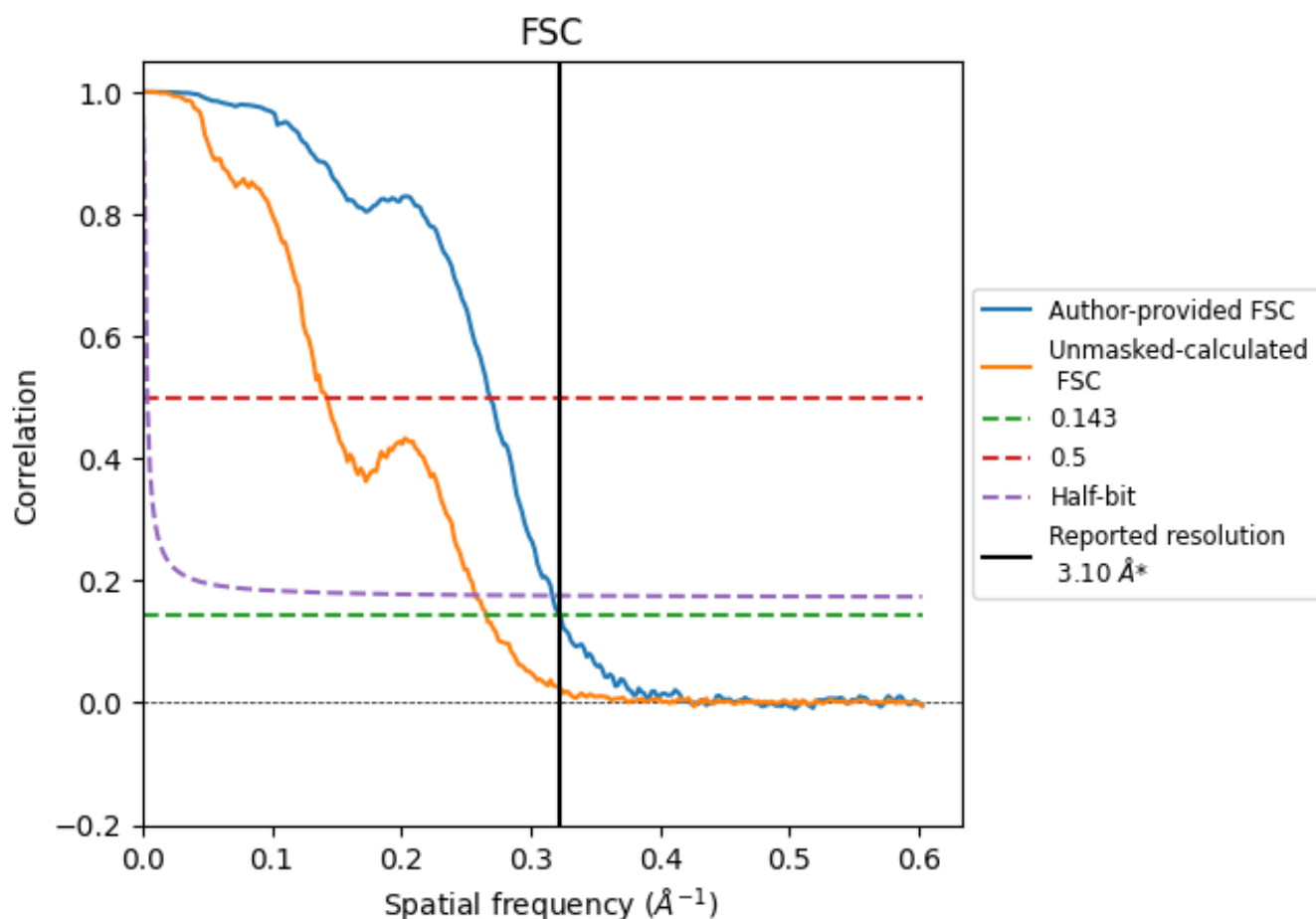


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

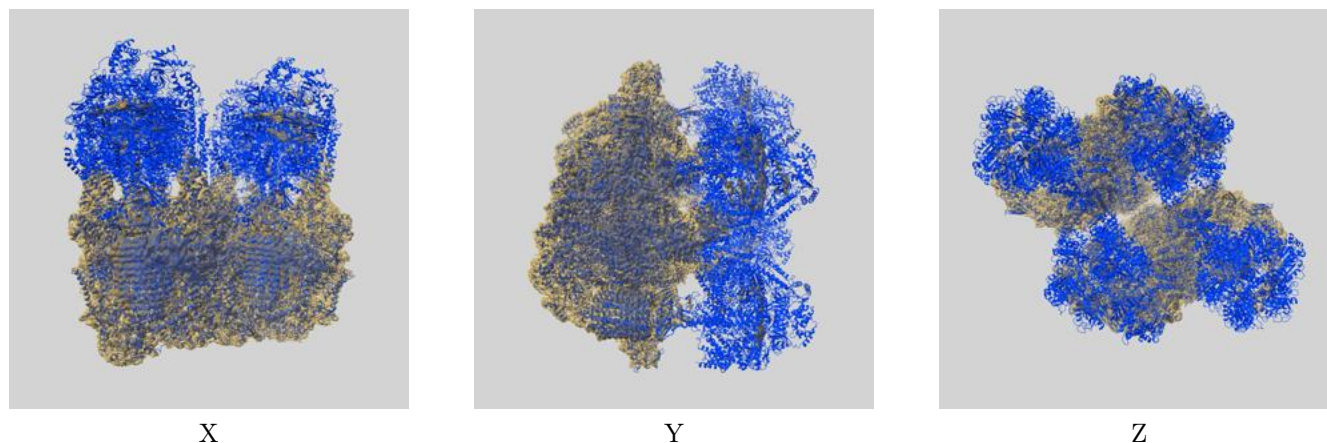
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.72	3.16
Unmasked-calculated*	3.76	7.01	3.89

*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 3.76 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

