



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 03:56 AM UTC

PDB ID : 6TDU / pdb_00006tdu
EMDB ID : EMD-10467
Title : Cryo-EM structure of Euglena gracilis mitochondrial ATP synthase, full dimer, rotational states 1
Authors : Muhleip, A.; Amunts, A.
Deposited on : 2019-11-10
Resolution : 4.32 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

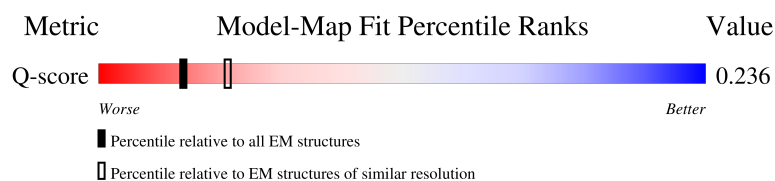
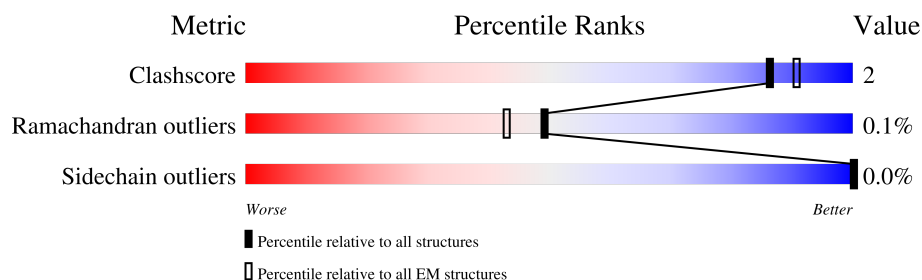
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.32 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.



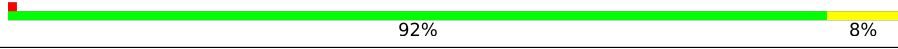
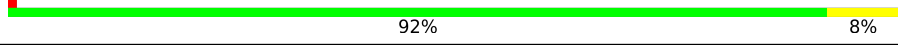
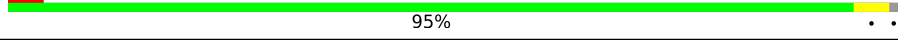
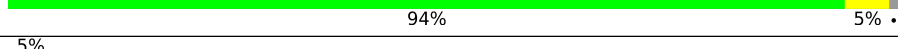
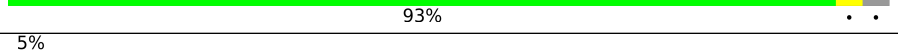
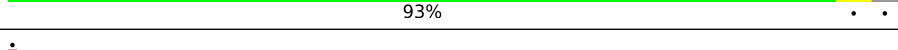
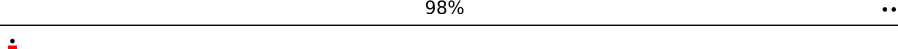
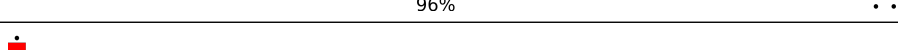
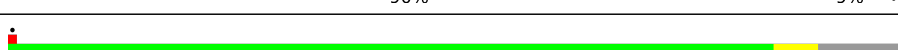
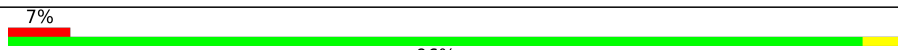
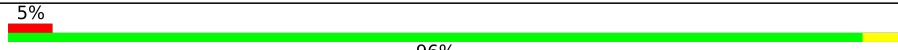
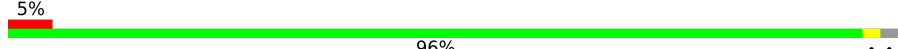
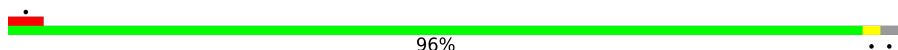
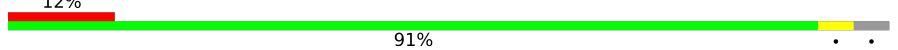
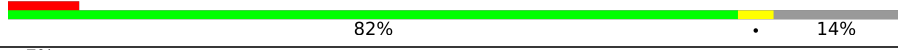
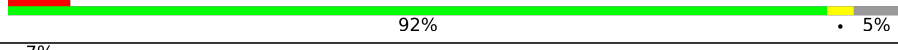
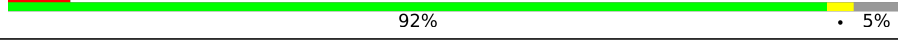
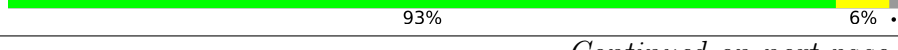
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3853 (3.83 - 4.82)

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	487	93% 6%
1	a	487	93% 6%
2	D	187	90% 9% .
2	d	187	90% 9% .

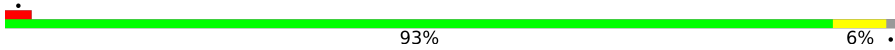
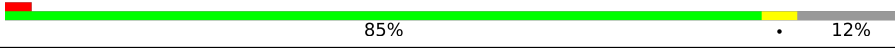
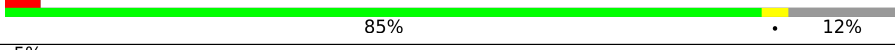
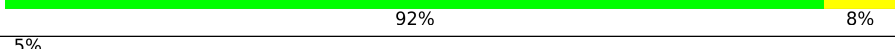
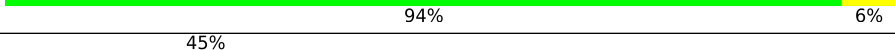
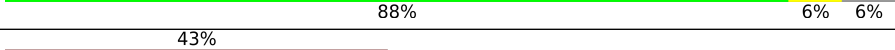
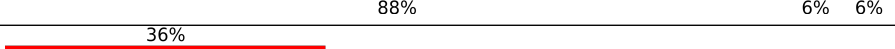
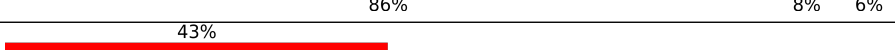
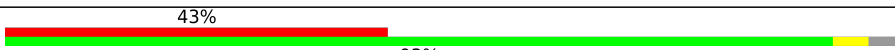
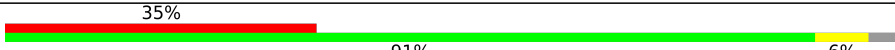
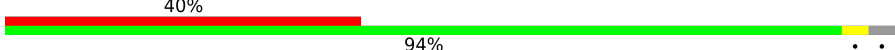
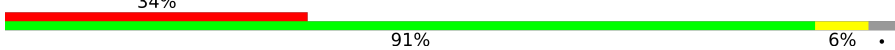
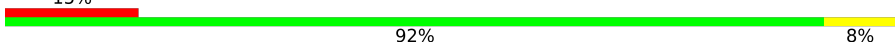
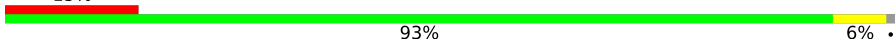
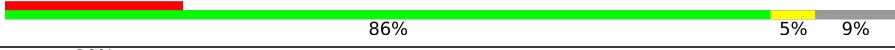
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Mol	Chain	Length	Quality of chain
3	E	97	
3	e	97	
4	F	274	
4	f	274	
5	G	112	
5	g	112	
6	H	476	
6	h	476	
7	I	98	
7	i	98	
8	J	104	
8	j	104	
9	K	113	
9	k	113	
10	L	57	
10	l	57	
11	M	169	
11	m	169	
12	N	137	
12	n	137	
13	O	116	
13	o	116	
14	P	120	
14	p	120	
15	Q	90	

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Mol	Chain	Length	Quality of chain
15	q	90	
16	R	78	
16	r	78	
17	S	74	
17	s	74	
18	T	66	
18	t	66	
19	AA	561	
19	AB	561	
19	AC	561	
19	BA	561	
19	BB	561	
19	BC	561	
20	AD	501	
20	AE	501	
20	AF	501	
20	BD	501	
20	BE	501	
20	BF	501	
21	AG	306	
21	BG	306	
22	AH	176	
22	BH	176	
23	AI	76	
23	BI	76	

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Mol	Chain	Length	Quality of chain
24	AJ	192	
24	AK	192	
24	AL	192	
24	BJ	192	
24	BK	192	
24	BL	192	
25	AM	267	
25	BM	267	
26	AN	103	
26	BN	103	
27	AO	104	
27	AP	104	
27	AQ	104	
27	AR	104	
27	AS	104	
27	AT	104	
27	AU	104	
27	AV	104	
27	AW	104	
27	AX	104	
27	BO	104	
27	BP	104	
27	BQ	104	
27	BR	104	
27	BS	104	

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Mol	Chain	Length	Quality of chain
27	BT	104	
27	BU	104	
27	BV	104	
27	BW	104	
27	BX	104	
28	B	338	
28	b	338	
29	C	169	
29	c	169	

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 271331 atoms, of which 136237 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 ATPTB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	486	Total	C	H	N	O	S	0	0
			7864	2525	3919	677	733	10		
1	a	486	Total	C	H	N	O	S	0	0
			7864	2525	3919	677	733	10		

- Molecule 2 is a protein called ATPTB6.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	186	Total	C	H	N	O	S	0	0
			3040	977	1519	269	267	8		
2	d	186	Total	C	H	N	O	S	0	0
			3040	977	1519	269	267	8		

- Molecule 3 is a protein called ATPTB12.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	96	Total	C	H	N	O	S	0	0
			1577	510	779	144	141	3		
3	e	96	Total	C	H	N	O	S	0	0
			1577	510	779	144	141	3		

- Molecule 4 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	F	274	Total	C	H	N	O	S	0	0
			4642	1566	2329	342	391	14		
4	f	274	Total	C	H	N	O	S	0	0
			4642	1566	2329	342	391	14		

- Molecule 5 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	G	111	Total	C	H	N	O	S	0	0
			1803	566	924	160	146	7		
5	g	111	Total	C	H	N	O	S	0	0
			1803	566	924	160	146	7		

- Molecule 6 is a protein called ATP synthase subunit d.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	H	460	Total	C	H	N	O	S	0	0
			7302	2343	3637	607	705	10		
6	h	460	Total	C	H	N	O	S	0	0
			7302	2343	3637	607	705	10		

- Molecule 7 is a protein called ATP synthase subunit f.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	97	Total	C	H	N	O	S	0	0
			1553	504	771	140	135	3		
7	i	97	Total	C	H	N	O	S	0	0
			1553	504	771	140	135	3		

- Molecule 8 is a protein called ATP synthase subunit i/j.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	103	Total	C	H	N	O	S	0	0
			1734	581	853	151	146	3		
8	j	103	Total	C	H	N	O	S	0	0
			1734	581	853	151	146	3		

- Molecule 9 is a protein called ATP synthase subunit k.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K	103	Total	C	H	N	O	S	0	0
			1637	530	821	136	144	6		
9	k	103	Total	C	H	N	O	S	0	0
			1637	530	821	136	144	6		

- Molecule 10 is a protein called ATP synthase subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	L	57	Total	C	H	N	O		0	0
			1008	350	507	69	82			

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	57	Total	C	H	N	O	0	0
			1008	350	507	69	82		

- Molecule 11 is a protein called ATPEG1.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	M	166	Total	C	H	N	O	S	0	0
			2717	887	1354	228	240	8		
11	m	166	Total	C	H	N	O	S	0	0
			2717	887	1354	228	240	8		

- Molecule 12 is a protein called ATPEG2.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	N	131	Total	C	H	N	O	S	0	0
			2168	714	1071	198	182	3		
12	n	131	Total	C	H	N	O	S	0	0
			2168	714	1071	198	182	3		

- Molecule 13 is a protein called ATPEG3.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	O	100	Total	C	H	N	O	S	0	0
			1652	556	803	146	145	2		
13	o	100	Total	C	H	N	O	S	0	0
			1652	556	803	146	145	2		

- Molecule 14 is a protein called ATPEG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	P	114	Total	C	H	N	O	S	0	0
			1838	601	912	159	160	6		
14	p	114	Total	C	H	N	O	S	0	0
			1838	601	912	159	160	6		

- Molecule 15 is a protein called ATPEG5.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	Q	89	Total	C	H	N	O	S	0	0
			1476	475	723	137	137	4		
15	q	89	Total	C	H	N	O	S	0	0
			1476	475	723	137	137	4		

- Molecule 16 is a protein called ATPEG6.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	R	69	Total	C	H	N	O	S	0	0
			1160	374	581	106	97	2		
16	r	69	Total	C	H	N	O	S	0	0
			1160	374	581	106	97	2		

- Molecule 17 is a protein called ATPEG7.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	S	65	Total	C	H	N	O	S	0	0
			1092	371	541	90	89	1		
17	s	65	Total	C	H	N	O	S	0	0
			1092	371	541	90	89	1		

- Molecule 18 is a protein called ATPEG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	T	66	Total	C	H	N	O	S	0	0
			1080	349	552	95	83	1		
18	t	66	Total	C	H	N	O	S	0	0
			1080	349	552	95	83	1		

- Molecule 19 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	AA	526	Total	C	H	N	O	S	0	0
			8291	2611	4196	700	766	18		
19	AB	526	Total	C	H	N	O	S	0	0
			8292	2611	4197	700	766	18		
19	AC	529	Total	C	H	N	O	S	0	0
			8336	2625	4219	703	771	18		
19	BA	526	Total	C	H	N	O	S	0	0
			8291	2611	4196	700	766	18		
19	BB	526	Total	C	H	N	O	S	0	0
			8292	2611	4197	700	766	18		
19	BC	529	Total	C	H	N	O	S	0	0
			8336	2625	4219	703	771	18		

- Molecule 20 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	AD	487	Total	C	H	N	O	S	0	0
			7407	2318	3729	620	713	27		
20	AE	487	Total	C	H	N	O	S	0	0
			7408	2318	3730	620	713	27		
20	AF	487	Total	C	H	N	O	S	0	0
			7407	2318	3729	620	713	27		
20	BD	487	Total	C	H	N	O	S	0	0
			7407	2318	3729	620	713	27		
20	BE	487	Total	C	H	N	O	S	0	0
			7408	2318	3730	620	713	27		
20	BF	487	Total	C	H	N	O	S	0	0
			7407	2318	3729	620	713	27		

- Molecule 21 is a protein called ATP synthase subunit gamma.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	AG	303	Total	C	H	N	O	S	0	0
			4898	1543	2462	420	459	14		
21	BG	303	Total	C	H	N	O	S	0	0
			4898	1543	2462	420	459	14		

- Molecule 22 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	AH	160	Total	C	H	N	O	S	0	0
			2448	787	1202	207	251	1		
22	BH	160	Total	C	H	N	O	S	0	0
			2448	787	1202	207	251	1		

- Molecule 23 is a protein called ATP synthase subunit epsilon.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	AI	66	Total	C	H	N	O	S	0	0
			1077	346	541	91	98	1		
23	BI	66	Total	C	H	N	O	S	0	0
			1077	346	541	91	98	1		

- Molecule 24 is a protein called p18.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AJ	170	Total	C	H	N	O	S	0	0
			2596	829	1294	217	249	7		

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Mol	Chain	Residues	Atoms						AltConf	Trace
24	AK	170	Total	C	H	N	O	S	0	0
			2596	829	1294	217	249	7		
24	AL	170	Total	C	H	N	O	S	0	0
			2596	829	1294	217	249	7		
24	BJ	170	Total	C	H	N	O	S	0	0
			2596	829	1294	217	249	7		
24	BK	170	Total	C	H	N	O	S	0	0
			2596	829	1294	217	249	7		
24	BL	170	Total	C	H	N	O	S	0	0
			2596	829	1294	217	249	7		

- Molecule 25 is a protein called oligomycin sensitivity conferring protein (OSCP).

Mol	Chain	Residues	Atoms						AltConf	Trace
25	AM	243	Total	C	H	N	O	S	0	0
			3778	1212	1885	310	370	1		
25	BM	243	Total	C	H	N	O	S	0	0
			3778	1212	1885	310	370	1		

- Molecule 26 is a protein called inhibitor of F1 (IF1).

Mol	Chain	Residues	Atoms						AltConf	Trace
26	AN	49	Total	C	H	N	O	S	0	0
			802	247	399	72	82	2		
26	BN	49	Total	C	H	N	O	S	0	0
			802	247	399	72	82	2		

- Molecule 27 is a protein called ATP synthase subunit c.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	AO	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
27	AP	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
27	AQ	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
27	AR	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
27	AS	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
27	AT	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
27	AU	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
27	AV	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
27	AW	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
27	AX	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
27	BO	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
27	BP	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
27	BQ	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
27	BR	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
27	BS	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
27	BT	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
27	BU	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
27	BV	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
27	BW	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		
27	BX	81	Total	C	H	N	O	S	0	0
			1185	383	605	89	102	6		

- Molecule 28 is a protein called ATPTB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	B	326	Total	C	H	N	O	S	0	0
			4813	1508	2421	405	474	5		
28	b	326	Total	C	H	N	O	S	0	0
			4813	1508	2421	405	474	5		

- Molecule 29 is a protein called ATPTB4.

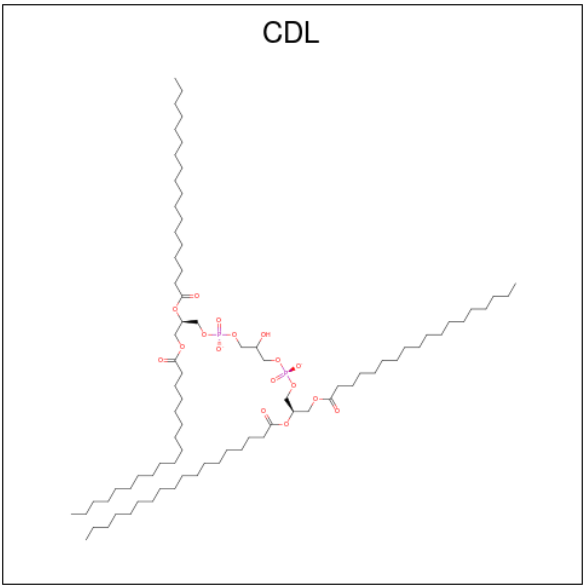
Mol	Chain	Residues	Atoms						AltConf	Trace
29	C	157	Total	C	H	N	O	S	0	0
			2472	781	1241	211	237	2		

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Mol	Chain	Residues	Atoms						AltConf	Trace
29	c	157	Total	C	H	N	O	S	0	0
			2472	781	1241	211	237	2		

- Molecule 30 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



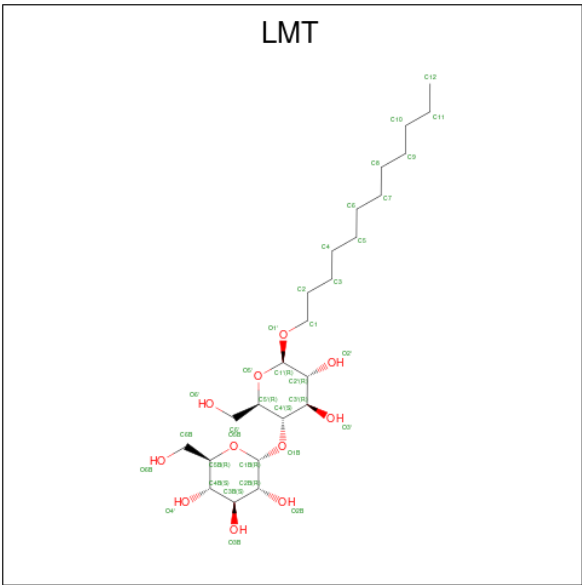
Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total 183	C 62	H 102	O 17	P 2	0
30	A	1	Total 170	C 62	H 89	O 17	P 2	0
30	A	1	Total 184	C 63	H 102	O 17	P 2	0
30	A	1	Total 99	C 44	H 36	O 17	P 2	0
30	A	1	Total 184	C 67	H 98	O 17	P 2	0
30	D	1	Total 228	C 72	H 137	O 17	P 2	0
30	E	1	Total 95	C 44	H 32	O 17	P 2	0
30	M	1	Total 80	C 34	H 27	O 17	P 2	0
30	M	1	Total 152	C 58	H 75	O 17	P 2	0
30	M	1	Total 80	C 34	H 27	O 17	P 2	0

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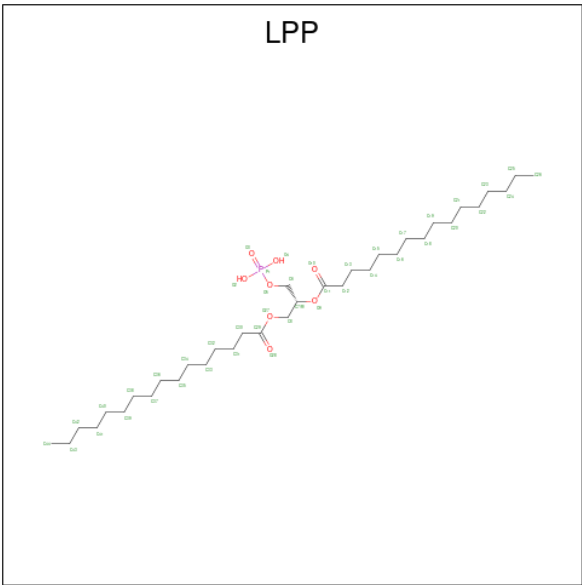
Mol	Chain	Residues	Atoms					AltConf
30	O	1	Total	C	H	O	P	0
			124	46	59	17	2	
30	P	1	Total	C	H	O	P	0
			75	29	27	17	2	
30	P	1	Total	C	H	O	P	0
			244	79	146	17	2	
30	R	1	Total	C	H	O	P	0
			150	57	74	17	2	
30	a	1	Total	C	H	O	P	0
			183	62	102	17	2	
30	a	1	Total	C	H	O	P	0
			170	62	89	17	2	
30	a	1	Total	C	H	O	P	0
			184	63	102	17	2	
30	a	1	Total	C	H	O	P	0
			99	44	36	17	2	
30	a	1	Total	C	H	O	P	0
			184	67	98	17	2	
30	d	1	Total	C	H	O	P	0
			228	72	137	17	2	
30	e	1	Total	C	H	O	P	0
			95	44	32	17	2	
30	m	1	Total	C	H	O	P	0
			152	58	75	17	2	
30	o	1	Total	C	H	O	P	0
			124	46	59	17	2	
30	p	1	Total	C	H	O	P	0
			75	29	27	17	2	
30	r	1	Total	C	H	O	P	0
			150	57	74	17	2	

- Molecule 31 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



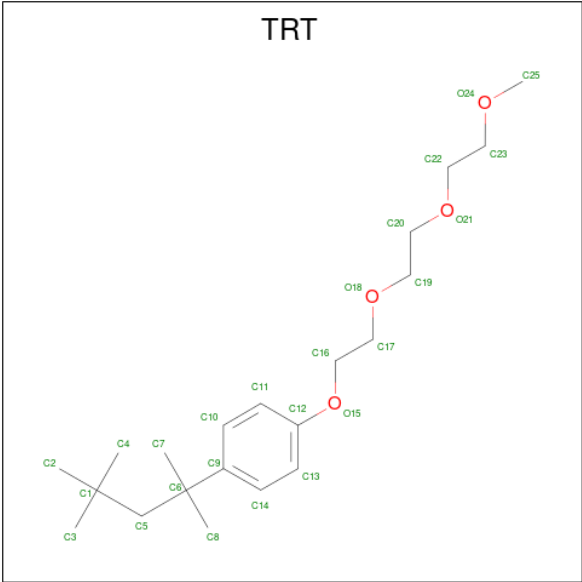
Mol	Chain	Residues	Atoms				AltConf
31	D	1	Total	C	H	O	0
			81	24	46	11	
31	F	1	Total	C	H	O	0
			81	24	46	11	
31	N	1	Total	C	H	O	0
			81	24	46	11	
31	Q	1	Total	C	H	O	0
			81	24	46	11	
31	d	1	Total	C	H	O	0
			81	24	46	11	
31	g	1	Total	C	H	O	0
			81	24	46	11	
31	n	1	Total	C	H	O	0
			81	24	46	11	
31	q	1	Total	C	H	O	0
			81	24	46	11	

- Molecule 32 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: C₃₅H₆₉O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
32	F	1	Total	C	H	O	P	0
			41	15	17	8	1	
32	I	1	Total	C	H	O	P	0
			111	35	67	8	1	
32	K	1	Total	C	H	O	P	0
			48	22	17	8	1	
32	N	1	Total	C	H	O	P	0
			43	17	17	8	1	
32	O	1	Total	C	H	O	P	0
			40	14	17	8	1	
32	O	1	Total	C	H	O	P	0
			74	23	42	8	1	
32	f	1	Total	C	H	O	P	0
			41	15	17	8	1	
32	i	1	Total	C	H	O	P	0
			111	35	67	8	1	
32	k	1	Total	C	H	O	P	0
			48	22	17	8	1	
32	n	1	Total	C	H	O	P	0
			43	17	17	8	1	
32	o	1	Total	C	H	O	P	0
			40	14	17	8	1	
32	o	1	Total	C	H	O	P	0
			74	23	42	8	1	

- Molecule 33 is FRAGMENT OF TRITON X-100 (CCD ID: TRT) (formula: C₂₁H₃₆O₄).