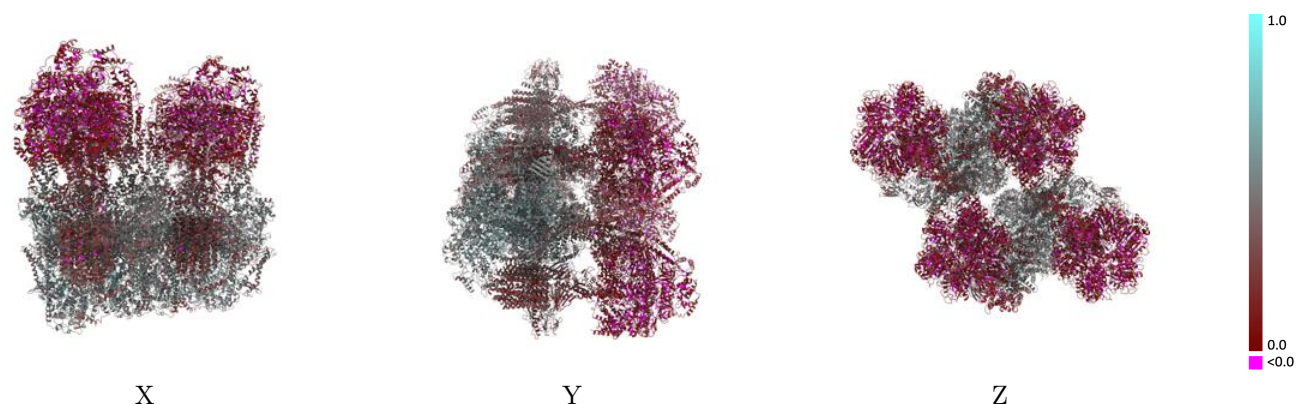
This section contains information regarding the fit between EMDB map EMD-10861 and PDB model 6YNZ. Per-residue inclusion information can be found in section 3 on page 32.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