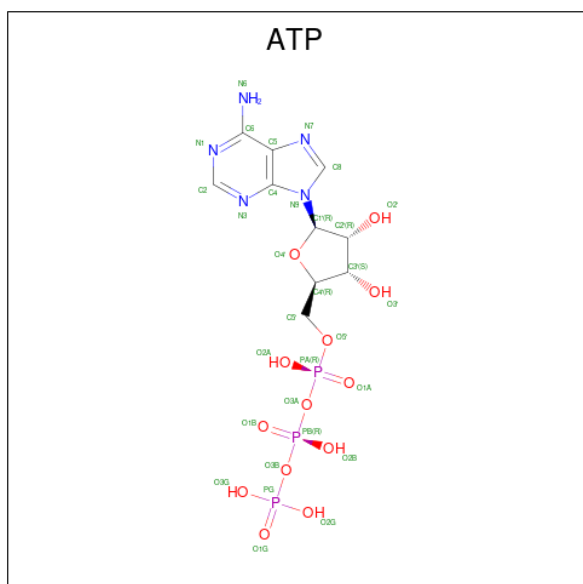
Mol	Chain	Residues	Atoms				AltConf
33	G	1	Total	C	H	O	0
			61	21	36	4	
33	G	1	Total	C	H	O	0
			61	21	36	4	
33	M	1	Total	C	H	O	0
			61	21	36	4	
33	M	1	Total	C	H	O	0
			61	21	36	4	
33	N	1	Total	C	H	O	0
			61	21	36	4	
33	N	1	Total	C	H	O	0
			61	21	36	4	
33	P	1	Total	C	H	O	0
			61	21	36	4	
33	g	1	Total	C	H	O	0
			61	21	36	4	
33	g	1	Total	C	H	O	0
			61	21	36	4	
33	m	1	Total	C	H	O	0
			61	21	36	4	
33	m	1	Total	C	H	O	0
			61	21	36	4	
33	n	1	Total	C	H	O	0
			61	21	36	4	
33	n	1	Total	C	H	O	0
			61	21	36	4	
33	p	1	Total	C	H	O	0
			61	21	36	4	

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Mol	Chain	Residues	Atoms				AltConf
33	AE	1	Total	C	H	O	0
			61	21	36	4	
33	AR	1	Total	C	H	O	0
			61	21	36	4	
33	BE	1	Total	C	H	O	0
			61	21	36	4	
33	BR	1	Total	C	H	O	0
			61	21	36	4	

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
34	AA	1	Total	C	H	N	O	P	0
			35	10	4	5	13	3	
34	AB	1	Total	C	H	N	O	P	0
			35	10	4	5	13	3	
34	AC	1	Total	C	H	N	O	P	0
			35	10	4	5	13	3	
34	AF	1	Total	C	H	N	O	P	0
			35	10	4	5	13	3	
34	BA	1	Total	C	H	N	O	P	0
			35	10	4	5	13	3	
34	BB	1	Total	C	H	N	O	P	0
			35	10	4	5	13	3	
34	BC	1	Total	C	H	N	O	P	0
			35	10	4	5	13	3	

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Mol	Chain	Residues	Atoms						AltConf
34	BF	1	Total	C	H	N	O	P	0
			35	10	4	5	13	3	

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

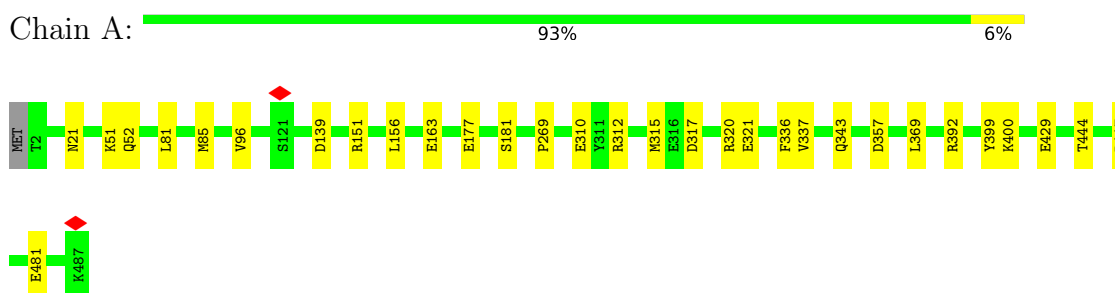
Mol	Chain	Residues	Atoms		AltConf
35	AA	1	Total	Mg	0
			1	1	
35	AB	1	Total	Mg	0
			1	1	
35	AC	1	Total	Mg	0
			1	1	
35	AD	1	Total	Mg	0
			1	1	
35	AF	1	Total	Mg	0
			1	1	
35	BA	1	Total	Mg	0
			1	1	
35	BB	1	Total	Mg	0
			1	1	
35	BC	1	Total	Mg	0
			1	1	
35	BD	1	Total	Mg	0
			1	1	
35	BF	1	Total	Mg	0
			1	1	

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

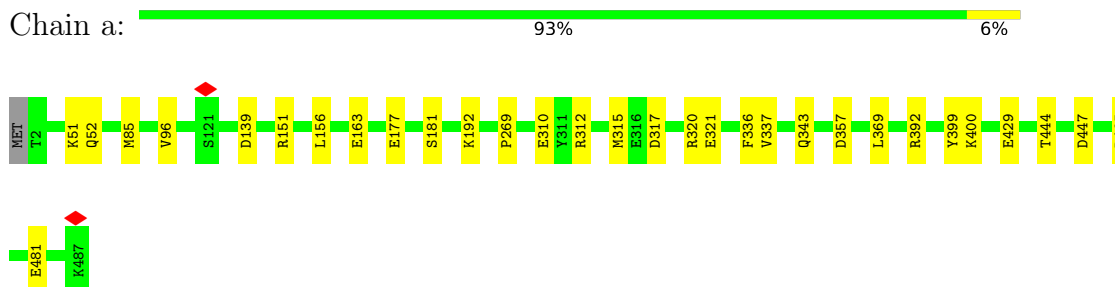
3 Residue-property plots [i](#)

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.

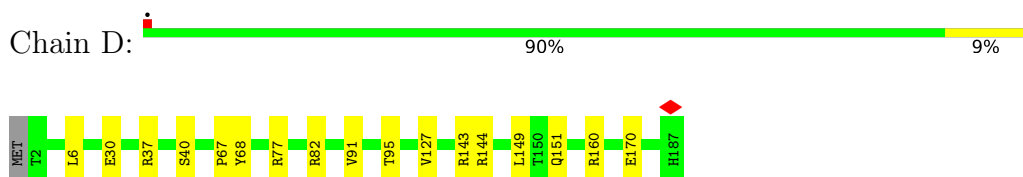
- Molecule 1: ATPTB1



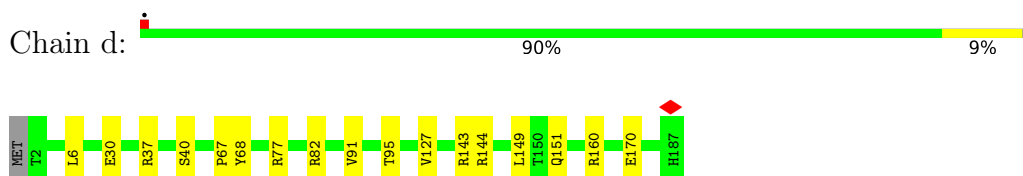
- Molecule 1: ATPTB1



- Molecule 2: ATPTB6



- Molecule 2: ATPTB6



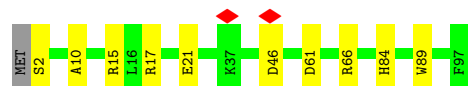
- Molecule 3: ATPTB12

Chain E:  85% 14%

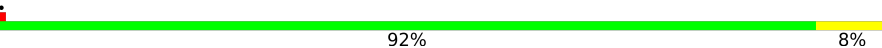


- Molecule 3: ATPTB12

Chain e:  89% 10%



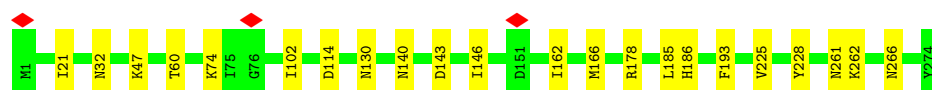
- Molecule 4: ATP synthase subunit a

Chain F:  92% 8%

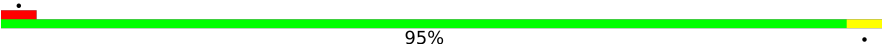


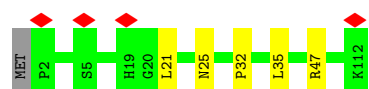
- Molecule 4: ATP synthase subunit a

Chain f:  92% 8%

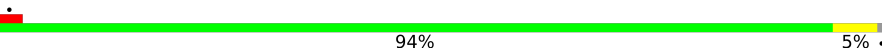


- Molecule 5: ATP synthase subunit b

Chain G:  95% 5%

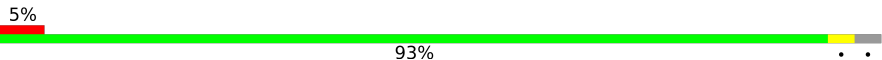


- Molecule 5: ATP synthase subunit b

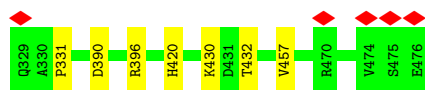
Chain g:  94% 5%



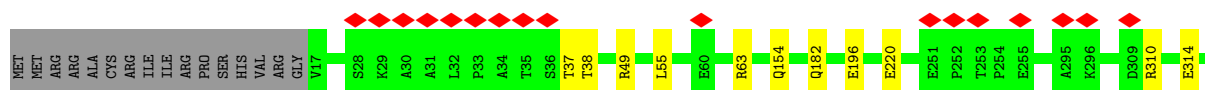
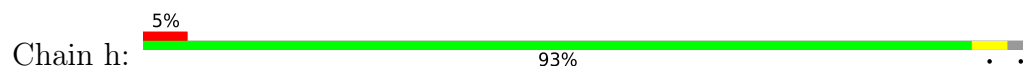
- Molecule 6: ATP synthase subunit d

Chain H:  5% 93%





- Molecule 6: ATP synthase subunit d



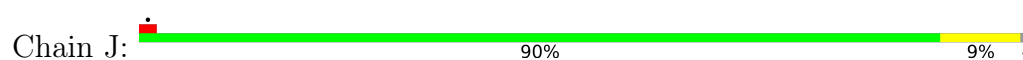
- Molecule 7: ATP synthase subunit f



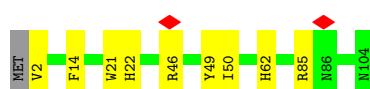
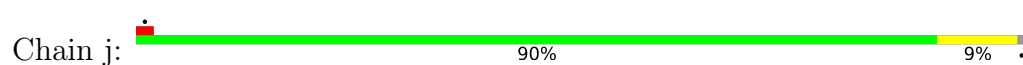
- Molecule 7: ATP synthase subunit f



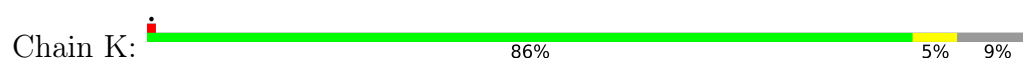
- Molecule 8: ATP synthase subunit i/j



- Molecule 8: ATP synthase subunit i/j

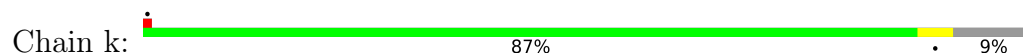


- Molecule 9: ATP synthase subunit k

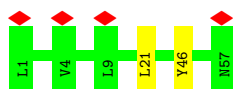




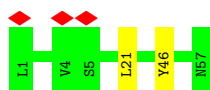
- Molecule 9: ATP synthase subunit k



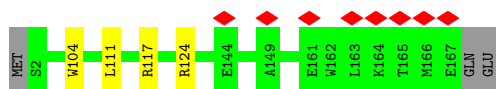
- Molecule 10: ATP synthase subunit 8



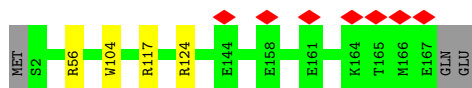
- Molecule 10: ATP synthase subunit 8



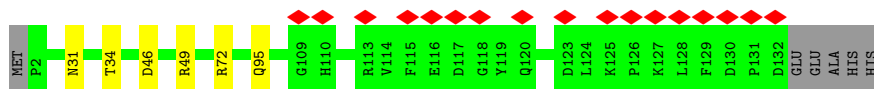
- Molecule 11: ATPEG1



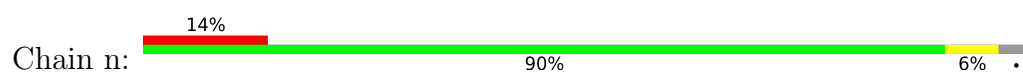
- Molecule 11: ATPEG1



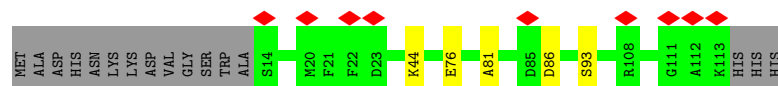
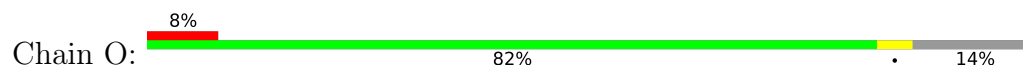
- Molecule 12: ATPEG2



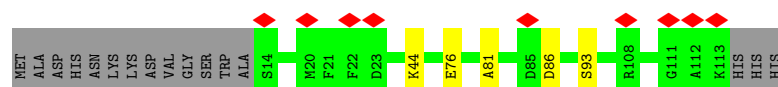
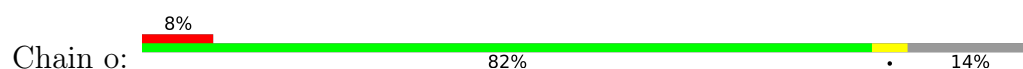
- Molecule 12: ATPEG2



• Molecule 13: ATPEG3



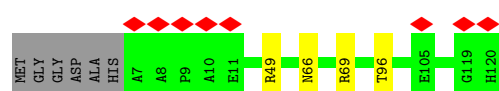
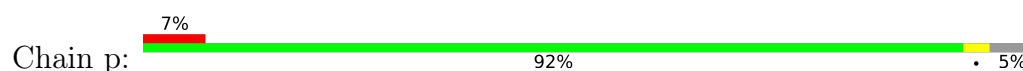
• Molecule 13: ATPEG3



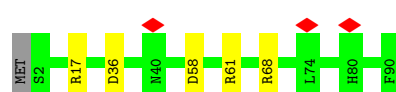
• Molecule 14: ATPEG4



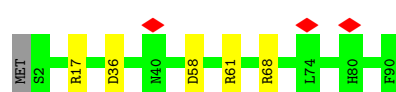
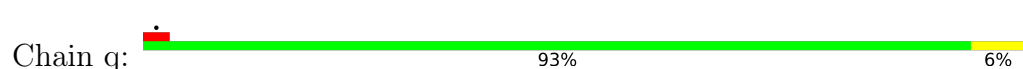
• Molecule 14: ATPEG4



• Molecule 15: ATPEG5

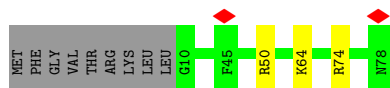


• Molecule 15: ATPEG5



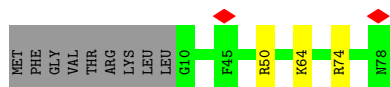
- Molecule 16: ATPEG6

Chain R:  85% 12%



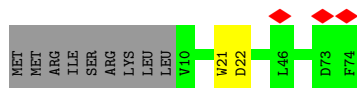
- Molecule 16: ATPEG6

Chain r:  85% 12%



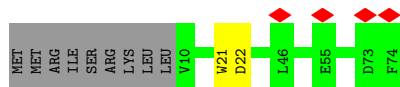
- Molecule 17: ATPEG7

Chain S:  85% 12%

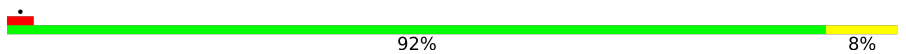


- Molecule 17: ATPEG7

Chain s:  5% 85% 12%

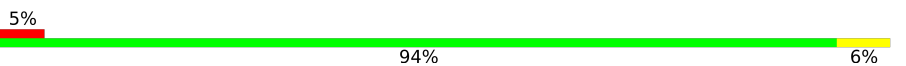


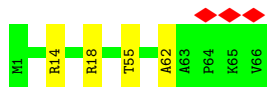
- Molecule 18: ATPEG8

Chain T:  92% 8%

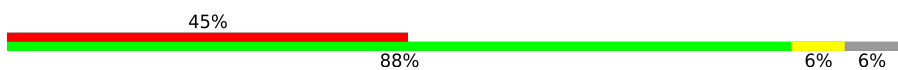


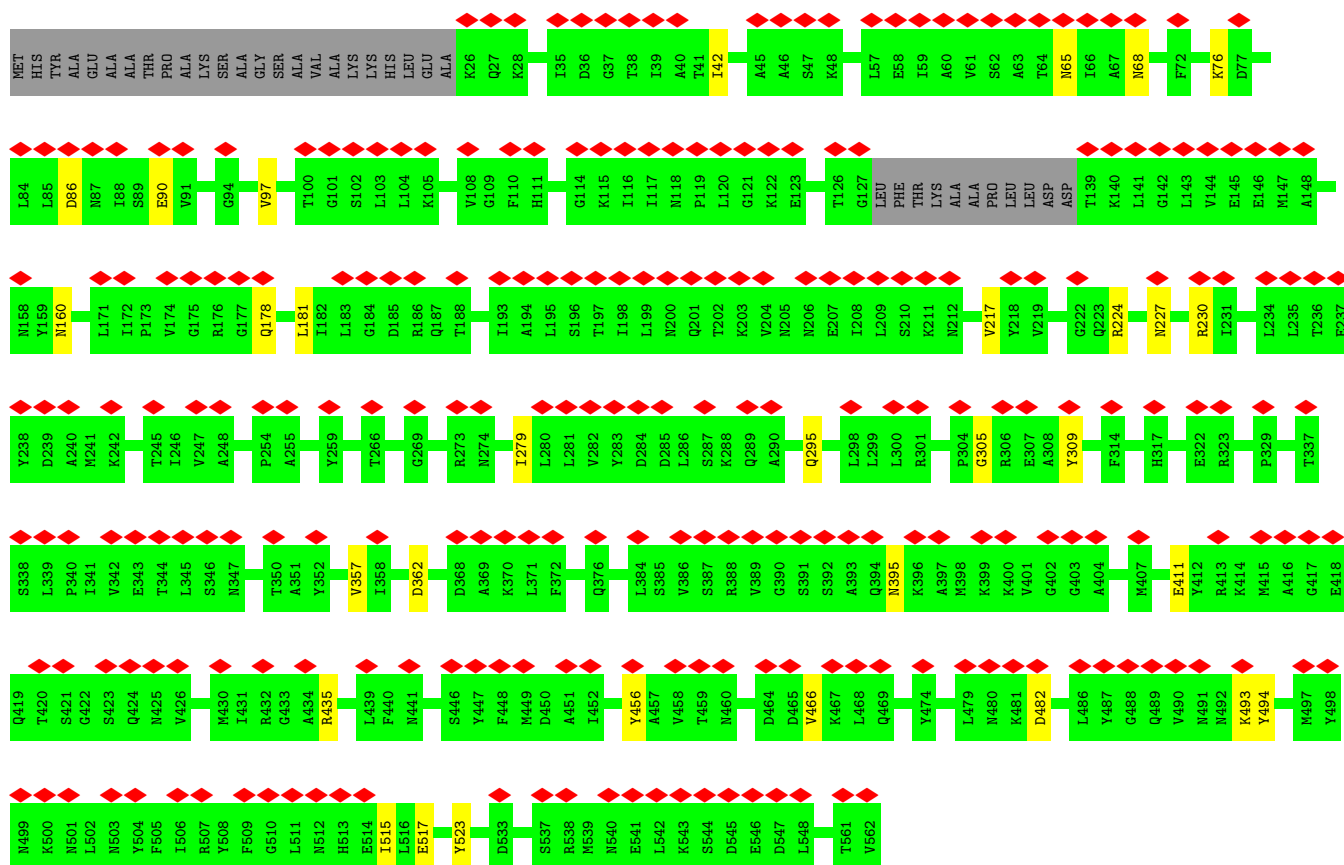
- Molecule 18: ATPEG8

Chain t:  5% 94% 6%

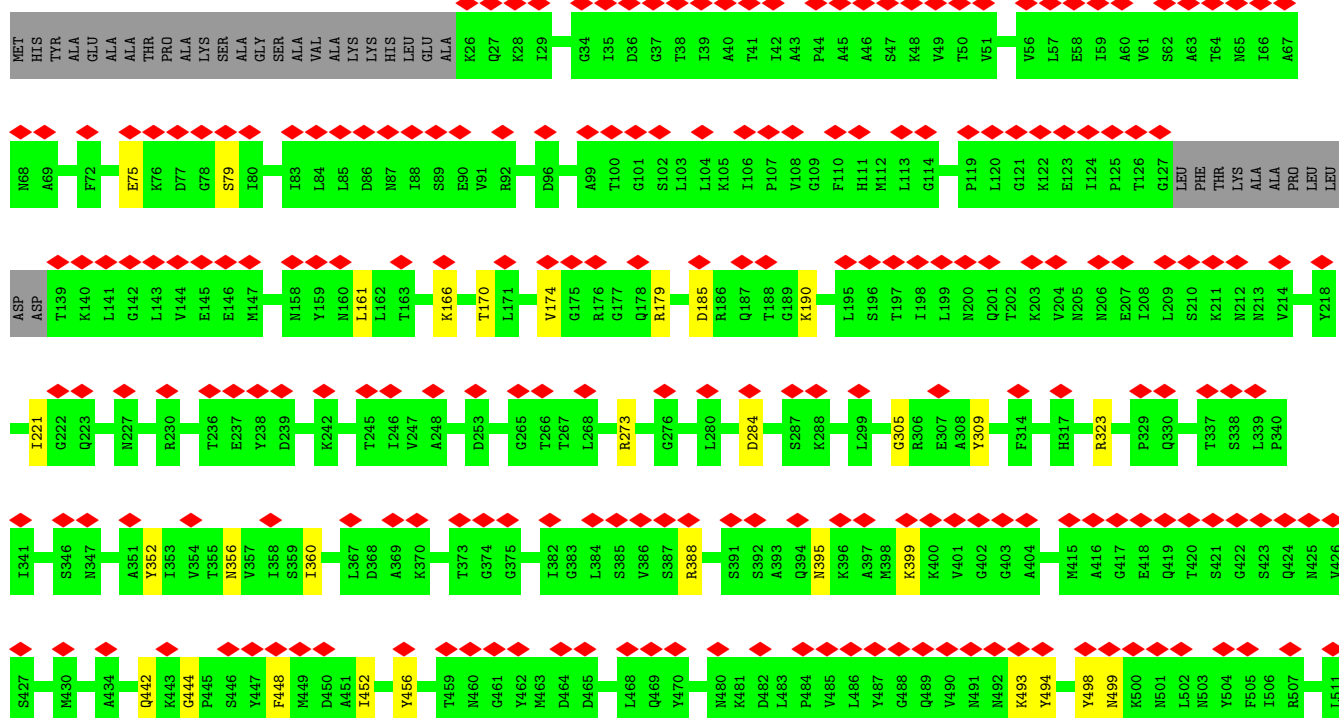
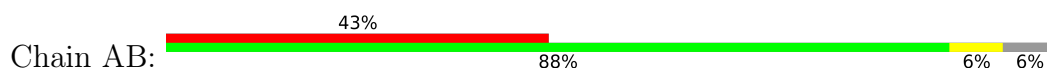


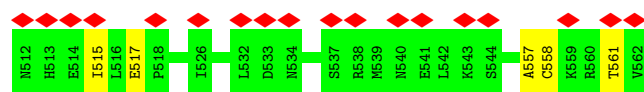
- Molecule 19: ATP synthase subunit alpha

Chain AA:  45% 88% 6% 6%



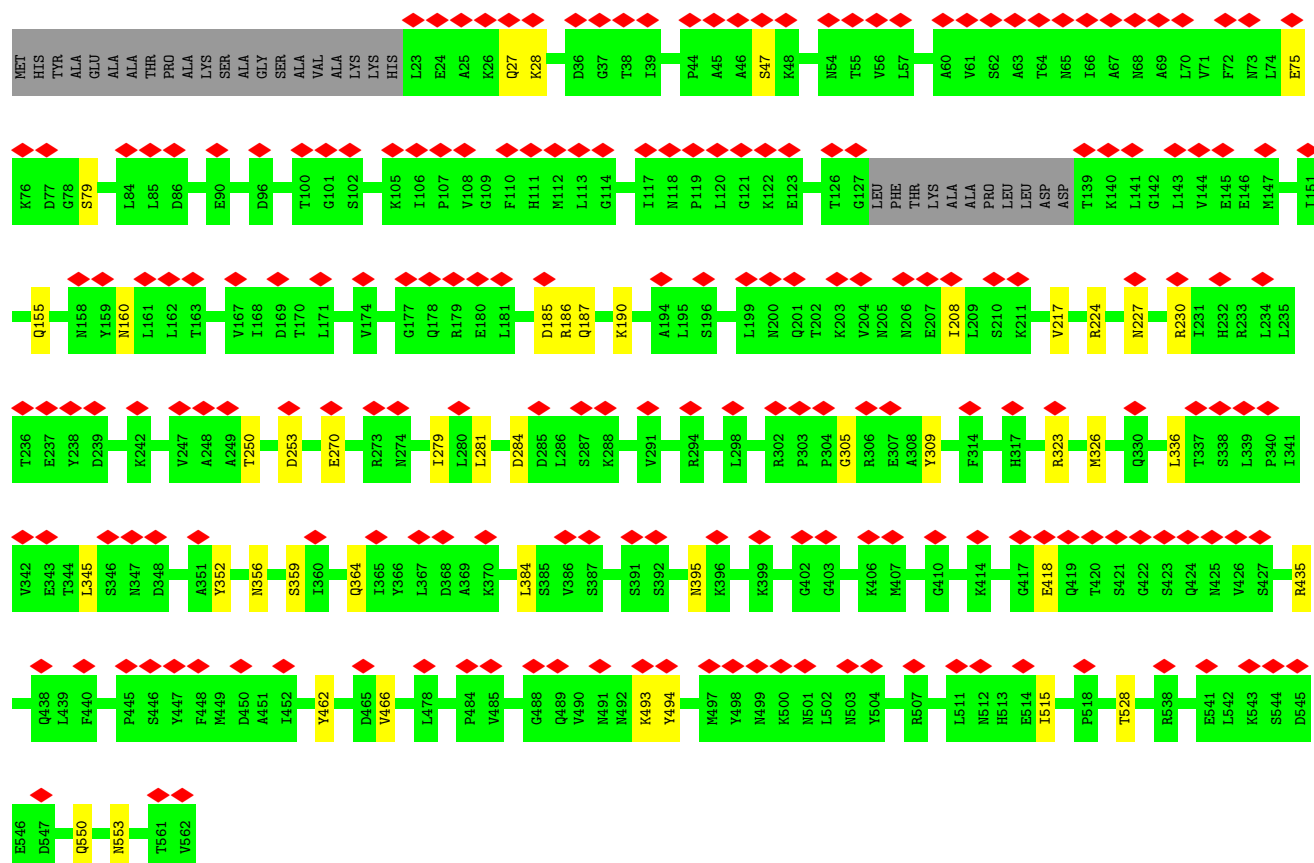
• Molecule 19: ATP synthase subunit alpha





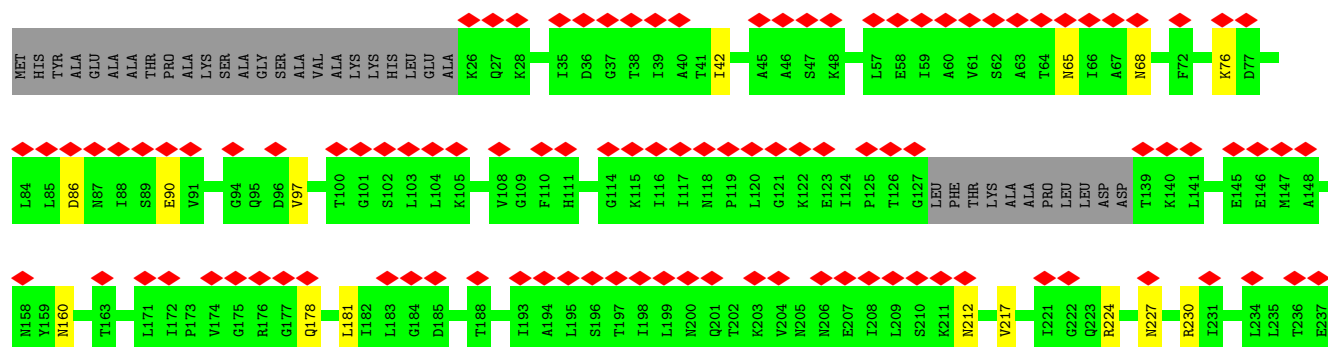
• Molecule 19: ATP synthase subunit alpha

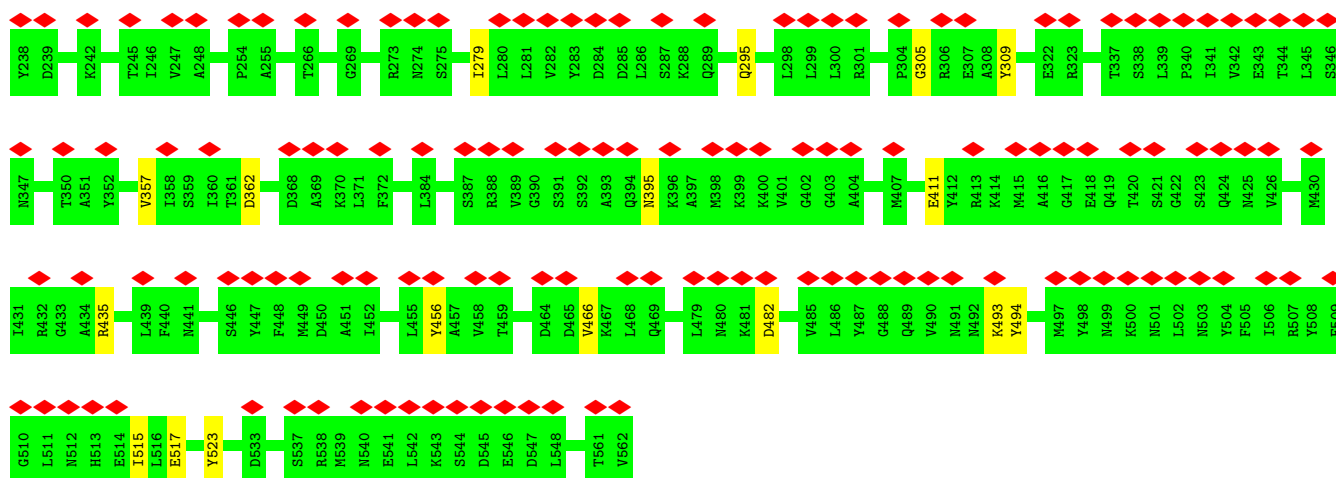
Chain AC: 36% 86% 8% 6%



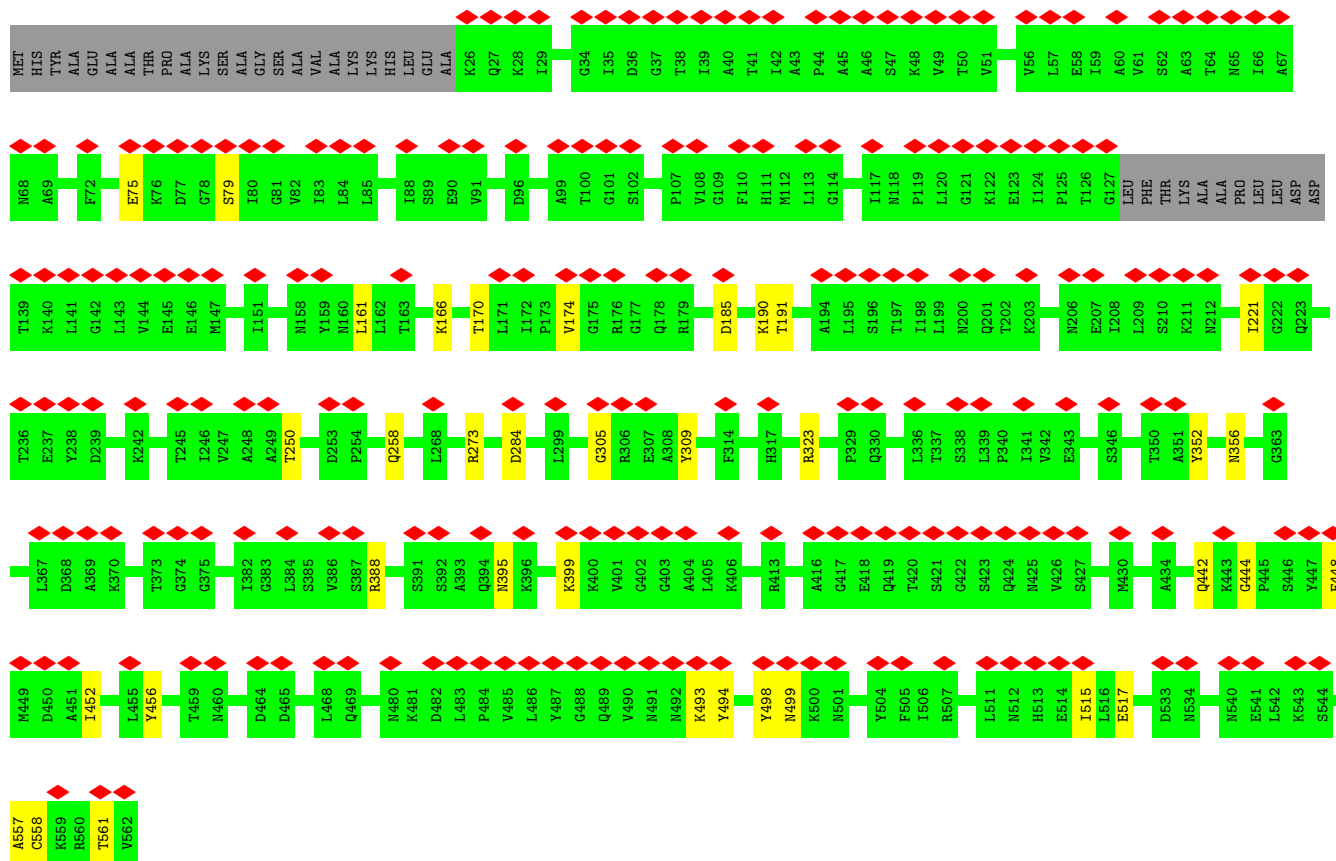
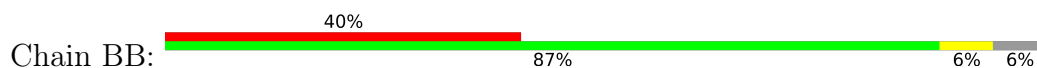
• Molecule 19: ATP synthase subunit alpha

Chain BA: 43% 88% 6% 6%

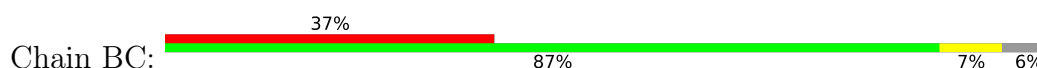


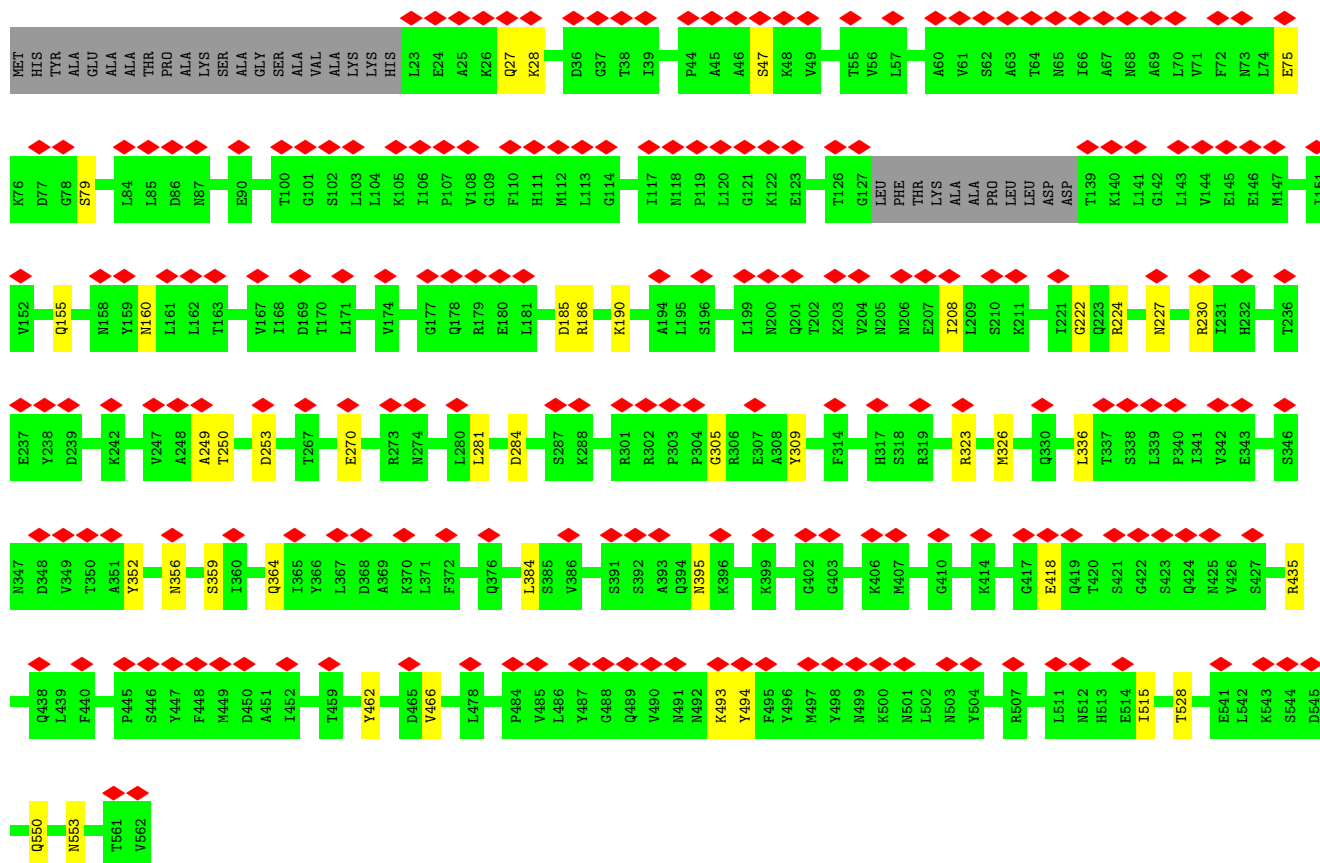


• Molecule 19: ATP synthase subunit alpha

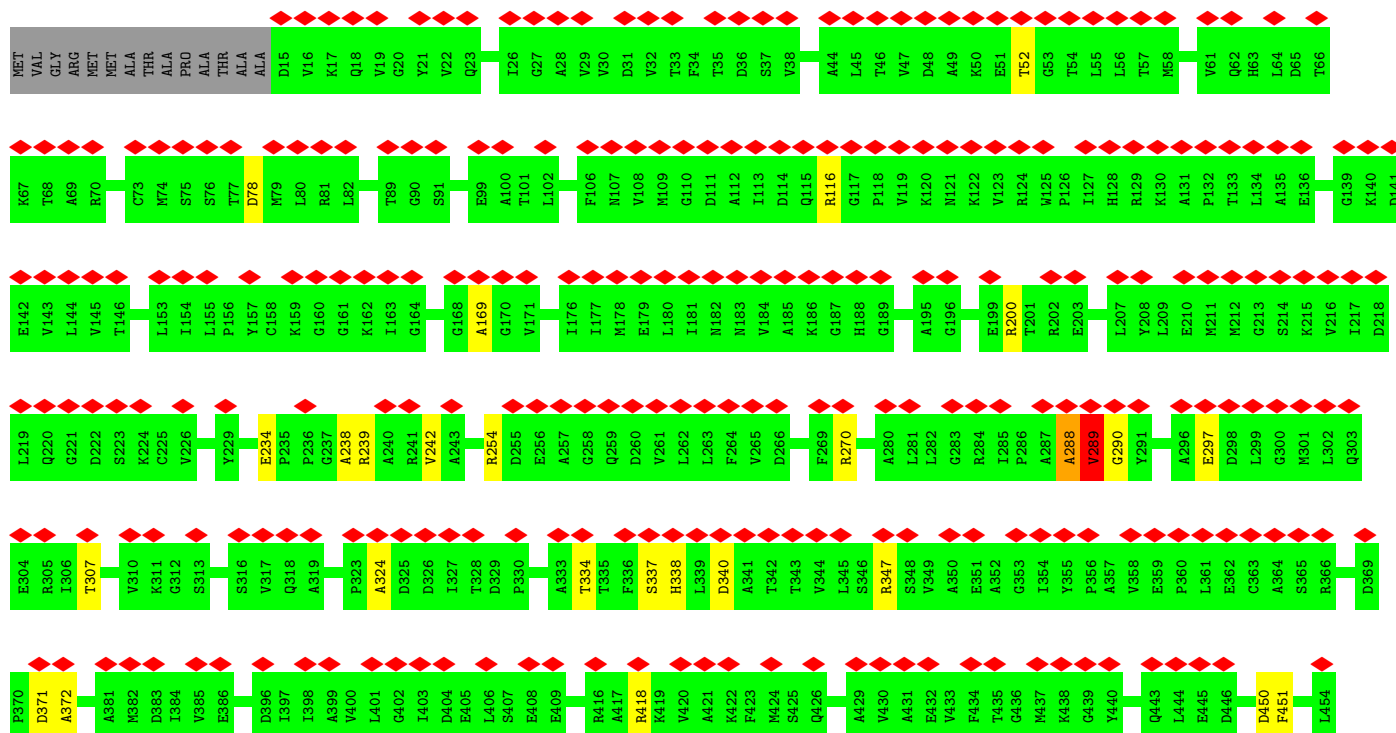
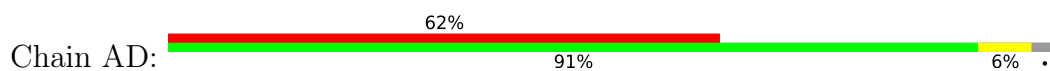


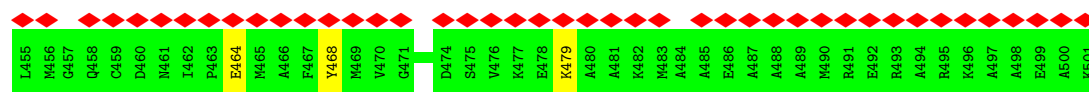
• Molecule 19: ATP synthase subunit alpha