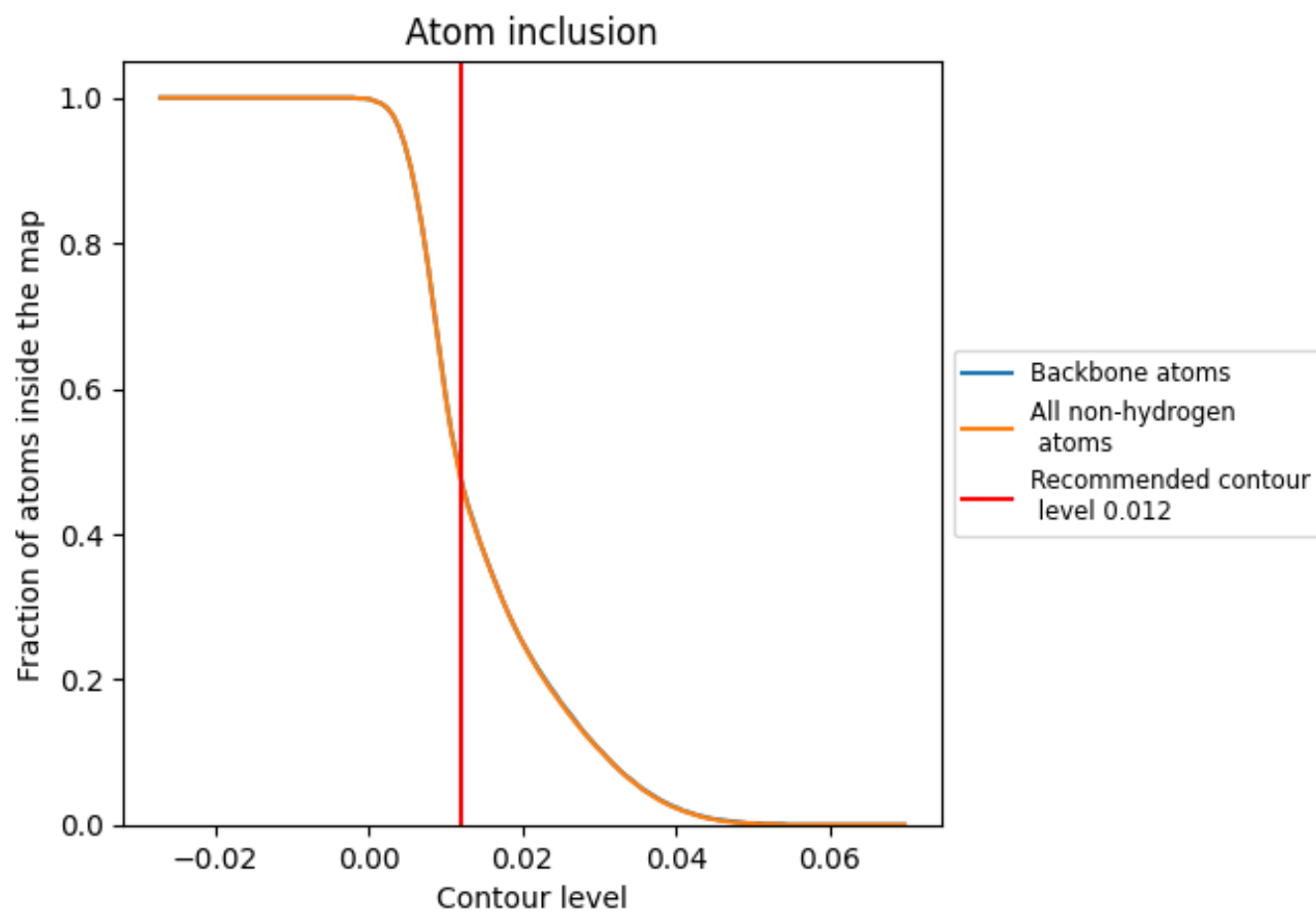


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 47% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4740	 0.3170
A	 0.8900	 0.5390
A1	 0.1400	 0.1480
A2	 0.0490	 0.1350
A3	 0.8860	 0.5350
A4	 0.0500	 0.1360
A5	 0.1440	 0.1460
B	 0.4990	 0.3720
B1	 0.0720	 0.1030
B2	 0.0260	 0.0960
B3	 0.4380	 0.3590
B4	 0.0260	 0.0910
B5	 0.0750	 0.1090
C	 0.9210	 0.5390
C1	 0.0110	 0.1020
C2	 0.0100	 0.0850
C3	 0.9010	 0.5170
C4	 0.0100	 0.0910
C5	 0.0110	 0.0980
D	 0.6370	 0.4190
D1	 0.0110	 0.1130
D2	 0.0140	 0.1060
D3	 0.5740	 0.4000
D4	 0.0150	 0.1120
D5	 0.0110	 0.1070
E	 0.6940	 0.3810
E1	 0.0850	 0.1090
E2	 0.0070	 0.0990
E3	 0.5910	 0.3760
E4	 0.0060	 0.0930
E5	 0.0840	 0.1120
F	 0.8620	 0.5330
F1	 0.0330	 0.1050
F2	 0.0300	 0.0930
F3	 0.8620	 0.5410