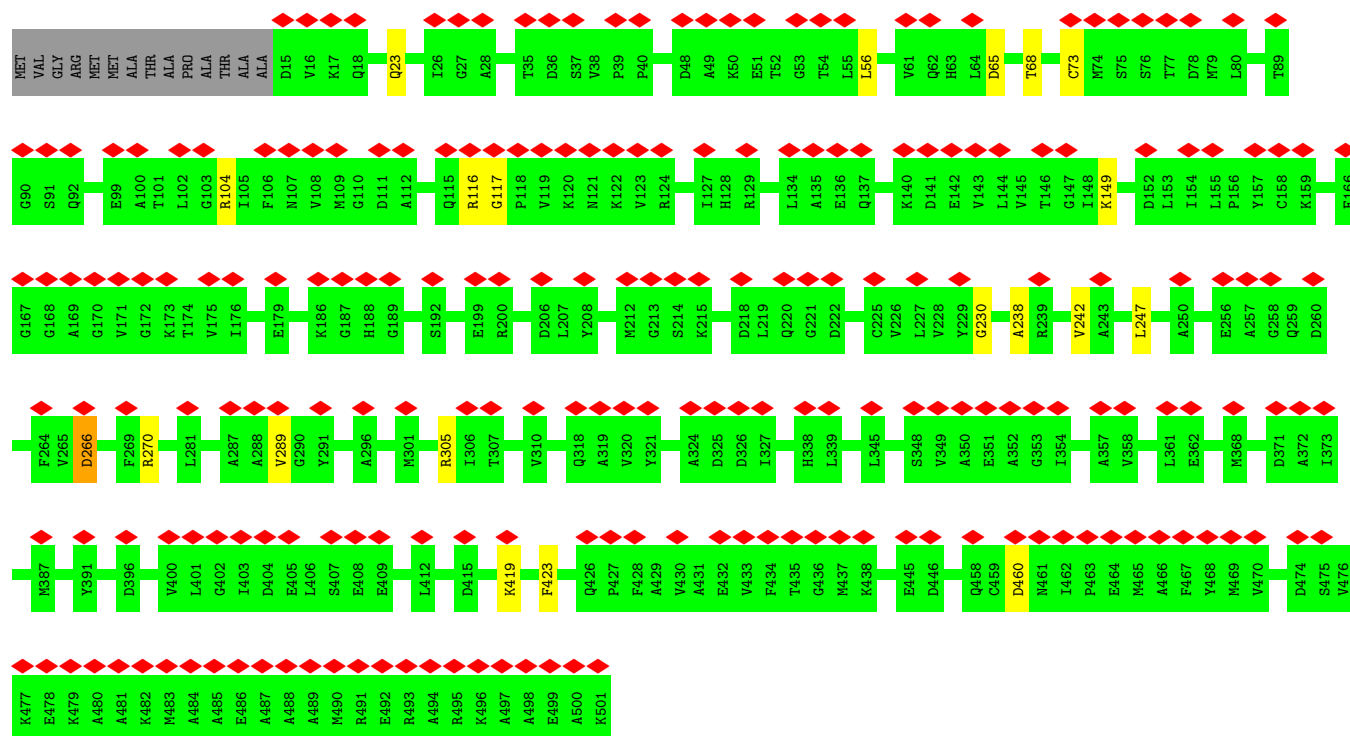


• Molecule 20: ATP synthase subunit beta

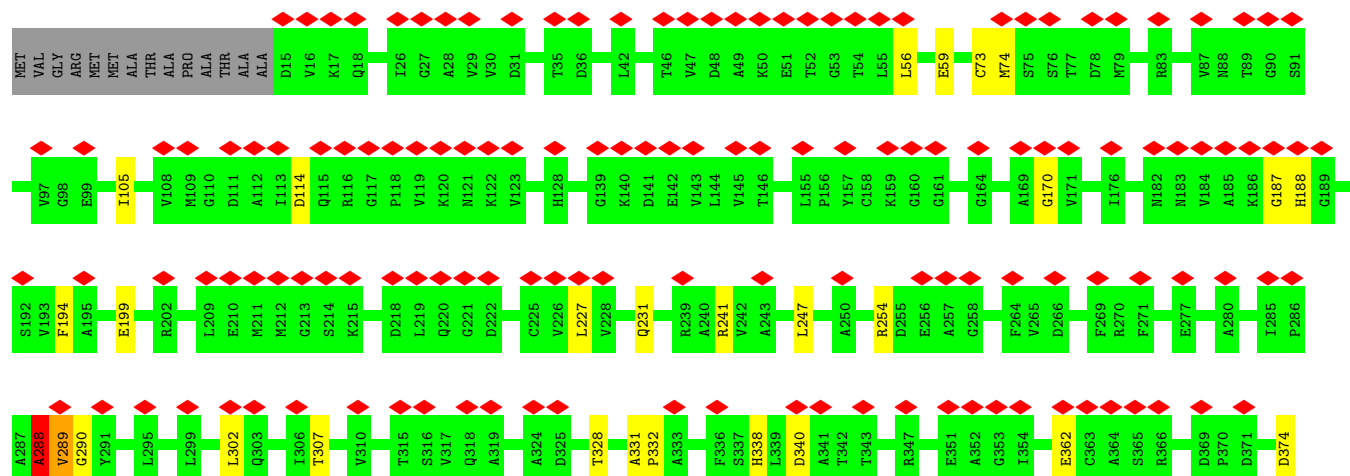
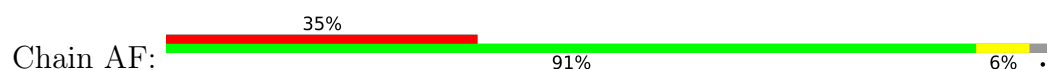


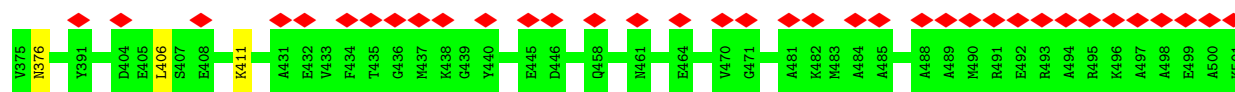


• Molecule 20: ATP synthase subunit beta

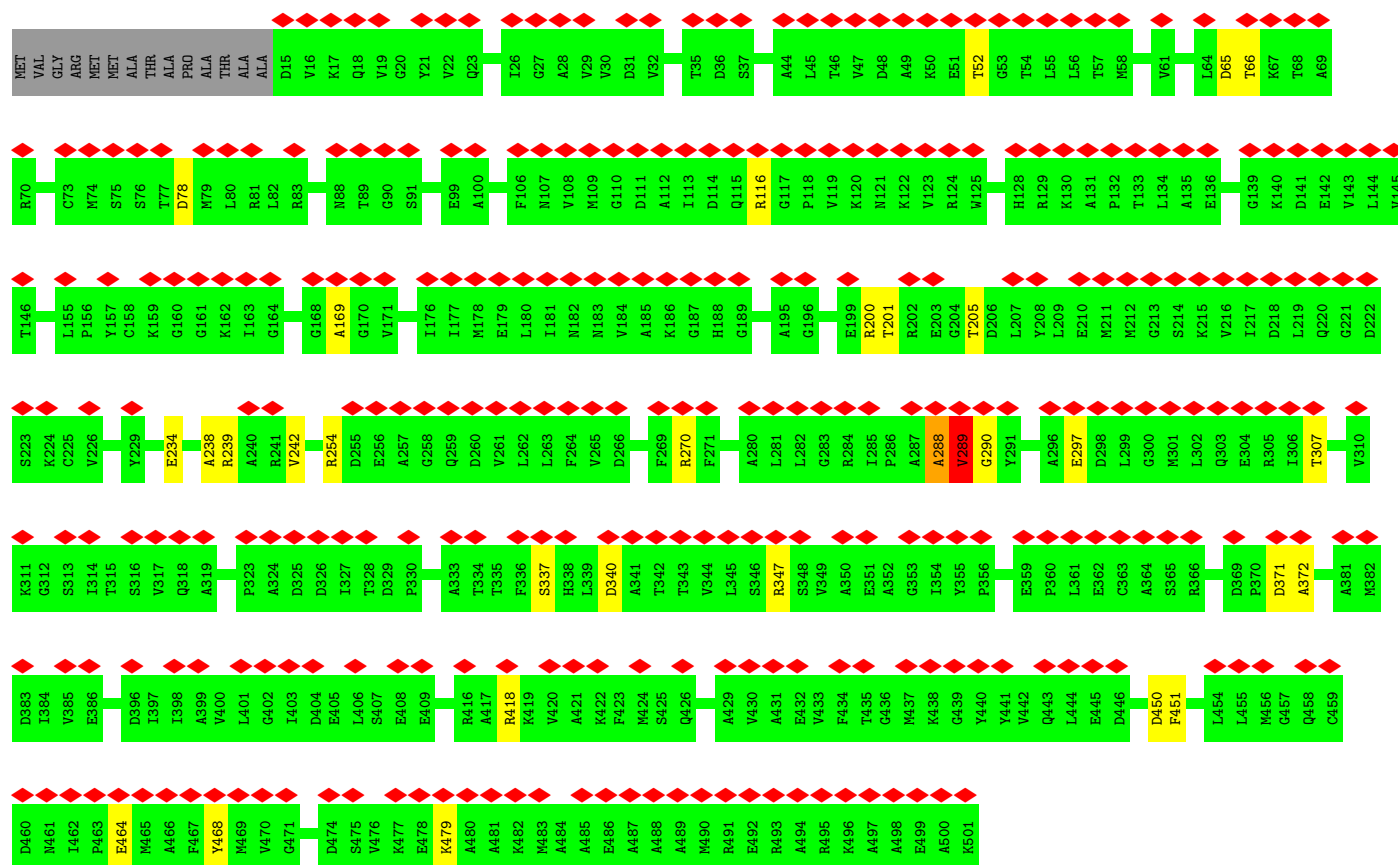


• Molecule 20: ATP synthase subunit beta

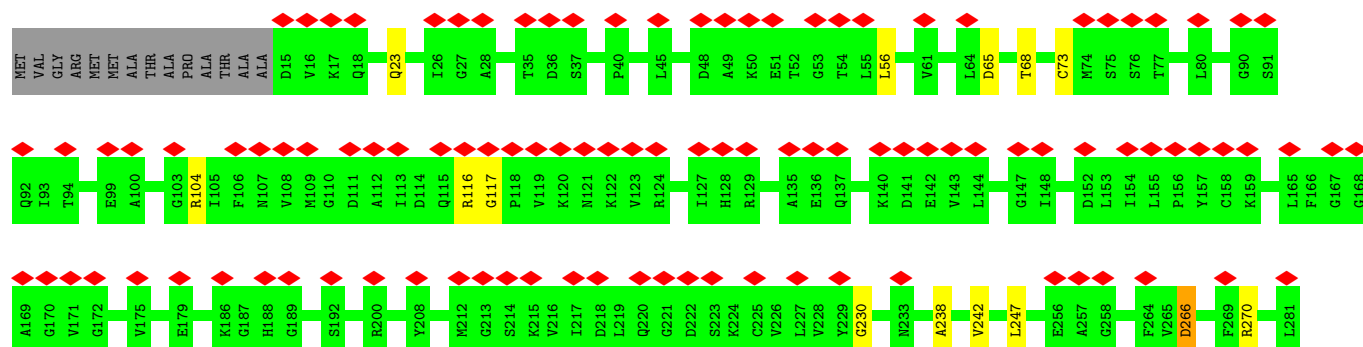


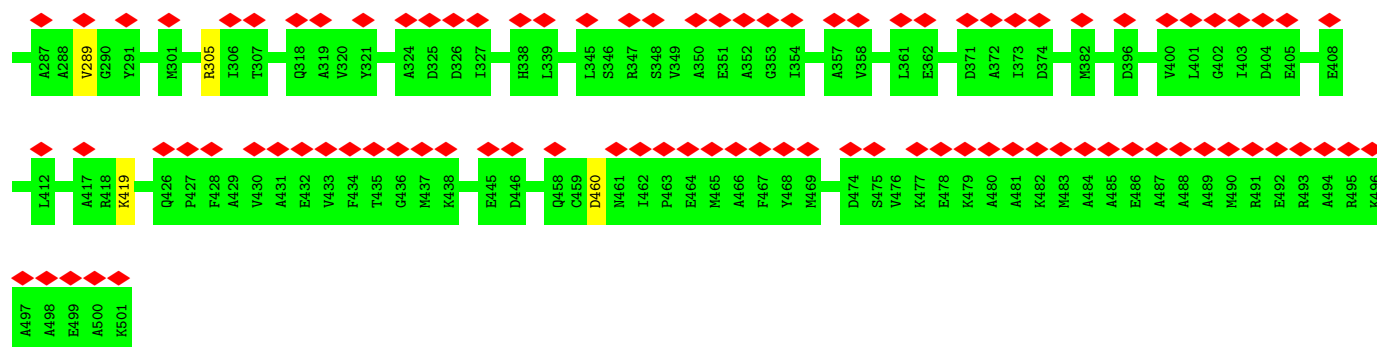


• Molecule 20: ATP synthase subunit beta

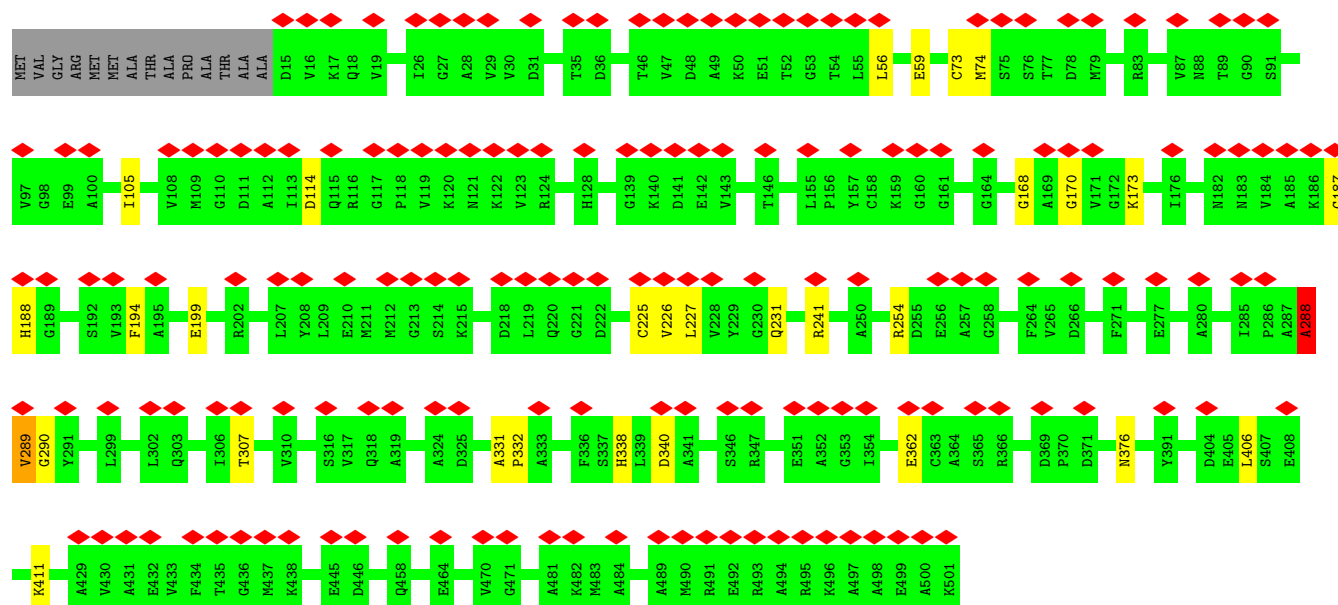


• Molecule 20: ATP synthase subunit beta

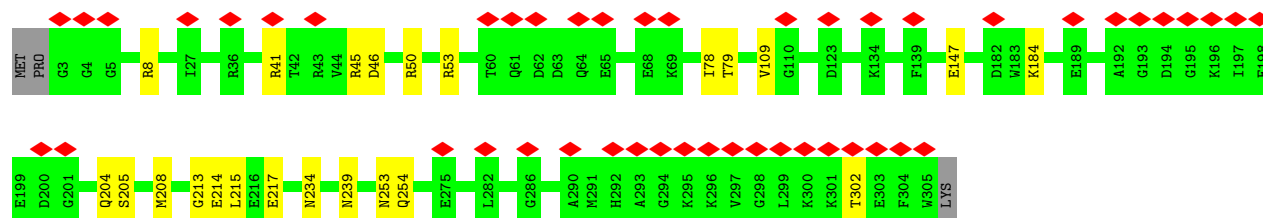




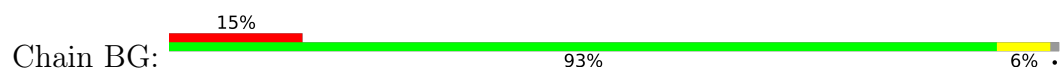
• Molecule 20: ATP synthase subunit beta

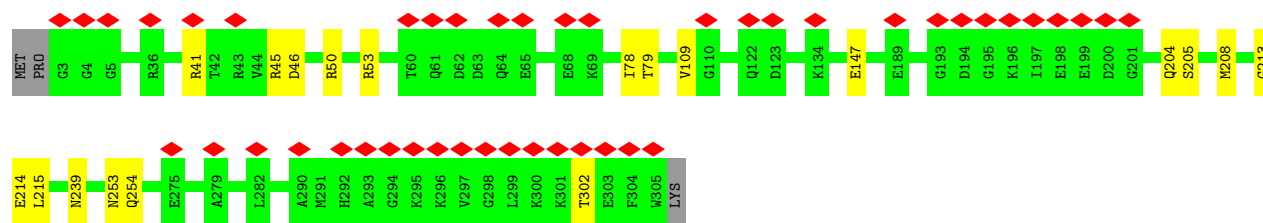


• Molecule 21: ATP synthase subunit gamma

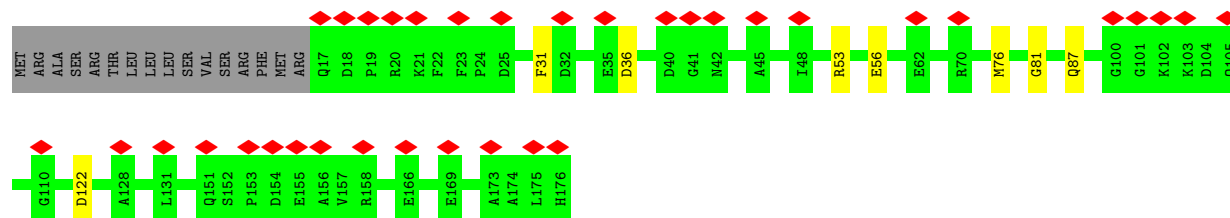
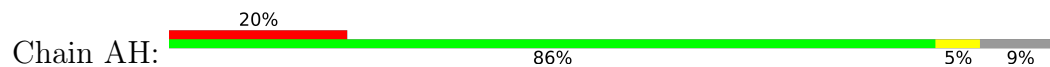


• Molecule 21: ATP synthase subunit gamma

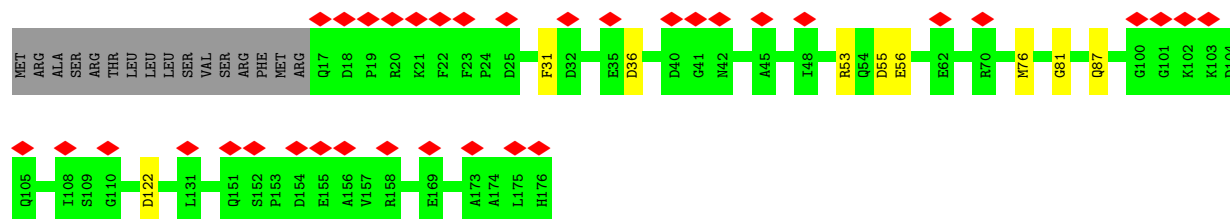
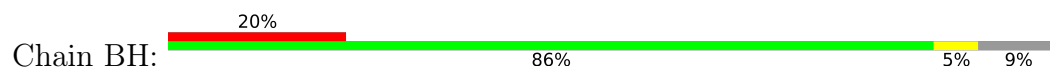




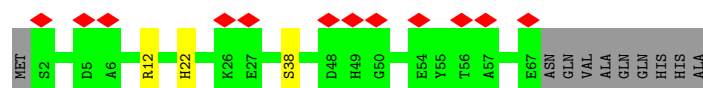
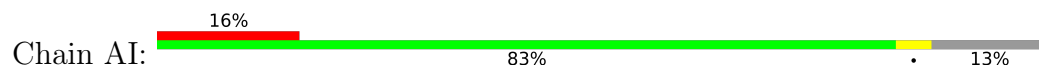
• Molecule 22: ATP synthase subunit delta



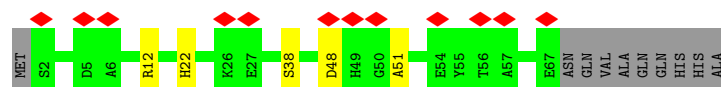
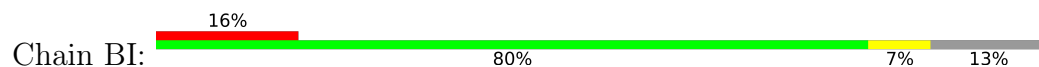
• Molecule 22: ATP synthase subunit delta



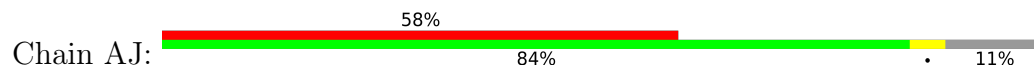
• Molecule 23: ATP synthase subunit epsilon

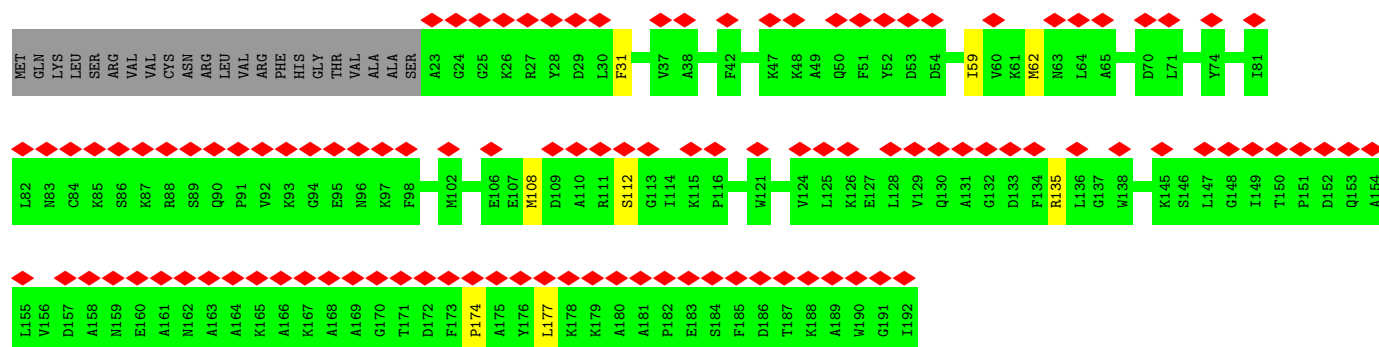


• Molecule 23: ATP synthase subunit epsilon

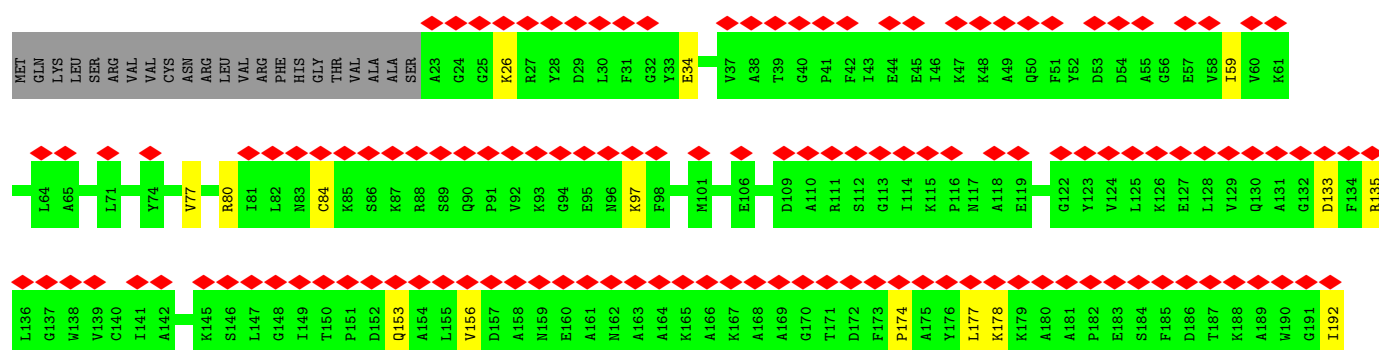
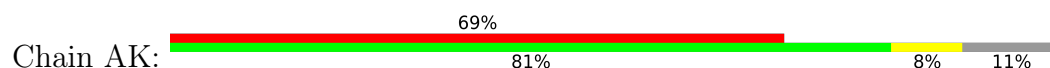


• Molecule 24: p18

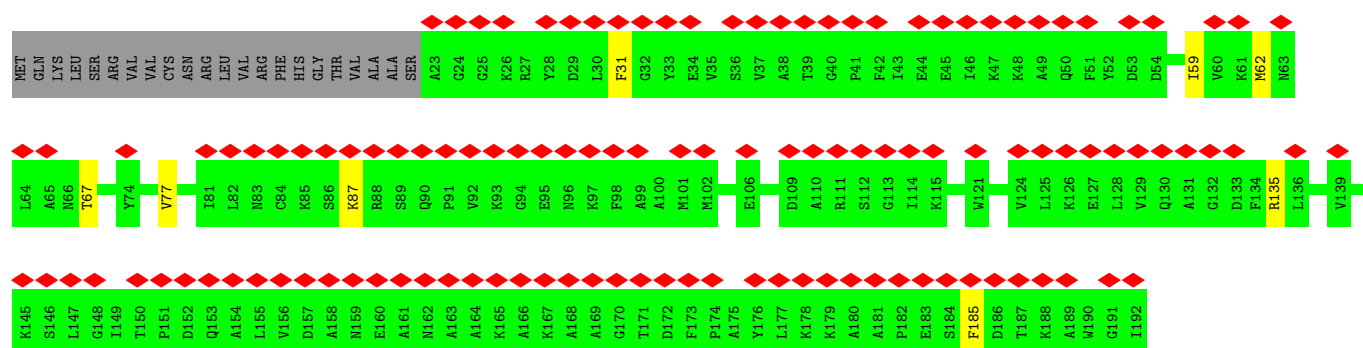
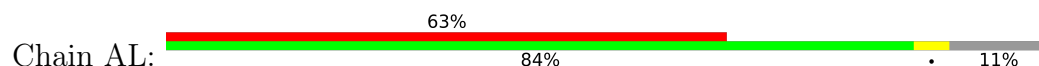




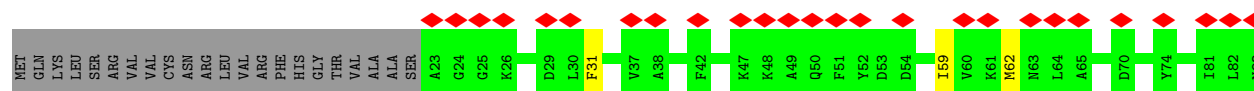
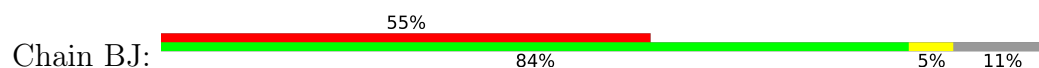
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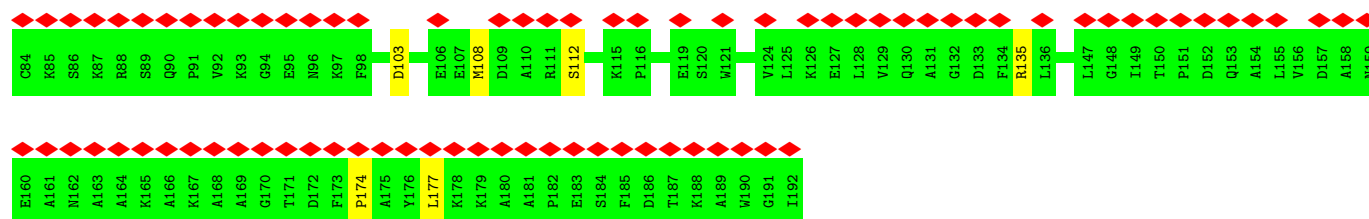


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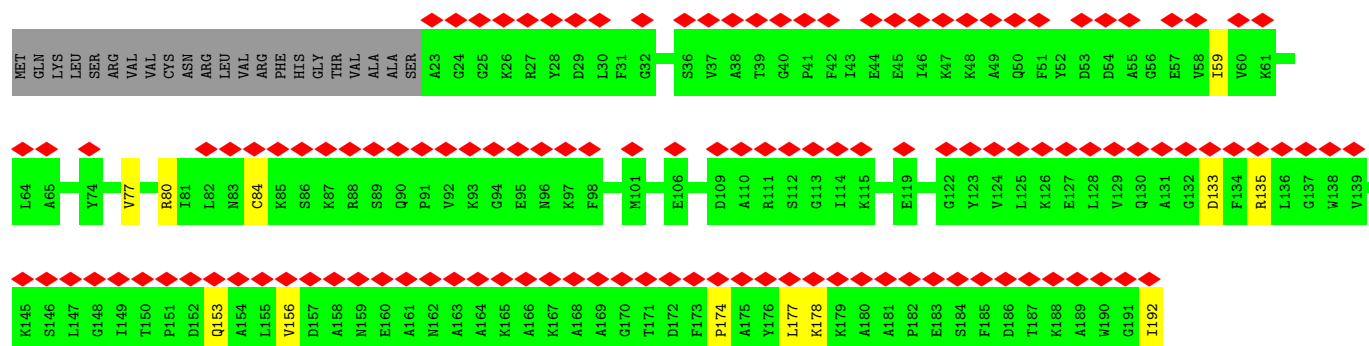
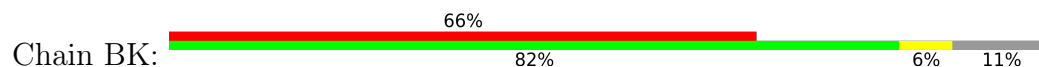


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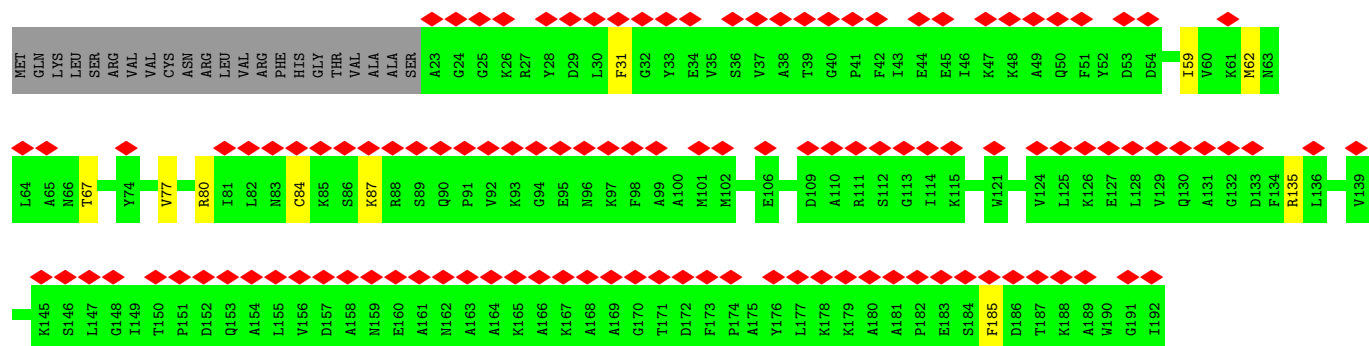
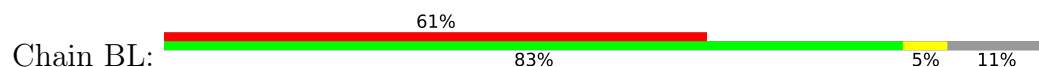




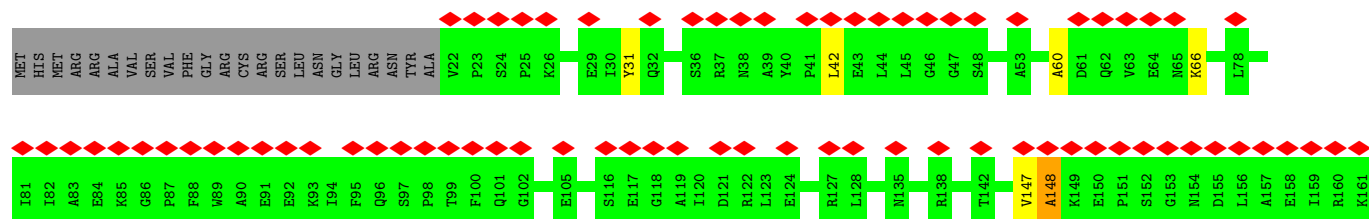
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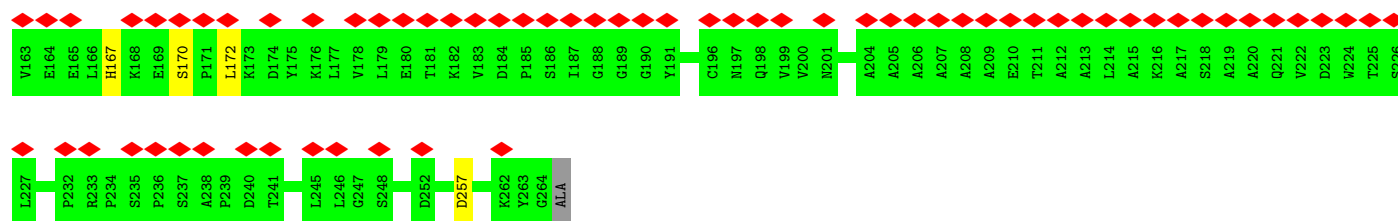


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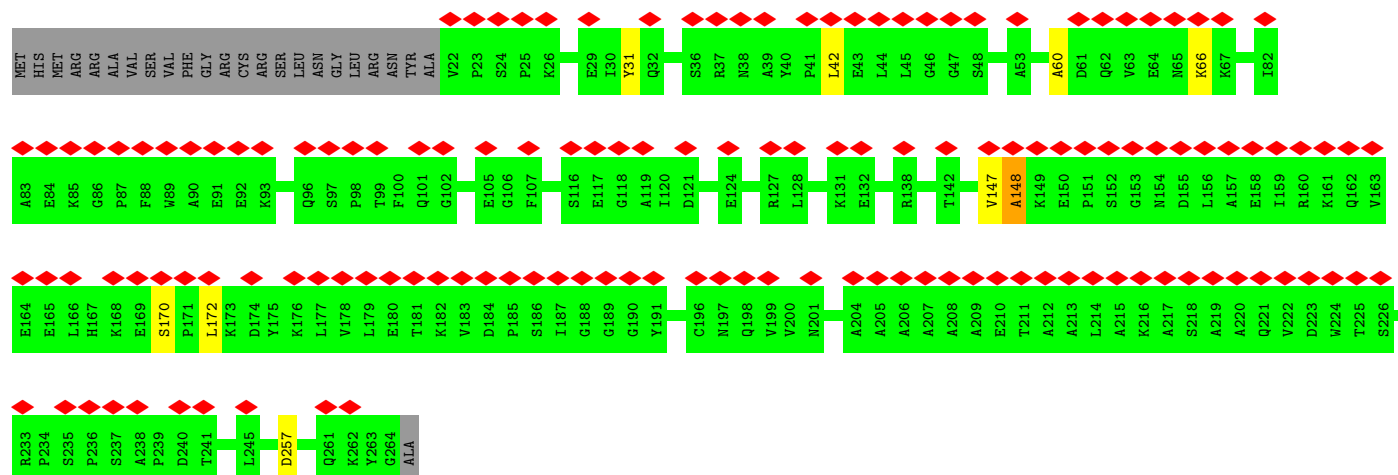
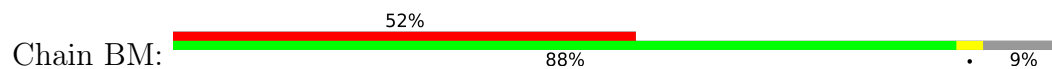


• Molecule 25: oligomycin sensitivity conferring protein (OSCP)

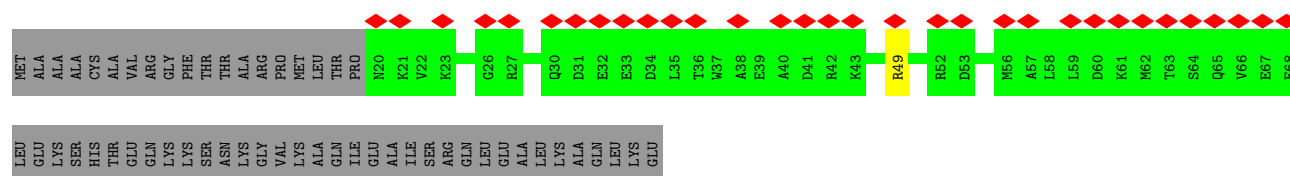




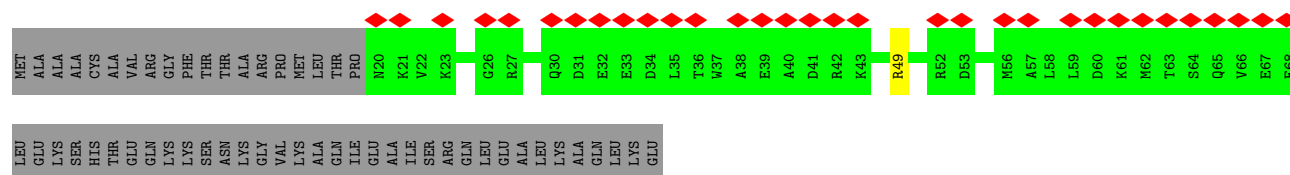
- Molecule 25: oligomycin sensitivity conferring protein (OSCP)



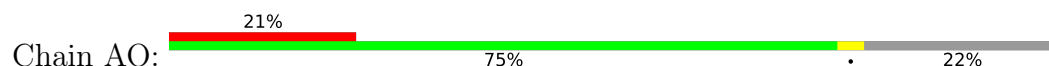
- Molecule 26: inhibitor of F1 (IF1)

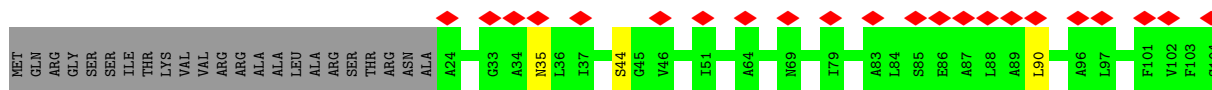


- Molecule 26: inhibitor of F1 (IF1)

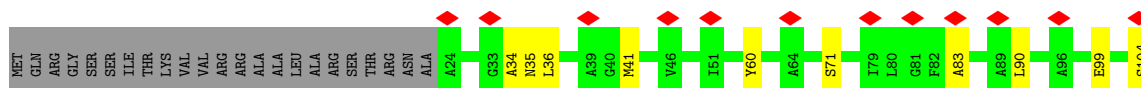
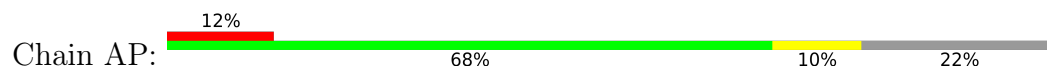


- Molecule 27: ATP synthase subunit c

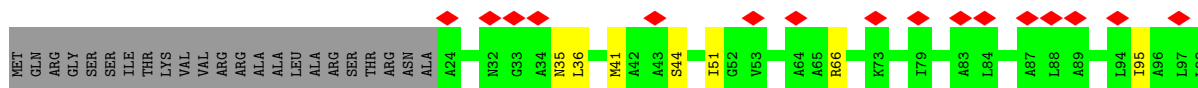
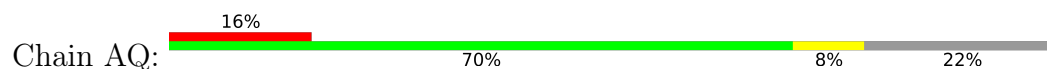




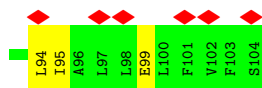
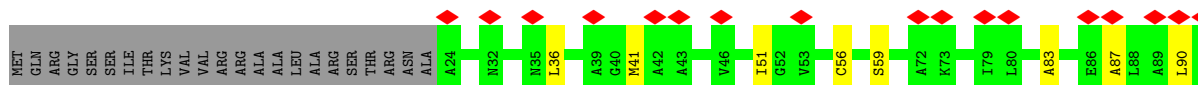
- Molecule 27: ATP synthase subunit c



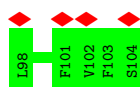
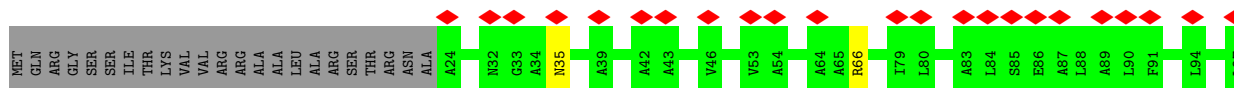
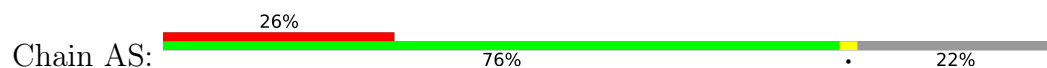
- Molecule 27: ATP synthase subunit c



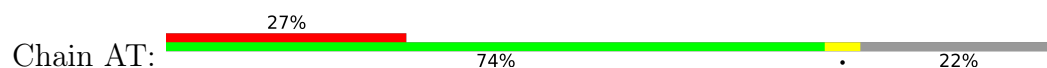
- Molecule 27: ATP synthase subunit c

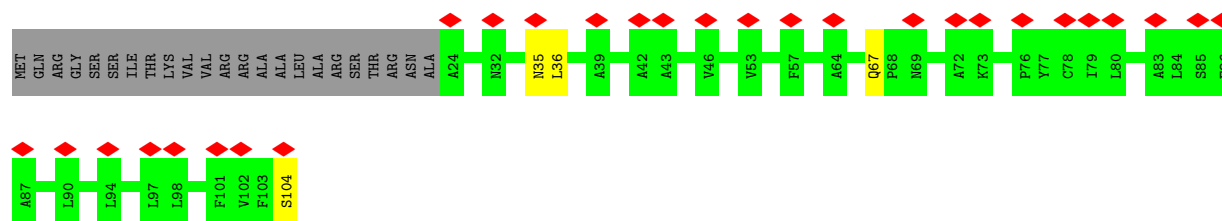


- Molecule 27: ATP synthase subunit c

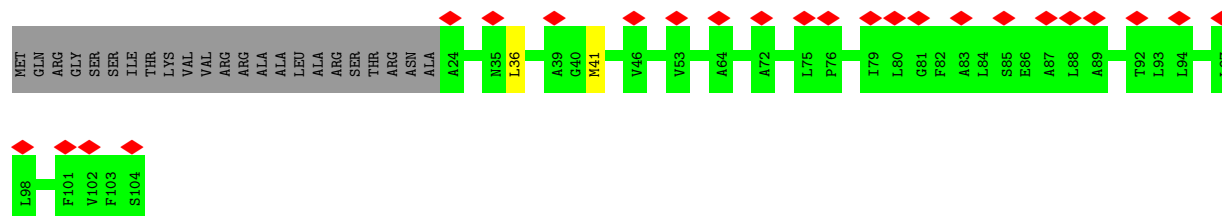
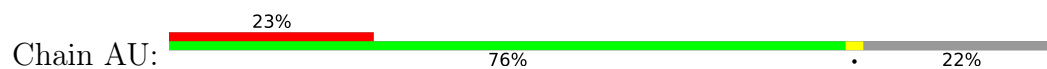


- Molecule 27: ATP synthase subunit c

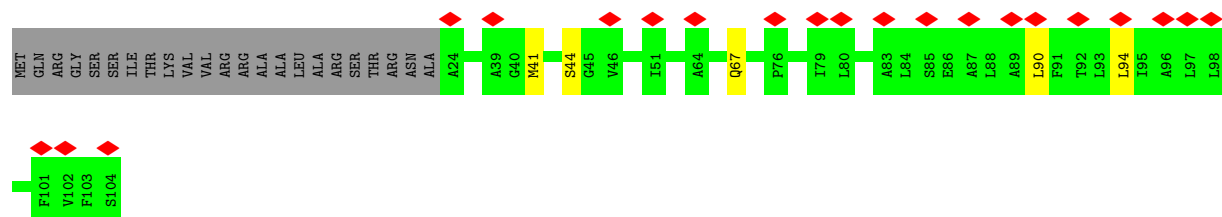
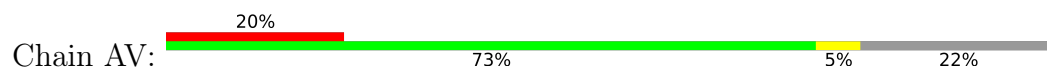




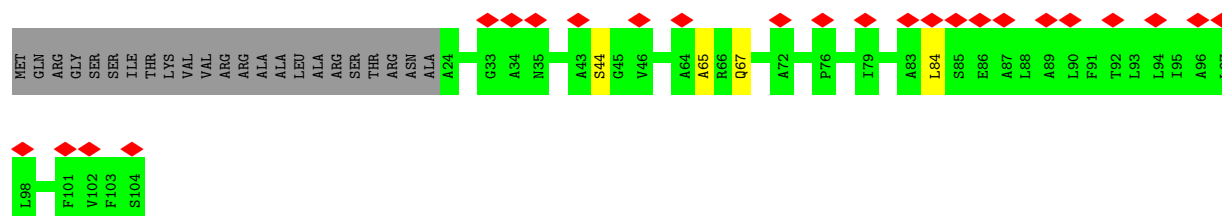
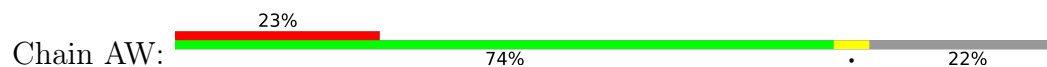
- Molecule 27: ATP synthase subunit c



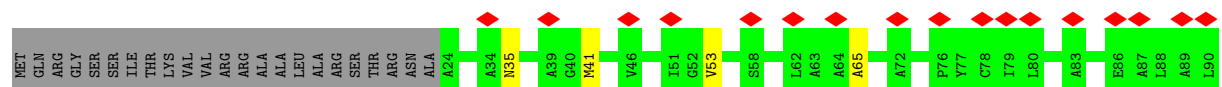
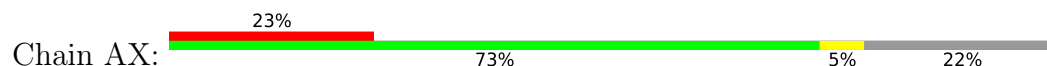
- Molecule 27: ATP synthase subunit c

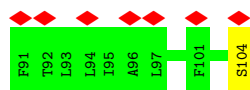


- Molecule 27: ATP synthase subunit c

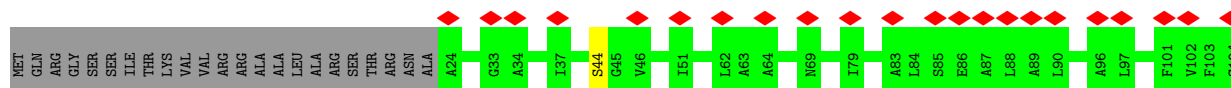
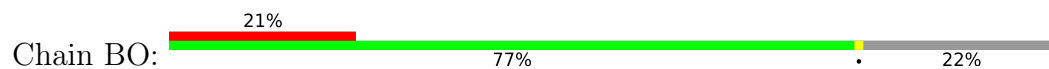


- Molecule 27: ATP synthase subunit c

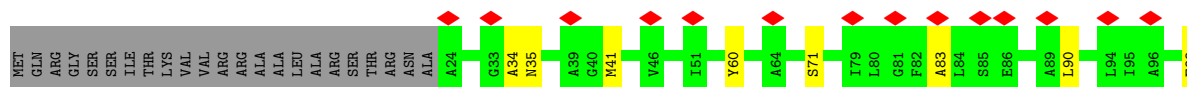




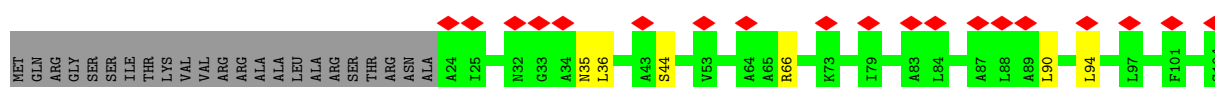
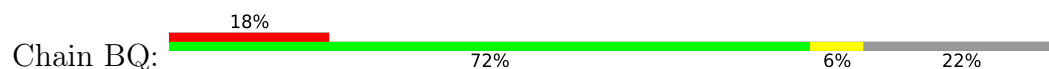
- Molecule 27: ATP synthase subunit c



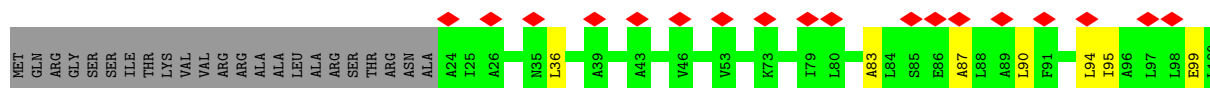
- Molecule 27: ATP synthase subunit c



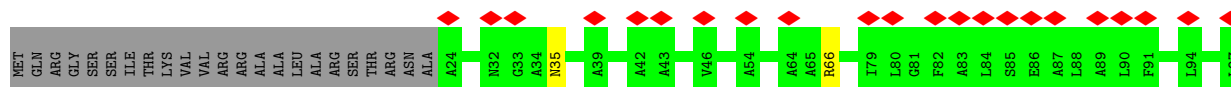
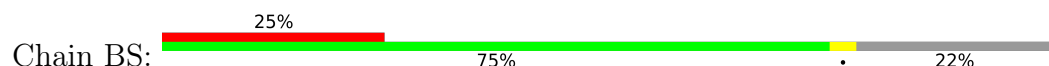
- Molecule 27: ATP synthase subunit c