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Chain	Atom inclusion	Q-score
F4	 0.0270	 0.0900
F5	 0.0340	 0.1070
G	 0.8260	 0.4910
G1	 0.0000	 0.1100
G2	 0.0000	 0.1040
G3	 0.7570	 0.4600
G4	 0.0000	 0.1020
G5	 0.0000	 0.1110
H	 0.8440	 0.4920
H1	 0.7070	 0.3200
H2	 0.7480	 0.3540
H3	 0.7470	 0.4600
H4	 0.7370	 0.3510
H5	 0.7070	 0.3140
I	 0.8520	 0.5090
I1	 0.6670	 0.3080
I2	 0.7480	 0.3210
I3	 0.7920	 0.4940
I4	 0.7480	 0.3170
I5	 0.6640	 0.3040
J	 0.8320	 0.4970
J1	 0.5780	 0.3010
J2	 0.7500	 0.3050
J3	 0.8030	 0.4820
J4	 0.7420	 0.3020
J5	 0.5730	 0.3020
K	 0.7860	 0.4370
K1	 0.5560	 0.2960
K2	 0.6910	 0.2760
K3	 0.7690	 0.4430
K4	 0.6960	 0.2740
K5	 0.5510	 0.2980
L	 0.8910	 0.5260
L1	 0.5580	 0.3000
L2	 0.7080	 0.2540
L3	 0.8580	 0.5160
L4	 0.7000	 0.2520
L5	 0.5730	 0.3000
M	 0.9330	 0.5270
M1	 0.6370	 0.2900
M2	 0.7510	 0.2800
M3	 0.9140	 0.5170

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Chain	Atom inclusion	Q-score
M4	 0.7580	 0.2820
M5	 0.6350	 0.2930
N	 0.9300	 0.5530
N1	 0.6210	 0.2830
N2	 0.7460	 0.2890
N3	 0.9090	 0.5410
N4	 0.7530	 0.2920
N5	 0.6230	 0.2860
O	 0.8700	 0.4970
O1	 0.6400	 0.2950
O2	 0.6960	 0.2760
O3	 0.8960	 0.4930
O4	 0.6920	 0.2730
O5	 0.6420	 0.2900
P	 0.7080	 0.4440
P1	 0.6820	 0.3080
P2	 0.6800	 0.3040
P3	 0.7280	 0.4340
P4	 0.6780	 0.3030
P5	 0.6890	 0.3090
Q	 0.7870	 0.4740
Q1	 0.6800	 0.3010
Q2	 0.7120	 0.3370
Q3	 0.6750	 0.4400
Q4	 0.7190	 0.3330
Q5	 0.6670	 0.3010
R	 0.8680	 0.5130
R3	 0.8260	 0.5040
S	 0.7340	 0.4300
S3	 0.6440	 0.4040
a	 0.8850	 0.5360
a3	 0.8680	 0.5290
b	 0.4400	 0.3580
b3	 0.5050	 0.3720
c	 0.8960	 0.5180
c3	 0.9180	 0.5400
d	 0.5720	 0.3980
d1	 0.2940	 0.2560
d2	 0.3590	 0.2310
d3	 0.6370	 0.4210
d4	 0.3510	 0.2340
d5	 0.2900	 0.2610

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Chain	Atom inclusion	Q-score
e	 0.5840	 0.3730
e1	 0.2350	 0.2080
e2	 0.2600	 0.2250
e3	 0.6960	 0.3810
e4	 0.2630	 0.2310
e5	 0.2270	 0.2020
f	 0.7670	 0.5250
f3	 0.8120	 0.5360
g	 0.7460	 0.4620
g1	 0.1590	 0.2070
g2	 0.1950	 0.2080
g3	 0.8180	 0.4890
g4	 0.1970	 0.2050
g5	 0.1610	 0.2050
h	 0.7220	 0.4690
h3	 0.8190	 0.5010
i	 0.8250	 0.4940
i1	 0.0400	 0.1780
i2	 0.0700	 0.1820
i3	 0.8470	 0.5160
i4	 0.0910	 0.2000
i5	 0.0300	 0.1910
j	 0.8010	 0.4810
j3	 0.8380	 0.4910
k	 0.7840	 0.4400
k3	 0.7920	 0.4370
l	 0.8520	 0.5170
l3	 0.8930	 0.5230
m	 0.9040	 0.5140
m3	 0.9320	 0.5230
n	 0.9070	 0.5410
n3	 0.9280	 0.5530
o	 0.8960	 0.4970
o3	 0.8580	 0.4950
p	 0.7170	 0.4310
p3	 0.7090	 0.4430
q	 0.6780	 0.4440
q3	 0.7860	 0.4720
r	 0.7860	 0.4940
r3	 0.8700	 0.5200
s	 0.5440	 0.3940
s3	 0.7000	 0.4300

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Chain	Atom inclusion	Q-score
t	 0.5330	 0.3790
t3	 0.6050	 0.4000