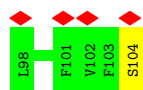


- Molecule 27: ATP synthase subunit c

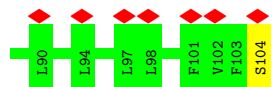
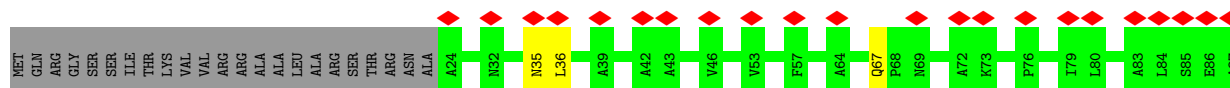
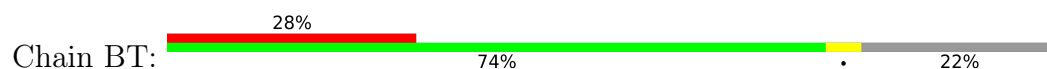


- Molecule 27: ATP synthase subunit c

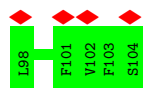
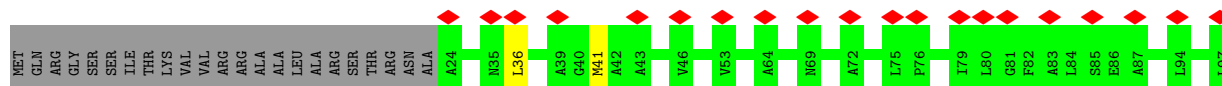
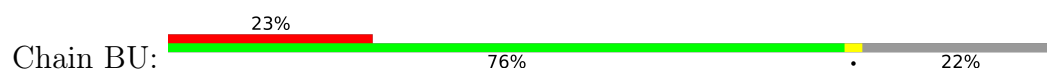




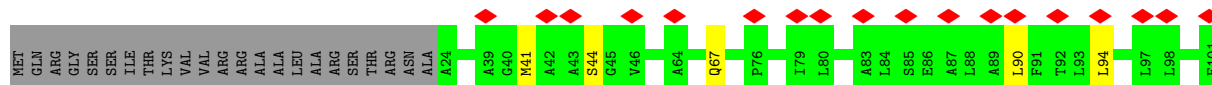
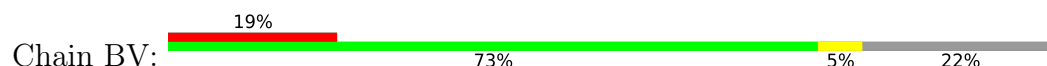
- Molecule 27: ATP synthase subunit c



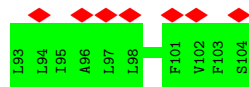
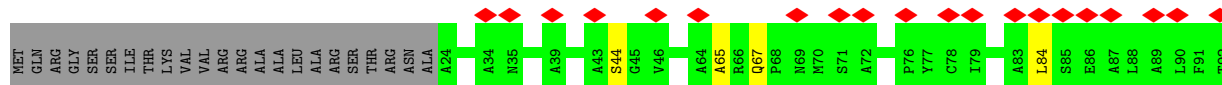
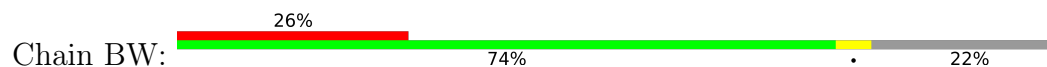
- Molecule 27: ATP synthase subunit c



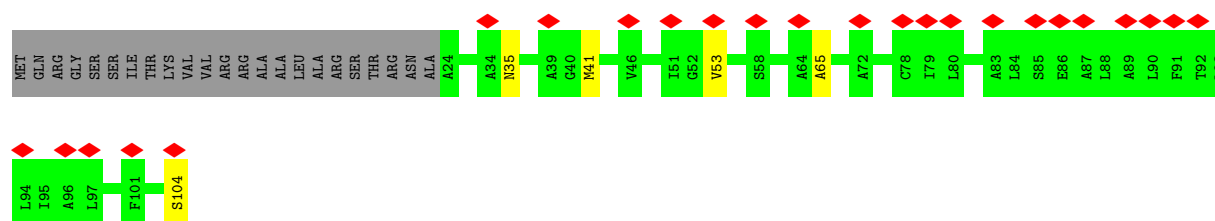
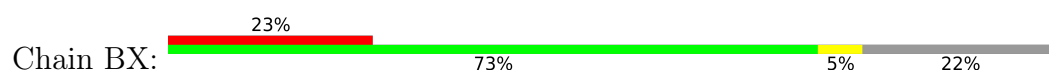
- Molecule 27: ATP synthase subunit c



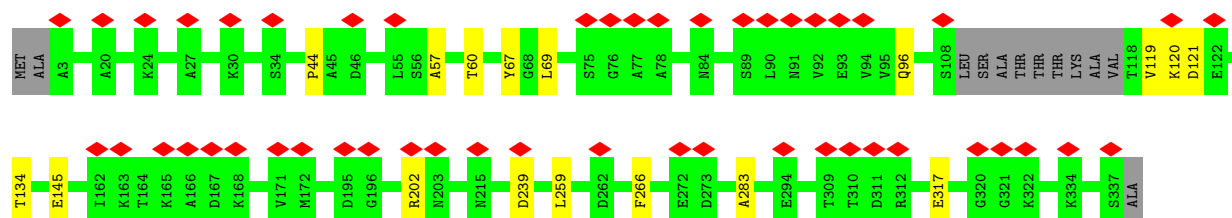
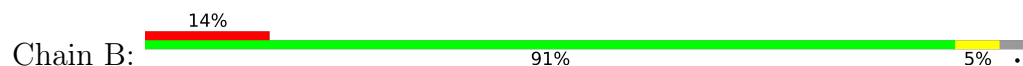
- Molecule 27: ATP synthase subunit c



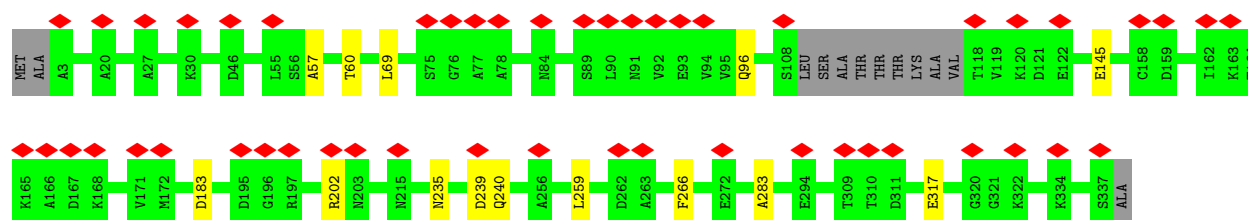
- Molecule 27: ATP synthase subunit c



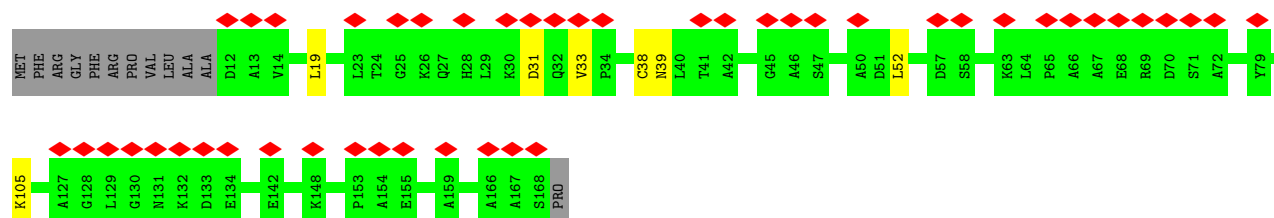
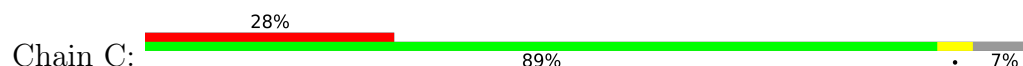
- Molecule 28: ATPTB3



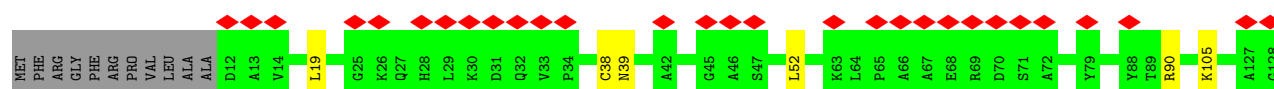
- Molecule 28: ATPTB3

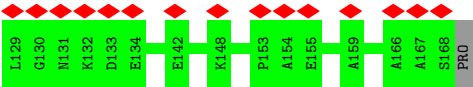


- Molecule 29: ATPTB4



- Molecule 29: ATPTB4





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	27232	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 ($e^-/\text{\AA}^2$)	36.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.129	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	461.99997, 461.99997, 461.99997	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LPP, TRT, ADP, LMT, MG, CDL, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.24	0/4047	0.40	0/5500
1	a	0.24	0/4047	0.40	0/5500
2	D	0.21	0/1559	0.38	0/2106
2	d	0.21	0/1559	0.38	0/2106
3	E	0.17	0/821	0.38	0/1100
3	e	0.17	0/821	0.37	0/1100
4	F	0.27	0/2379	0.43	0/3233
4	f	0.27	0/2379	0.41	0/3233
5	G	0.26	0/901	0.43	0/1218
5	g	0.26	0/901	0.43	0/1218
6	H	0.22	0/3755	0.39	0/5132
6	h	0.22	0/3755	0.40	0/5132
7	I	0.24	0/804	0.43	0/1084
7	i	0.24	0/804	0.43	0/1084
8	J	0.23	0/918	0.39	0/1255
8	j	0.23	0/918	0.39	0/1255
9	K	0.18	0/839	0.34	0/1135
9	k	0.18	0/839	0.35	0/1135
10	L	0.26	0/518	0.40	0/711
10	l	0.26	0/518	0.40	0/711
11	M	0.25	0/1399	0.36	0/1895
11	m	0.25	0/1399	0.37	0/1895
12	N	0.24	0/1137	0.34	0/1540
12	n	0.24	0/1137	0.34	0/1540
13	O	0.19	0/881	0.37	0/1193
13	o	0.19	0/881	0.36	0/1193
14	P	0.26	0/955	0.38	0/1292
14	p	0.26	0/955	0.38	0/1292
15	Q	0.17	0/774	0.42	0/1040
15	q	0.17	0/774	0.41	0/1040
16	R	0.17	0/594	0.38	0/798
16	r	0.17	0/594	0.38	0/798

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	S	0.21	0/575	0.40	0/785
17	s	0.21	0/575	0.39	0/785
18	T	0.20	0/543	0.36	0/730
18	t	0.20	0/543	0.36	0/730
19	AA	0.17	0/4164	0.41	0/5635
19	AB	0.17	0/4164	0.40	0/5635
19	AC	0.17	0/4186	0.41	0/5665
19	BA	0.17	0/4164	0.41	0/5635
19	BB	0.17	0/4164	0.40	0/5635
19	BC	0.17	0/4186	0.41	0/5665
20	AD	0.21	0/3732	0.44	1/5056 (0.0%)
20	AE	0.18	0/3732	0.42	0/5056
20	AF	0.20	0/3732	0.44	1/5056 (0.0%)
20	BD	0.21	0/3732	0.45	1/5056 (0.0%)
20	BE	0.18	0/3732	0.42	0/5056
20	BF	0.20	0/3732	0.44	1/5056 (0.0%)
21	AG	0.17	0/2476	0.42	0/3337
21	BG	0.17	0/2476	0.42	0/3337
22	AH	0.17	0/1270	0.39	0/1720
22	BH	0.16	0/1270	0.38	0/1720
23	AI	0.17	0/549	0.41	0/744
23	BI	0.17	0/549	0.41	0/744
24	AJ	0.15	0/1328	0.37	0/1792
24	AK	0.16	0/1328	0.39	0/1792
24	AL	0.16	0/1328	0.40	0/1792
24	BJ	0.15	0/1328	0.37	0/1792
24	BK	0.16	0/1328	0.39	0/1792
24	BL	0.16	0/1328	0.40	0/1792
25	AM	0.18	0/1933	0.44	0/2623
25	BM	0.18	0/1933	0.45	0/2623
26	AN	0.16	0/408	0.44	0/547
26	BN	0.16	0/408	0.44	0/547
27	AO	0.21	0/590	0.44	0/802
27	AP	0.19	0/590	0.43	0/802
27	AQ	0.22	0/590	0.43	0/802
27	AR	0.19	0/590	0.43	0/802
27	AS	0.16	0/590	0.37	0/802
27	AT	0.16	0/590	0.39	0/802
27	AU	0.15	0/590	0.37	0/802
27	AV	0.16	0/590	0.36	0/802
27	AW	0.16	0/590	0.40	0/802
27	AX	0.17	0/590	0.38	0/802
27	BO	0.20	0/590	0.44	0/802

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	BP	0.19	0/590	0.42	0/802
27	BQ	0.21	0/590	0.41	0/802
27	BR	0.18	0/590	0.43	0/802
27	BS	0.16	0/590	0.37	0/802
27	BT	0.16	0/590	0.39	0/802
27	BU	0.16	0/590	0.37	0/802
27	BV	0.16	0/590	0.36	0/802
27	BW	0.16	0/590	0.40	0/802
27	BX	0.17	0/590	0.38	0/802
28	B	0.16	0/2428	0.41	0/3298
28	b	0.16	0/2428	0.40	0/3298
29	C	0.16	0/1253	0.37	0/1691
29	c	0.16	0/1253	0.38	0/1691
All	All	0.20	0/134620	0.41	4/182412 (0.0%)

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
19	AC	0	1
19	BC	0	1
20	AE	0	1
20	AF	0	1
20	BE	0	1
20	BF	0	1
25	AM	0	2
25	BM	0	2
All	All	0	10

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	BF	289	VAL	N-CA-C	5.91	121.63	109.34
20	AF	289	VAL	N-CA-C	5.88	121.56	109.34
20	AD	289	VAL	N-CA-C	5.55	120.88	109.34
20	BD	289	VAL	N-CA-C	5.53	120.84	109.34

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	AC	284	ASP	Peptide
20	AE	266	ASP	Peptide
20	AF	288	ALA	Peptide
25	AM	147	VAL	Peptide
25	AM	148	ALA	Peptide
19	BC	284	ASP	Peptide
20	BE	266	ASP	Peptide
20	BF	288	ALA	Peptide
25	BM	147	VAL	Peptide
25	BM	148	ALA	Peptide

5.2 Too-close contacts [i](#)

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	3945	3919	3919	20	0
1	a	3945	3919	3919	22	0
2	D	1521	1519	1519	12	0
2	d	1521	1519	1519	12	0
3	E	798	779	779	12	0
3	e	798	779	779	9	0
4	F	2313	2329	2329	16	0
4	f	2313	2329	2329	16	0
5	G	879	924	924	3	0
5	g	879	924	924	4	0
6	H	3665	3637	3637	10	0
6	h	3665	3637	3637	11	0
7	I	782	771	771	1	0
7	i	782	771	771	2	0
8	J	881	853	852	7	0
8	j	881	853	852	8	0
9	K	816	821	821	5	0
9	k	816	821	821	4	0
10	L	501	507	507	2	0
10	l	501	507	507	2	0
11	M	1363	1354	1354	3	0
11	m	1363	1354	1354	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	N	1097	1071	1070	4	0
12	n	1097	1071	1070	6	0
13	O	849	803	803	4	0
13	o	849	803	803	5	0
14	P	926	912	912	3	0
14	p	926	912	912	3	0
15	Q	753	723	723	4	0
15	q	753	723	723	4	0
16	R	579	581	581	4	0
16	r	579	581	581	4	0
17	S	551	541	541	2	0
17	s	551	541	541	2	0
18	T	528	552	552	5	0
18	t	528	552	552	4	0
19	AA	4095	4196	4197	19	0
19	AB	4095	4197	4197	20	0
19	AC	4117	4219	4219	29	0
19	BA	4095	4196	4197	20	0
19	BB	4095	4197	4197	21	0
19	BC	4117	4219	4219	27	0
20	AD	3678	3729	3729	19	0
20	AE	3678	3730	3730	11	0
20	AF	3678	3729	3729	20	0
20	BD	3678	3729	3729	19	0
20	BE	3678	3730	3730	10	0
20	BF	3678	3729	3729	19	0
21	AG	2436	2462	2462	17	0
21	BG	2436	2462	2462	15	0
22	AH	1246	1202	1202	6	0
22	BH	1246	1202	1202	7	0
23	AI	536	541	541	3	0
23	BI	536	541	541	4	0
24	AJ	1302	1294	1294	5	0
24	AK	1302	1294	1294	10	0
24	AL	1302	1294	1294	6	0
24	BJ	1302	1294	1294	6	0
24	BK	1302	1294	1294	8	0
24	BL	1302	1294	1294	7	0
25	AM	1893	1885	1885	6	0
25	BM	1893	1885	1885	5	0
26	AN	403	399	399	1	0
26	BN	403	399	399	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	AO	580	605	605	3	0
27	AP	580	605	605	9	0
27	AQ	580	605	605	9	0
27	AR	580	605	605	7	0
27	AS	580	605	605	2	0
27	AT	580	605	605	4	0
27	AU	580	605	605	2	0
27	AV	580	605	605	4	0
27	AW	580	605	605	4	0
27	AX	580	605	605	4	0
27	BO	580	605	605	1	0
27	BP	580	605	605	7	0
27	BQ	580	605	605	7	0
27	BR	580	605	605	4	0
27	BS	580	605	605	3	0
27	BT	580	605	605	4	0
27	BU	580	605	605	2	0
27	BV	580	605	605	4	0
27	BW	580	605	605	4	0
27	BX	580	605	605	4	0
28	B	2392	2421	2421	12	0
28	b	2392	2421	2421	11	0
29	C	1231	1241	1241	4	0
29	c	1231	1241	1241	4	0
30	A	393	427	515	13	0
30	D	91	137	135	2	0
30	E	63	32	73	6	0
30	M	183	129	201	6	0
30	O	65	59	77	2	0
30	P	146	173	189	2	0
30	R	76	74	99	2	0
30	a	393	427	515	16	0
30	d	91	137	135	2	0
30	e	63	32	73	6	0
30	m	77	75	101	2	0
30	o	65	59	77	3	0
30	p	48	27	40	1	0
30	r	76	74	99	3	0
31	D	35	46	45	0	0
31	F	35	46	45	2	0
31	N	35	46	44	0	0
31	Q	35	46	45	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	d	35	46	45	0	0
31	g	35	46	45	3	0
31	n	35	46	44	0	0
31	q	35	46	45	1	0
32	F	24	17	21	0	0
32	I	44	67	67	0	0
32	K	31	17	35	1	0
32	N	26	17	25	0	0
32	O	55	59	59	0	0
32	f	24	17	21	0	0
32	i	44	67	67	0	0
32	k	31	17	35	2	0
32	n	26	17	25	0	0
32	o	55	59	59	0	0
33	AE	25	36	36	0	0
33	AR	25	36	36	0	0
33	BE	25	36	36	0	0
33	BR	25	36	36	0	0
33	G	50	72	72	1	0
33	M	50	72	72	0	0
33	N	50	72	72	1	0
33	P	25	36	36	0	0
33	g	50	72	72	1	0
33	m	50	72	72	0	0
33	n	50	72	72	1	0
33	p	25	36	36	0	0
34	AA	31	4	12	0	0
34	AB	31	4	12	1	0
34	AC	31	4	12	1	0
34	AF	31	4	12	2	0
34	BA	31	4	12	0	0
34	BB	31	4	12	2	0
34	BC	31	4	12	0	0
34	BF	31	4	12	2	0
35	AA	1	0	0	0	0
35	AB	1	0	0	0	0
35	AC	1	0	0	0	0
35	AD	1	0	0	0	0
35	AF	1	0	0	0	0
35	BA	1	0	0	0	0
35	BB	1	0	0	0	0
35	BC	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	BD	1	0	0	0	0
35	BF	1	0	0	0	0
36	AD	27	7	12	0	0
36	BD	27	8	12	0	0
All	All	135094	136237	136825	579	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 2.

All (579) 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)
3:E:27:HIS:HD1	3:E:51:THR:HG1	1.18	0.83
20:AF:187:GLY:O	28:b:202:ARG:NH2	2.17	0.77
21:BG:214:GLU:OE1	27:BS:66:ARG:NH1	2.18	0.77
28:B:202:ARG:NH2	20:BF:187:GLY:O	2.19	0.76
21:AG:214:GLU:OE1	27:AS:66:ARG:NH1	2.18	0.75
6:H:319:ARG:NH2	25:BM:257:ASP:OD1	2.20	0.74
1:a:369:LEU:O	1:a:392:ARG:NH1	2.21	0.73
1:A:369:LEU:O	1:A:392:ARG:NH1	2.21	0.73
6:h:319:ARG:NH2	25:AM:257:ASP:OD1	2.20	0.73
27:BP:41:MET:O	27:BQ:44:SER:OG	2.06	0.73
21:AG:213:GLY:O	27:AQ:66:ARG:NH2	2.23	0.72
21:BG:213:GLY:O	27:BQ:66:ARG:NH2	2.22	0.72
27:AP:41:MET:O	27:AQ:44:SER:OG	2.08	0.71
20:BD:234:GLU:O	20:BD:239:ARG:NH2	2.24	0.71
21:BG:204:GLN:NE2	22:BH:36:ASP:O	2.24	0.71
14:p:49:ARG:NH1	30:p:201:CDL:OA3	2.24	0.70
19:AA:224:ARG:NH2	20:AD:340:ASP:OD1	2.25	0.70
19:AC:270:GLU:OE2	19:AC:323:ARG:NH2	2.25	0.70
19:BA:227:ASN:OD1	19:BA:230:ARG:NH2	2.24	0.70
19:AC:494:TYR:OH	19:AC:515:ILE:O	2.09	0.70
24:BL:59:ILE:HD11	24:BL:77:VAL:HG21	1.73	0.70
11:m:117:ARG:O	11:m:124:ARG:NH2	2.25	0.69
20:AF:254:ARG:NH1	20:AF:307:THR:O	2.25	0.69
21:AG:204:GLN:NE2	22:AH:36:ASP:O	2.25	0.69
19:AA:227:ASN:OD1	19:AA:230:ARG:NH2	2.24	0.69
19:BC:270:GLU:OE2	19:BC:323:ARG:NH2	2.26	0.69
6:H:420:HIS:NE2	6:H:432:THR:OG1	2.24	0.69
11:M:117:ARG:O	11:M:124:ARG:NH2	2.26	0.69
14:P:49:ARG:NH1	30:P:201:CDL:OA3	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:BF:254:ARG:NH1	20:BF:307:THR:O	2.25	0.69
6:H:430:LYS:O	10:L:46:TYR:OH	2.11	0.69
6:h:420:HIS:NE2	6:h:432:THR:OG1	2.25	0.69
19:BA:435:ARG:NH2	19:BA:466:VAL:O	2.26	0.69
19:BC:227:ASN:OD1	19:BC:230:ARG:NH2	2.25	0.69
3:e:2:SER:N	13:o:93:SER:HG	1.91	0.68
30:A:505:CDL:H822	2:D:127:VAL:HG13	1.76	0.68
24:AL:59:ILE:HD11	24:AL:77:VAL:HG21	1.73	0.68
27:AP:35:ASN:ND2	27:AP:104:SER:O	2.27	0.68
19:BA:224:ARG:NH2	20:BD:340:ASP:OD1	2.27	0.68
27:AO:44:SER:OG	27:AX:41:MET:O	2.11	0.68
19:BC:494:TYR:OH	19:BC:515:ILE:O	2.10	0.68
1:A:269:PRO:O	2:D:82:ARG:NH1	2.27	0.68
20:AD:234:GLU:O	20:AD:239:ARG:NH2	2.26	0.68
4:F:114:ASP:OD2	18:T:14:ARG:NH2	2.27	0.67
28:B:317:GLU:O	29:C:105:LYS:NZ	2.27	0.67
19:AA:435:ARG:NH2	19:AA:466:VAL:O	2.26	0.67
1:a:151:ARG:NH2	1:a:321:GLU:OE1	2.27	0.67
6:h:430:LYS:O	10:l:46:TYR:OH	2.11	0.67
19:AB:493:LYS:O	24:AK:135:ARG:NH1	2.28	0.67
19:AC:227:ASN:OD1	19:AC:230:ARG:NH2	2.27	0.67
22:BH:81:GLY:O	27:BT:67:GLN:NE2	2.27	0.67
19:BB:493:LYS:O	24:BK:135:ARG:NH1	2.27	0.67
4:f:114:ASP:OD2	18:t:14:ARG:NH2	2.27	0.67
21:BG:79:THR:OG1	21:BG:109:VAL:O	2.11	0.67
1:A:151:ARG:NH2	1:A:321:GLU:OE1	2.27	0.67
28:B:119:VAL:O	28:B:121:ASP:N	2.28	0.67
4:F:74:LYS:NZ	31:F:302:LMT:O2B	2.27	0.66
27:AX:35:ASN:ND2	27:AX:104:SER:O	2.28	0.66
28:b:317:GLU:O	29:c:105:LYS:NZ	2.27	0.66
27:BX:35:ASN:ND2	27:BX:104:SER:O	2.28	0.66
30:a:505:CDL:H822	2:d:127:VAL:HG13	1.78	0.66
27:BP:35:ASN:ND2	27:BP:104:SER:O	2.28	0.66
1:a:269:PRO:O	2:d:82:ARG:NH1	2.28	0.66
9:k:22:ARG:NH2	30:r:101:CDL:O1	2.28	0.66
22:AH:81:GLY:O	27:AT:67:GLN:NE2	2.28	0.66
32:K:201:LPP:O3	16:R:50:ARG:NH1	2.28	0.66
19:BC:435:ARG:NH2	19:BC:466:VAL:O	2.29	0.66
4:f:74:LYS:NZ	31:g:201:LMT:O2B	2.29	0.65
20:BD:254:ARG:NH1	20:BD:307:THR:O	2.30	0.65
27:BO:44:SER:OG	27:BX:41:MET:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AC:75:GLU:OE1	19:AC:79:SER:OG	2.15	0.64
19:BC:75:GLU:OE1	19:BC:79:SER:OG	2.15	0.64
1:a:400:LYS:NZ	1:a:481:GLU:OE2	2.30	0.64
20:AD:254:ARG:NH1	20:AD:307:THR:O	2.30	0.64
32:k:201:LPP:O3	16:r:50:ARG:NH1	2.30	0.64
19:BB:75:GLU:OE1	19:BB:79:SER:OG	2.16	0.64
19:AC:435:ARG:NH2	19:AC:466:VAL:O	2.31	0.64
19:AB:75:GLU:OE1	19:AB:79:SER:OG	2.16	0.63
28:B:96:GLN:NE2	28:B:239:ASP:OD1	2.31	0.63
2:D:151:GLN:O	2:D:160:ARG:NH1	2.32	0.63
19:AC:553:ASN:ND2	20:AF:376:ASN:OD1	2.32	0.63
21:AG:147:GLU:OE1	23:AI:12:ARG:NH1	2.32	0.63
5:G:47:ARG:NH2	6:H:196:GLU:OE2	2.32	0.62
19:BC:553:ASN:ND2	20:BF:376:ASN:OD1	2.32	0.62
21:BG:78:ILE:O	21:BG:239:ASN:ND2	2.31	0.62
19:AA:493:LYS:O	24:AJ:135:ARG:NH2	2.33	0.62
1:A:400:LYS:NZ	1:A:481:GLU:OE2	2.30	0.62
9:K:22:ARG:NH2	30:R:101:CDL:O1	2.33	0.62
19:AC:224:ARG:NH2	20:AF:340:ASP:OD1	2.33	0.62
21:BG:147:GLU:OE1	23:BI:12:ARG:NH1	2.33	0.62
19:BB:494:TYR:OH	19:BB:515:ILE:O	2.18	0.61
20:BD:288:ALA:O	20:BD:290:GLY:N	2.31	0.61
19:BA:493:LYS:O	24:BJ:135:ARG:NH2	2.32	0.61
27:BT:35:ASN:ND2	27:BT:104:SER:O	2.33	0.61
21:AG:79:THR:OG1	21:AG:109:VAL:O	2.09	0.61
20:BE:419:LYS:NZ	20:BE:460:ASP:O	2.33	0.61
9:K:11:SER:OG	18:T:7:GLU:OE1	2.13	0.61
2:d:151:GLN:O	2:d:160:ARG:NH1	2.32	0.61
19:AB:494:TYR:OH	19:AB:515:ILE:O	2.18	0.61
21:AG:78:ILE:O	21:AG:239:ASN:ND2	2.34	0.61
1:A:139:ASP:OD1	17:S:21:TRP:NE1	2.34	0.61
19:AC:418:GLU:OE2	26:AN:49:ARG:NH2	2.33	0.61
15:Q:58:ASP:OD1	15:Q:61:ARG:NH1	2.34	0.60
5:g:47:ARG:NH2	6:h:196:GLU:OE2	2.32	0.60
1:a:139:ASP:OD1	17:s:21:TRP:NE1	2.34	0.60
19:BB:185:ASP:O	19:BB:190:LYS:NZ	2.33	0.60
19:BC:224:ARG:NH2	20:BF:340:ASP:OD1	2.33	0.60
19:BC:418:GLU:OE2	26:BN:49:ARG:NH2	2.34	0.60
19:AB:166:LYS:O	19:AB:170:THR:OG1	2.15	0.60
19:BA:42:ILE:HD12	19:BA:97:VAL:HG21	1.83	0.60
20:BF:288:ALA:O	20:BF:290:GLY:N	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:r:50:ARG:NH2	30:r:101:CDL:OB4	2.34	0.59
3:E:2:SER:N	13:O:93:SER:HG	1.99	0.59
19:AC:208:ILE:O	24:AL:87:LYS:NZ	2.35	0.59
1:A:177:GLU:O	1:A:181:SER:OG	2.20	0.59
19:AA:42:ILE:HD12	19:AA:97:VAL:HG21	1.84	0.59
24:AK:80:ARG:NE	24:AK:84:CYS:SG	2.76	0.59
1:a:177:GLU:O	1:a:181:SER:OG	2.20	0.59
20:AD:288:ALA:O	20:AD:290:GLY:N	2.31	0.59
19:AB:388:ARG:CZ	34:AF:601:ATP:H5'2	2.32	0.59
3:e:46:ASP:OD2	8:j:85:ARG:NH2	2.36	0.58
23:BI:22:HIS:ND1	23:BI:38:SER:OG	2.36	0.58
3:E:46:ASP:OD2	8:J:85:ARG:NH2	2.37	0.58
15:q:58:ASP:OD1	15:q:61:ARG:NH1	2.36	0.58
21:AG:53:ARG:NH1	22:AH:31:PHE:O	2.36	0.58
21:BG:53:ARG:NH1	22:BH:31:PHE:O	2.37	0.58
30:M:205:CDL:O1	30:M:205:CDL:H522	2.04	0.58
22:AH:76:MET:SD	22:AH:87:GLN:NE2	2.77	0.58
28:b:96:GLN:NE2	28:b:239:ASP:OD1	2.36	0.57
1:a:156:LEU:O	1:a:312:ARG:NH2	2.37	0.57
19:AA:411:GLU:OE1	19:AA:411:GLU:N	2.38	0.57
23:AI:22:HIS:ND1	23:AI:38:SER:OG	2.37	0.57
16:R:50:ARG:NH2	30:R:101:CDL:OB4	2.37	0.57
1:a:357:ASP:OD1	1:a:399:TYR:OH	2.19	0.57
6:h:49:ARG:NH1	28:b:145:GLU:OE2	2.38	0.57
6:H:49:ARG:NH1	28:B:145:GLU:OE2	2.38	0.57
27:BT:35:ASN:HA	27:BU:36:LEU:HD23	1.87	0.57
20:AD:52:THR:OG1	20:AD:78:ASP:O	2.18	0.57
19:BA:224:ARG:NH1	20:BD:337:SER:O	2.38	0.57
15:Q:36:ASP:OD1	15:Q:68:ARG:NH1	2.38	0.57
20:AE:419:LYS:NZ	20:AE:460:ASP:O	2.37	0.57
3:E:17:ARG:NH1	3:E:21:GLU:OE2	2.37	0.57
12:n:72:ARG:NH1	14:p:96:THR:O	2.37	0.57
19:AB:185:ASP:O	19:AB:190:LYS:NZ	2.37	0.56
20:AD:468:TYR:O	20:AD:479:LYS:NZ	2.38	0.56
1:A:357:ASP:OD1	1:A:399:TYR:OH	2.20	0.56
4:F:185:LEU:HD12	27:BP:90:LEU:HD21	1.87	0.56
30:a:503:CDL:H732	30:a:503:CDL:H771	1.88	0.56
19:AB:456:TYR:OH	19:AB:517:GLU:OE2	2.24	0.56
2:d:68:TYR:O	2:d:77:ARG:NH1	2.38	0.56
20:AF:170:GLY:HA2	34:AF:601:ATP:H5'1	1.88	0.56
22:BH:76:MET:SD	22:BH:87:GLN:NE2	2.77	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:72:ARG:NH1	14:P:96:THR:O	2.38	0.56
19:BA:411:GLU:N	19:BA:411:GLU:OE1	2.38	0.56
19:BB:273:ARG:NH2	19:BB:323:ARG:O	2.38	0.56
19:BB:388:ARG:CZ	34:BF:601:ATP:H5'2	2.35	0.56
6:h:390:ASP:OD1	6:h:396:ARG:NH1	2.39	0.56
27:BU:41:MET:O	27:BV:44:SER:OG	2.24	0.56
19:BC:208:ILE:O	24:BL:87:LYS:NZ	2.36	0.56
24:BK:80:ARG:NE	24:BK:84:CYS:SG	2.76	0.56
1:a:317:ASP:O	4:f:47:LYS:NZ	2.39	0.56
20:BD:468:TYR:O	20:BD:479:LYS:NZ	2.39	0.56
30:M:201:CDL:O1	30:M:201:CDL:H522	2.06	0.55
15:q:36:ASP:OD1	15:q:68:ARG:NH1	2.40	0.55
4:f:32:ASN:ND2	4:f:60:THR:OG1	2.40	0.55
19:BA:456:TYR:OH	19:BA:517:GLU:OE2	2.25	0.55
3:e:17:ARG:NH1	3:e:21:GLU:OE2	2.39	0.55
19:AA:456:TYR:OH	19:AA:517:GLU:OE2	2.24	0.55
6:H:390:ASP:OD1	6:H:396:ARG:NH1	2.39	0.55
19:AC:359:SER:OG	20:AD:270:ARG:NH2	2.40	0.55
24:BK:153:GLN:HA	24:BK:156:VAL:HG12	1.89	0.55
27:AT:35:ASN:HA	27:AU:36:LEU:HD23	1.88	0.54
19:BC:359:SER:OG	20:BD:270:ARG:NH2	2.40	0.54
2:D:68:TYR:O	2:D:77:ARG:NH1	2.40	0.54
30:A:503:CDL:H441	30:O:201:CDL:H731	1.88	0.54
24:AK:153:GLN:HA	24:AK:156:VAL:HG12	1.89	0.54
20:BE:104:ARG:NH2	20:BE:117:GLY:O	2.41	0.54
20:BF:170:GLY:HA2	34:BF:601:ATP:H5'1	1.88	0.54
19:BB:456:TYR:OH	19:BB:517:GLU:OE2	2.25	0.54
1:a:429:GLU:OE1	7:i:2:ALA:N	2.40	0.54
22:AH:53:ARG:NH1	22:AH:56:GLU:OE2	2.41	0.53
27:AP:60:TYR:HH	27:AP:71:SER:HG	1.55	0.53
19:BA:178:GLN:NE2	19:BA:362:ASP:O	2.40	0.53
27:BR:83:ALA:O	27:BR:87:ALA:N	2.38	0.53
27:BV:41:MET:O	27:BW:44:SER:OG	2.26	0.53
8:j:49:TYR:OH	12:n:113:ARG:NH2	2.41	0.53
19:AB:273:ARG:NH2	19:AB:323:ARG:O	2.41	0.53
22:BH:53:ARG:NH1	22:BH:56:GLU:OE2	2.41	0.53
3:e:89:TRP:CH2	30:e:101:CDL:H731	2.43	0.53
19:AB:161:LEU:N	19:AB:174:VAL:O	2.41	0.53
27:AQ:35:ASN:HA	27:AR:36:LEU:HD23	1.90	0.53
20:BE:65:ASP:OD1	20:BE:68:THR:N	2.41	0.53
1:A:156:LEU:O	1:A:312:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BB:161:LEU:N	19:BB:174:VAL:O	2.41	0.53
20:AE:104:ARG:NH2	20:AE:117:GLY:O	2.42	0.53
20:AF:288:ALA:O	20:AF:290:GLY:N	2.30	0.53
3:e:61:ASP:OD1	8:j:46:ARG:NH1	2.42	0.53
1:A:96:VAL:HG12	30:A:505:CDL:H831	1.90	0.53
21:AG:215:LEU:O	27:AQ:66:ARG:NH2	2.42	0.53
27:AR:90:LEU:O	27:AR:94:LEU:N	2.42	0.53
4:F:32:ASN:ND2	4:F:60:THR:OG1	2.41	0.52
19:AB:442:GLN:NE2	19:AB:444:GLY:O	2.41	0.52
27:AT:35:ASN:ND2	27:AT:104:SER:O	2.43	0.52
2:D:170:GLU:OE1	2:D:170:GLU:N	2.43	0.52
9:k:87:VAL:HA	9:k:90:ILE:HD12	1.91	0.52
19:AC:187:GLN:NE2	34:AC:601:ATP:O3G	2.43	0.52
19:BA:305:GLY:N	19:BA:309:TYR:O	2.43	0.52
15:q:17:ARG:NH2	31:q:101:LMT:O6B	2.42	0.52
19:AA:494:TYR:OH	19:AA:515:ILE:O	2.27	0.52
4:f:185:LEU:HD12	27:AP:90:LEU:HD21	1.90	0.52
20:AE:65:ASP:OD1	20:AE:68:THR:N	2.41	0.52
30:E:101:CDL:H661	30:E:101:CDL:H621	1.91	0.52
30:a:503:CDL:H441	30:o:201:CDL:H731	1.90	0.52
19:BB:305:GLY:N	19:BB:309:TYR:O	2.43	0.52
27:BV:67:GLN:NE2	27:BW:65:ALA:O	2.43	0.52
1:A:429:GLU:OE1	7:I:2:ALA:N	2.43	0.52
20:AE:230:GLY:HA3	20:AE:242:VAL:HG21	1.92	0.52
9:K:87:VAL:HA	9:K:90:ILE:HD12	1.91	0.51
19:AB:305:GLY:N	19:AB:309:TYR:O	2.43	0.51
21:BG:147:GLU:OE2	23:BI:12:ARG:NE	2.43	0.51
20:AD:169:ALA:O	20:AD:347:ARG:NH2	2.43	0.51
27:AR:83:ALA:O	27:AR:87:ALA:N	2.40	0.51
20:AD:116:ARG:NH2	24:AL:31:PHE:O	2.43	0.51
2:d:170:GLU:OE1	2:d:170:GLU:N	2.43	0.51
27:BQ:35:ASN:HA	27:BR:36:LEU:HD23	1.93	0.51
30:e:101:CDL:H661	30:e:101:CDL:H621	1.92	0.51
27:AV:67:GLN:NE2	27:AW:65:ALA:O	2.44	0.51
20:BE:230:GLY:HA3	20:BE:242:VAL:HG21	1.93	0.51
19:AA:224:ARG:NH1	20:AD:337:SER:O	2.44	0.51
27:AU:41:MET:O	27:AV:44:SER:OG	2.29	0.51
20:AF:56:LEU:HD11	20:AF:73:CYS:HB3	1.93	0.51
20:BD:116:ARG:NH2	24:BL:31:PHE:O	2.43	0.51
21:AG:184:LYS:NZ	21:AG:217:GLU:OE1	2.44	0.50
27:BR:90:LEU:O	27:BR:94:LEU:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:69:LEU:HD13	28:b:259:LEU:HB3	1.93	0.50
1:A:317:ASP:O	4:F:47:LYS:NZ	2.40	0.50
2:d:30:GLU:OE2	2:d:144:ARG:NH1	2.44	0.50
21:AG:147:GLU:OE2	23:AI:12:ARG:NE	2.45	0.50
4:f:143:ASP:HA	4:f:146:ILE:HD12	1.93	0.50
19:AC:359:SER:O	20:AD:200:ARG:NH2	2.45	0.50
19:BA:494:TYR:OH	19:BA:515:ILE:O	2.29	0.50
19:AA:178:GLN:NE2	19:AA:362:ASP:O	2.44	0.50
34:AB:601:ATP:O3G	34:AB:601:ATP:O2B	2.29	0.50
20:BD:52:THR:OG1	20:BD:78:ASP:O	2.21	0.50
19:AC:364:GLN:NE2	19:AC:384:LEU:O	2.45	0.49
24:AK:59:ILE:HD11	24:AK:77:VAL:HG21	1.94	0.49
19:BB:442:GLN:NE2	19:BB:444:GLY:O	2.42	0.49
19:AA:305:GLY:N	19:AA:309:TYR:O	2.44	0.49
1:a:51:LYS:O	1:a:52:GLN:NE2	2.46	0.49
3:e:2:SER:N	13:o:93:SER:OG	2.44	0.49
19:BB:221:ILE:N	19:BB:284:ASP:O	2.45	0.49
1:a:310:GLU:O	18:t:18:ARG:NH2	2.46	0.49
4:f:178:ARG:NH2	27:AP:83:ALA:O	2.45	0.49
19:AA:65:ASN:ND2	19:AA:90:GLU:OE1	2.46	0.49
19:BA:295:GLN:NE2	20:BD:297:GLU:OE1	2.45	0.49
24:BK:59:ILE:HD11	24:BK:77:VAL:HG21	1.94	0.49
4:F:143:ASP:HA	4:F:146:ILE:HD12	1.93	0.49
33:n:203:TRT:H7C2	33:n:204:TRT:H14	1.95	0.49
27:AV:41:MET:O	27:AW:44:SER:OG	2.30	0.49
3:E:89:TRP:CH2	30:E:101:CDL:H731	2.48	0.49
30:a:502:CDL:H712	30:d:201:CDL:H311	1.95	0.49
34:BB:601:ATP:O2B	34:BB:601:ATP:O3G	2.29	0.49
1:A:51:LYS:O	1:A:52:GLN:NE2	2.46	0.48
11:M:111:LEU:HD21	30:P:202:CDL:H632	1.94	0.48
1:a:96:VAL:HG12	30:a:505:CDL:H831	1.95	0.48
20:BD:450:ASP:OD1	20:BD:451:PHE:N	2.46	0.48
20:BF:56:LEU:HD11	20:BF:73:CYS:HB3	1.96	0.48
20:BF:406:LEU:O	20:BF:411:LYS:NZ	2.46	0.48
2:D:30:GLU:OE2	2:D:144:ARG:NH1	2.45	0.48
2:d:67:PRO:HD3	2:d:95:THR:HG22	1.96	0.48
19:BC:47:SER:HB2	25:BM:42:LEU:HD21	1.96	0.48
3:E:10:ALA:O	3:E:15:ARG:NH2	2.47	0.48
19:BA:65:ASN:ND2	19:BA:90:GLU:OE1	2.46	0.48
19:BC:364:GLN:NE2	19:BC:384:LEU:O	2.44	0.48
20:AF:59:GLU:OE2	20:AF:241:ARG:NE	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AA:295:GLN:NE2	20:AD:297:GLU:OE1	2.45	0.48
3:e:10:ALA:O	3:e:15:ARG:NH2	2.46	0.48
20:BD:169:ALA:O	20:BD:347:ARG:NH2	2.47	0.48
20:AD:450:ASP:OD1	20:AD:451:PHE:N	2.46	0.48
21:BG:302:THR:N	25:BM:31:TYR:OH	2.47	0.48
15:Q:17:ARG:NH2	31:Q:101:LMT:O6B	2.47	0.47
20:AF:74:MET:HE1	20:AF:241:ARG:HG3	1.96	0.47
20:BF:59:GLU:OE2	20:BF:241:ARG:NE	2.47	0.47
8:J:2:VAL:N	17:S:22:ASP:OD1	2.47	0.47
30:a:503:CDL:H712	30:a:503:CDL:H741	1.69	0.47
19:BC:359:SER:O	20:BD:200:ARG:NH2	2.47	0.47
2:D:67:PRO:HD3	2:D:95:THR:HG22	1.95	0.47
30:a:505:CDL:H751	30:a:505:CDL:H782	1.61	0.47
30:d:201:CDL:H341	9:k:70:VAL:HG13	1.97	0.47
4:f:130:ASN:OD1	4:f:140:ASN:ND2	2.45	0.47
3:E:61:ASP:OD1	8:J:46:ARG:NH1	2.48	0.47
30:e:101:CDL:H621	30:e:101:CDL:H591	1.74	0.47
31:g:201:LMT:O6B	31:g:201:LMT:O4'	2.25	0.47
19:BC:550:GLN:NE2	24:BL:185:PHE:O	2.47	0.47
1:A:310:GLU:O	18:T:18:ARG:NH2	2.47	0.47
30:A:504:CDL:H572	30:A:504:CDL:H541	1.74	0.47
19:AB:498:TYR:HB3	24:AK:177:LEU:HD11	1.95	0.47
20:AE:266:ASP:OD2	20:AE:270:ARG:NH2	2.46	0.47
27:AP:34:ALA:O	27:AQ:36:LEU:HD23	2.14	0.47
25:BM:170:SER:OG	25:BM:172:LEU:O	2.32	0.47
1:A:315:MET:HE2	1:A:343:GLN:HG2	1.97	0.47
27:AP:99:GLU:HG3	27:AQ:36:LEU:HD21	1.96	0.47
27:BV:90:LEU:O	27:BV:94:LEU:N	2.47	0.47
30:A:502:CDL:H712	30:D:201:CDL:H311	1.96	0.47
30:D:201:CDL:H341	9:K:70:VAL:HG13	1.97	0.47
4:F:130:ASN:OD1	4:F:140:ASN:ND2	2.46	0.47
30:a:502:CDL:H742	30:a:502:CDL:H772	1.37	0.47
6:h:310:ARG:NH2	6:h:314:GLU:OE2	2.47	0.47
21:BG:253:ASN:OD1	21:BG:254:GLN:N	2.48	0.47
28:b:240:GLN:OE1	29:c:90:ARG:NH1	2.47	0.47
2:D:149:LEU:HD22	18:T:62:ALA:HB2	1.97	0.47
2:d:143:ARG:NH2	18:t:55:THR:OG1	2.48	0.47
24:AK:174:PRO:O	24:AK:178:LYS:NZ	2.46	0.47
30:a:502:CDL:H791	30:a:502:CDL:H761	1.64	0.47
30:m:201:CDL:H781	30:m:201:CDL:H822	1.97	0.47
4:F:162:ILE:HD12	4:F:166:MET:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:444:THR:N	1:a:447:ASP:OD2	2.47	0.47
8:j:2:VAL:N	17:s:22:ASP:OD1	2.48	0.47
19:AC:47:SER:HB2	25:AM:42:LEU:HD21	1.95	0.47
4:F:178:ARG:NH2	27:BP:83:ALA:O	2.45	0.46
19:AC:550:GLN:NE2	24:AL:185:PHE:O	2.47	0.46
20:AD:238:ALA:O	20:AD:242:VAL:HG23	2.15	0.46
20:BF:105:ILE:HD12	20:BF:114:ASP:HB3	1.97	0.46
27:BW:67:GLN:NE2	27:BX:65:ALA:O	2.49	0.46
1:A:320:ARG:NH2	1:A:337:VAL:O	2.48	0.46
19:AB:499:ASN:ND2	24:AK:133:ASP:OD2	2.47	0.46
21:AG:253:ASN:OD1	21:AG:254:GLN:N	2.48	0.46
19:BB:166:LYS:O	19:BB:170:THR:OG1	2.25	0.46
12:N:46:ASP:OD1	12:N:49:ARG:NH1	2.47	0.46
25:BM:60:ALA:O	25:BM:66:LYS:N	2.48	0.46
30:E:101:CDL:H621	30:E:101:CDL:H591	1.73	0.46
27:AW:67:GLN:NE2	27:AX:65:ALA:O	2.49	0.46
12:N:95:GLN:OE1	12:N:95:GLN:N	2.49	0.46
2:d:149:LEU:HD22	18:t:62:ALA:HB2	1.96	0.46
21:AG:302:THR:N	25:AM:31:TYR:OH	2.49	0.46
24:BK:174:PRO:O	24:BK:178:LYS:NZ	2.46	0.46
20:AF:105:ILE:HD12	20:AF:114:ASP:HB3	1.98	0.46
19:BB:498:TYR:HB3	24:BK:177:LEU:HD11	1.97	0.46
30:A:502:CDL:H761	30:A:502:CDL:H791	1.66	0.46
1:a:315:MET:HE2	1:a:343:GLN:HG2	1.97	0.46
19:AB:395:ASN:O	19:AB:399:LYS:N	2.45	0.46
19:BC:222:GLY:N	19:BC:249:ALA:O	2.47	0.46
20:BF:74:MET:HE1	20:BF:241:ARG:HG3	1.97	0.46
27:BS:35:ASN:HA	27:BT:36:LEU:HD23	1.98	0.46
9:k:100:ILE:O	16:r:74:ARG:NH1	2.49	0.46
1:A:85:MET:HE2	30:A:505:CDL:H132	1.97	0.46
19:AB:221:ILE:N	19:AB:284:ASP:O	2.45	0.46
30:M:204:CDL:H822	30:M:204:CDL:H781	1.99	0.45
2:d:6:LEU:O	13:o:44:LYS:NZ	2.49	0.45
27:AS:35:ASN:HA	27:AT:36:LEU:HD23	1.98	0.45
28:B:317:GLU:OE1	28:B:317:GLU:N	2.50	0.45
19:BA:160:ASN:ND2	19:BA:395:ASN:OD1	2.49	0.45
27:BP:34:ALA:O	27:BQ:36:LEU:HD23	2.16	0.45
12:N:31:ASN:N	12:N:34:THR:OG1	2.47	0.45
24:AL:62:MET:O	24:AL:67:THR:OG1	2.31	0.45
27:AW:84:LEU:HD22	27:AX:53:VAL:HG11	1.97	0.45
19:BB:352:TYR:O	19:BB:356:ASN:ND2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:BE:116:ARG:NH1	24:BJ:31:PHE:O	2.50	0.45
1:a:85:MET:HE2	30:a:505:CDL:H132	1.97	0.45
4:f:21:ILE:HG21	10:l:21:LEU:HD11	1.98	0.45
6:h:154:GLN:O	6:h:182:GLN:NE2	2.49	0.45
12:n:95:GLN:OE1	12:n:95:GLN:N	2.49	0.45
15:q:17:ARG:NH1	16:r:64:LYS:O	2.48	0.45
20:AE:116:ARG:NH1	24:AJ:31:PHE:O	2.49	0.45
20:BD:238:ALA:O	20:BD:242:VAL:HG23	2.15	0.45
21:BG:215:LEU:O	27:BQ:66:ARG:NH2	2.49	0.45
19:AC:186:ARG:NH2	20:AF:362:GLU:O	2.47	0.45
20:BF:199:GLU:O	20:BF:231:GLN:NE2	2.49	0.45
27:BP:60:TYR:HH	27:BP:71:SER:HG	1.60	0.45
27:BP:99:GLU:HG3	27:BQ:36:LEU:HD21	1.99	0.45
30:A:502:CDL:C82	30:O:201:CDL:H742	2.47	0.45
19:AA:160:ASN:ND2	19:AA:395:ASN:OD1	2.50	0.45
20:AF:199:GLU:O	20:AF:231:GLN:NE2	2.49	0.45
2:D:6:LEU:O	13:O:44:LYS:NZ	2.50	0.45
33:N:201:TRT:H7C2	33:N:202:TRT:H14	1.99	0.45
4:f:162:ILE:HD12	4:f:166:MET:HE3	1.98	0.45
19:AB:352:TYR:O	19:AB:356:ASN:ND2	2.50	0.45
20:AF:406:LEU:O	20:AF:411:LYS:NZ	2.45	0.45
1:a:163:GLU:OE1	1:a:163:GLU:N	2.48	0.45
29:c:38:CYS:SG	29:c:39:ASN:N	2.90	0.45
4:F:102:ILE:HD13	8:J:22:HIS:HA	1.98	0.45
27:AV:90:LEU:O	27:AV:94:LEU:N	2.50	0.45
19:BC:493:LYS:O	24:BL:135:ARG:NH1	2.51	0.45
2:D:91:VAL:O	2:D:95:THR:HG23	2.17	0.44
19:AC:305:GLY:N	19:AC:309:TYR:O	2.50	0.44
28:B:57:ALA:O	28:B:60:THR:OG1	2.31	0.44
19:BC:160:ASN:ND2	19:BC:395:ASN:OD1	2.50	0.44
6:H:457:VAL:HG13	28:B:134:THR:HG23	1.99	0.44
30:a:505:CDL:H811	30:a:505:CDL:H781	1.86	0.44
6:h:55:LEU:O	6:h:63:ARG:NH2	2.49	0.44
19:AA:76:LYS:NZ	20:AE:23:GLN:OE1	2.43	0.44
20:BE:247:LEU:HD21	20:BE:305:ARG:HB2	1.99	0.44
30:A:503:CDL:H712	30:A:503:CDL:H741	1.72	0.44
19:AC:160:ASN:ND2	19:AC:395:ASN:OD1	2.50	0.44
9:K:100:ILE:O	16:R:74:ARG:NH1	2.50	0.44
2:d:91:VAL:O	2:d:95:THR:HG23	2.17	0.44
19:BA:181:LEU:HD13	19:BA:357:VAL:HG11	1.99	0.44
19:BB:499:ASN:ND2	24:BK:133:ASP:OD2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLU:OE1	1:A:163:GLU:N	2.49	0.44
12:n:46:ASP:OD1	12:n:49:ARG:NH1	2.49	0.44
19:AA:482:ASP:OD1	19:AA:523:TYR:OH	2.35	0.44
19:AC:27:GLN:NE2	19:AC:28:LYS:O	2.51	0.44
25:AM:60:ALA:O	25:AM:66:LYS:N	2.48	0.44
19:BB:250:THR:O	19:BB:258:GLN:NE2	2.50	0.44
20:BD:418:ARG:NE	20:BD:464:GLU:OE2	2.51	0.44
24:BL:62:MET:O	24:BL:67:THR:OG1	2.31	0.44
28:b:317:GLU:N	28:b:317:GLU:OE1	2.50	0.44
19:AC:493:LYS:O	24:AL:135:ARG:NH1	2.51	0.44
20:AD:418:ARG:NE	20:AD:464:GLU:OE2	2.51	0.44
2:D:37:ARG:O	2:D:40:SER:OG	2.35	0.44
30:E:101:CDL:H661	30:E:101:CDL:H591	2.00	0.44
21:AG:50:ARG:NH2	22:AH:122:ASP:OD1	2.50	0.44
15:Q:17:ARG:NH1	16:R:64:LYS:O	2.48	0.44
30:a:502:CDL:C82	30:o:201:CDL:H742	2.47	0.44
19:AC:155:GLN:N	19:AC:326:MET:O	2.50	0.44
27:AR:56:CYS:O	27:AR:59:SER:OG	2.36	0.44
19:BC:155:GLN:N	19:BC:326:MET:O	2.50	0.44
21:BG:45:ARG:NH2	21:BG:46:ASP:OD2	2.50	0.44
2:D:143:ARG:NH2	18:T:55:THR:OG1	2.49	0.44
11:M:104:TRP:CH2	30:M:205:CDL:H531	2.52	0.44
19:AA:181:LEU:HD13	19:AA:357:VAL:HG11	2.00	0.44
19:BC:281:LEU:HD11	19:BC:336:LEU:HD12	2.00	0.44
20:BF:168:GLY:O	20:BF:173:LYS:NZ	2.51	0.44
19:AC:281:LEU:HD11	19:AC:336:LEU:HD12	2.00	0.43
24:AK:84:CYS:O	24:AK:97:LYS:NZ	2.32	0.43
6:H:310:ARG:NH2	6:H:314:GLU:OE2	2.47	0.43
33:g:202:TRT:H3C2	33:g:202:TRT:H8C1	2.00	0.43
5:G:32:PRO:HA	5:G:35:LEU:HD12	1.99	0.43
6:H:55:LEU:O	6:H:63:ARG:NH2	2.49	0.43
5:g:59:ASN:ND2	6:h:220:GLU:OE1	2.52	0.43
19:BC:27:GLN:NE2	19:BC:28:LYS:O	2.51	0.43
20:AE:247:LEU:HD21	20:AE:305:ARG:HB2	1.99	0.43
30:A:503:CDL:H732	30:A:503:CDL:H771	2.01	0.43
6:H:154:GLN:O	6:H:182:GLN:NE2	2.51	0.43
30:a:504:CDL:H541	30:a:504:CDL:H572	1.74	0.43
8:j:62:HIS:O	8:j:62:HIS:ND1	2.52	0.43
24:AJ:174:PRO:HD2	24:AJ:177:LEU:HD12	2.01	0.43
19:BA:482:ASP:OD1	19:BA:523:TYR:OH	2.36	0.43
5:g:21:LEU:HD22	5:g:25:ASN:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:AG:45:ARG:NH2	21:AG:46:ASP:OD2	2.51	0.43
28:B:69:LEU:HD13	28:B:259:LEU:HB3	2.00	0.43
27:BS:35:ASN:ND2	27:BS:104:SER:O	2.52	0.43
3:E:84:HIS:CE1	30:E:101:CDL:H622	2.53	0.43
19:BB:395:ASN:O	19:BB:399:LYS:N	2.46	0.43
20:BF:194:PHE:HB2	20:BF:227:LEU:HD23	2.01	0.43
21:BG:50:ARG:NH2	22:BH:122:ASP:OD1	2.51	0.43
24:BJ:108:MET:O	24:BJ:112:SER:OG	2.36	0.43
14:P:66:ASN:OD1	14:P:69:ARG:NH2	2.48	0.43
3:e:84:HIS:CE1	30:e:101:CDL:H622	2.53	0.43
19:BA:217:VAL:HG23	19:BA:279:ILE:HD11	2.01	0.43
3:e:66:ARG:NH2	13:o:76:GLU:O	2.52	0.43
19:AB:558:CYS:HA	19:AB:561:THR:HG22	2.01	0.43
20:AE:149:LYS:NZ	20:AE:423:PHE:O	2.48	0.43
19:BA:76:LYS:NZ	20:BE:23:GLN:OE1	2.46	0.43
19:AC:224:ARG:NH1	20:AF:338:HIS:O	2.52	0.42
19:AC:462:TYR:HB3	19:AC:528:THR:HG21	2.01	0.42
24:AJ:108:MET:O	24:AJ:112:SER:OG	2.36	0.42
27:AO:35:ASN:HA	27:AP:36:LEU:HD23	2.01	0.42
27:BR:95:ILE:O	27:BR:99:GLU:N	2.51	0.42
20:AF:188:HIS:O	28:b:202:ARG:NH1	2.52	0.42
19:BA:68:ASN:N	19:BA:86:ASP:OD1	2.52	0.42
30:A:502:CDL:H742	30:A:502:CDL:H772	1.36	0.42
1:a:320:ARG:NH2	1:a:337:VAL:O	2.48	0.42
27:AR:95:ILE:O	27:AR:99:GLU:N	2.53	0.42
19:BC:224:ARG:NH1	20:BF:338:HIS:O	2.51	0.42
1:a:336:PHE:O	30:a:501:CDL:H721	2.19	0.42
24:BL:80:ARG:NE	24:BL:84:CYS:SG	2.93	0.42
8:J:62:HIS:ND1	8:J:62:HIS:O	2.52	0.42
8:j:14:PHE:O	8:j:21:TRP:NE1	2.50	0.42
19:AB:557:ALA:HB1	24:AK:192:ILE:HG21	2.02	0.42
24:AK:26:LYS:NZ	24:AK:34:GLU:OE2	2.46	0.42
25:AM:167:HIS:O	25:AM:170:SER:OG	2.32	0.42
19:BA:212:ASN:ND2	24:BJ:103:ASP:OD2	2.45	0.42
1:A:444:THR:N	1:A:447:ASP:OD2	2.49	0.42
1:a:447:ASP:O	1:a:465:ARG:NH1	2.53	0.42
14:p:66:ASN:OD1	14:p:69:ARG:NH2	2.48	0.42
20:AE:56:LEU:HD11	20:AE:73:CYS:SG	2.59	0.42
20:BF:225:CYS:SG	20:BF:226:VAL:N	2.91	0.42
24:BJ:59:ILE:HA	24:BJ:62:MET:HE3	2.00	0.42
27:AQ:41:MET:HE1	27:AR:41:MET:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:225:VAL:HG22	31:F:302:LMT:H32	2.02	0.42
5:g:32:PRO:HA	5:g:35:LEU:HD12	2.02	0.42
19:AC:352:TYR:O	19:AC:356:ASN:ND2	2.53	0.42
25:AM:170:SER:OG	25:AM:172:LEU:O	2.38	0.42
29:C:19:LEU:HD21	29:C:52:LEU:HD22	2.01	0.42
1:A:336:PHE:O	30:A:501:CDL:H721	2.20	0.42
33:G:201:TRT:H8C1	33:G:201:TRT:H3C2	2.01	0.42
4:f:193:PHE:CZ	27:AO:90:LEU:HD23	2.54	0.42
30:m:201:CDL:H711	30:m:201:CDL:H522	2.02	0.42
19:AA:68:ASN:N	19:AA:86:ASP:OD1	2.52	0.42
20:AD:324:ALA:O	21:AG:8:ARG:NH1	2.53	0.42
21:AG:41:ARG:NH1	21:AG:234:ASN:OD1	2.53	0.42
19:BB:557:ALA:HB1	24:BK:192:ILE:HG21	2.02	0.42
19:BB:558:CYS:HA	19:BB:561:THR:HG22	2.01	0.42
19:BC:462:TYR:HB3	19:BC:528:THR:HG21	2.02	0.42
4:f:186:HIS:CE1	4:f:228:TYR:HH	2.33	0.42
4:f:225:VAL:HG22	31:g:201:LMT:H32	2.01	0.42
27:AQ:95:ILE:O	27:AQ:99:GLU:N	2.52	0.42
20:BF:331:ALA:HB3	20:BF:332:PRO:HD3	2.02	0.42
24:BJ:174:PRO:HD2	24:BJ:177:LEU:HD12	2.01	0.42
3:E:53:ARG:NH2	4:F:1:MET:O	2.53	0.41
20:AF:247:LEU:HD11	20:AF:302:LEU:HD12	2.02	0.41
28:B:202:ARG:NH1	20:BF:188:HIS:O	2.53	0.41
8:J:14:PHE:O	8:J:21:TRP:NE1	2.51	0.41
30:M:205:CDL:OB4	11:m:56:ARG:NH2	2.48	0.41
19:AC:185:ASP:O	19:AC:190:LYS:NZ	2.54	0.41
29:C:38:CYS:SG	29:C:39:ASN:N	2.93	0.41
20:BD:371:ASP:OD1	20:BD:372:ALA:N	2.53	0.41
30:e:101:CDL:H661	30:e:101:CDL:H591	2.02	0.41
30:e:101:CDL:H572	30:e:101:CDL:H541	1.80	0.41
19:BC:186:ARG:NH2	20:BF:362:GLU:O	2.49	0.41
20:BE:56:LEU:HD11	20:BE:73:CYS:SG	2.60	0.41
19:AA:217:VAL:HG23	19:AA:279:ILE:HD11	2.01	0.41
19:AB:448:PHE:CE2	19:AB:452:ILE:HD11	2.56	0.41
28:B:266:PHE:HB3	28:B:283:ALA:HB1	2.03	0.41
19:BC:352:TYR:O	19:BC:356:ASN:ND2	2.53	0.41
20:BD:289:VAL:O	20:BD:289:VAL:HG12	2.21	0.41
21:BG:41:ARG:NE	22:BH:55:ASP:OD2	2.46	0.41
27:BW:84:LEU:HD22	27:BX:53:VAL:HG11	2.03	0.41
28:b:266:PHE:HB3	28:b:283:ALA:HB1	2.02	0.41
1:a:320:ARG:NH2	30:a:503:CDL:OB3	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:37:ARG:O	2:d:40:SER:OG	2.37	0.41
20:AF:194:PHE:HB2	20:AF:227:LEU:HD23	2.03	0.41
19:BC:305:GLY:N	19:BC:309:TYR:O	2.52	0.41
29:c:19:LEU:HD21	29:c:52:LEU:HD22	2.01	0.41
3:E:53:ARG:NH1	4:F:4:SER:O	2.54	0.41
30:E:101:CDL:H572	30:E:101:CDL:H541	1.77	0.41
30:M:201:CDL:H552	11:m:104:TRP:HZ3	1.85	0.41
13:O:81:ALA:HB3	13:O:86:ASP:HB2	2.03	0.41
12:n:31:ASN:N	12:n:34:THR:OG1	2.47	0.41
27:AQ:51:ILE:HG23	27:AR:51:ILE:HD13	2.01	0.41
20:BE:266:ASP:OD2	20:BE:270:ARG:NH2	2.49	0.41
23:BI:48:ASP:N	23:BI:51:ALA:O	2.45	0.41
19:AC:217:VAL:HG23	19:AC:279:ILE:HD11	2.03	0.41
20:AD:289:VAL:HG12	20:AD:289:VAL:O	2.21	0.41
20:BD:201:THR:O	20:BD:205:THR:HG23	2.21	0.41
27:BQ:90:LEU:O	27:BQ:94:LEU:N	2.48	0.41
4:F:21:ILE:HG21	10:L:21:LEU:HD11	2.03	0.41
8:j:50:ILE:N	12:n:118:GLY:O	2.54	0.41
32:k:201:LPP:H401	32:k:201:LPP:H371	1.25	0.41
19:BB:448:PHE:CE2	19:BB:452:ILE:HD11	2.56	0.41
3:E:66:ARG:NH2	13:O:76:GLU:O	2.53	0.41
4:F:261:ASN:OD1	4:F:262:LYS:N	2.54	0.41
1:a:177:GLU:OE1	1:a:192:LYS:NZ	2.32	0.41
30:a:502:CDL:H822	30:o:201:CDL:C75	2.51	0.41
6:h:420:HIS:CD2	6:h:432:THR:HG1	2.29	0.41
7:i:59:GLU:OE1	7:i:64:TRP:N	2.51	0.41
13:o:81:ALA:HB3	13:o:86:ASP:HB2	2.03	0.41
19:AB:179:ARG:NH1	19:AB:360:ILE:O	2.52	0.41
20:AD:334:THR:O	20:AD:338:HIS:ND1	2.51	0.41
20:AE:238:ALA:O	20:AE:242:VAL:HG23	2.21	0.41
21:AG:205:SER:HB2	21:AG:208:MET:HE2	2.03	0.41
24:AJ:59:ILE:HA	24:AJ:62:MET:HE3	2.01	0.41
19:BB:191:THR:OG1	34:BB:601:ATP:O2B	2.39	0.41
21:BG:205:SER:HB2	21:BG:208:MET:HE2	2.03	0.41
28:b:183:ASP:OD1	28:b:235:ASN:ND2	2.53	0.41
5:G:21:LEU:HD22	5:G:25:ASN:HB3	2.02	0.41
27:AP:60:TYR:OH	27:AP:71:SER:OG	2.29	0.41
20:BE:238:ALA:O	20:BE:242:VAL:HG23	2.21	0.41
4:F:266:ASN:N	4:F:266:ASN:OD1	2.54	0.40
30:r:101:CDL:H751	30:r:101:CDL:H572	2.03	0.40
19:AC:345:LEU:HD23	20:AF:328:THR:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AF:331:ALA:HB3	20:AF:332:PRO:HD3	2.02	0.40
29:C:31:ASP:HB3	29:C:33:VAL:HG23	2.04	0.40
4:f:266:ASN:OD1	4:f:266:ASN:N	2.54	0.40
30:A:505:CDL:H782	30:A:505:CDL:H751	1.59	0.40
3:E:71:ASP:OD1	3:E:71:ASP:N	2.55	0.40
8:J:70:ASP:HB3	8:J:73:LYS:HB3	2.03	0.40
4:f:261:ASN:OD1	4:f:262:LYS:N	2.55	0.40
20:AF:374:ASP:N	20:AF:374:ASP:OD1	2.55	0.40
28:B:44:PRO:O	28:B:67:TYR:OH	2.33	0.40
19:BC:250:THR:N	19:BC:253:ASP:OD2	2.48	0.40
28:b:57:ALA:O	28:b:60:THR:OG1	2.31	0.40
1:A:21:ASN:HB3	1:A:81:LEU:HD22	2.04	0.40
4:f:102:ILE:HD13	8:j:22:HIS:HA	2.02	0.40
19:AC:250:THR:N	19:AC:253:ASP:OD2	2.48	0.40
20:AD:371:ASP:OD1	20:AD:372:ALA:N	2.54	0.40
19:BC:185:ASP:O	19:BC:190:LYS:NZ	2.54	0.40
20:BD:65:ASP:OD1	20:BD:66:THR:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	484/487 (99%)	468 (97%)	16 (3%)	0	100	100
1	a	484/487 (99%)	468 (97%)	16 (3%)	0	100	100
2	D	184/187 (98%)	179 (97%)	5 (3%)	0	100	100
2	d	184/187 (98%)	179 (97%)	5 (3%)	0	100	100
3	E	94/97 (97%)	91 (97%)	3 (3%)	0	100	100
3	e	94/97 (97%)	91 (97%)	3 (3%)	0	100	100
4	F	272/274 (99%)	261 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	f	272/274 (99%)	262 (96%)	10 (4%)	0	100	100
5	G	109/112 (97%)	109 (100%)	0	0	100	100
5	g	109/112 (97%)	109 (100%)	0	0	100	100
6	H	458/476 (96%)	447 (98%)	10 (2%)	1 (0%)	43	77
6	h	458/476 (96%)	445 (97%)	10 (2%)	3 (1%)	18	55
7	I	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
7	i	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
8	J	101/104 (97%)	98 (97%)	3 (3%)	0	100	100
8	j	101/104 (97%)	98 (97%)	3 (3%)	0	100	100
9	K	101/113 (89%)	100 (99%)	1 (1%)	0	100	100
9	k	101/113 (89%)	100 (99%)	1 (1%)	0	100	100
10	L	55/57 (96%)	51 (93%)	4 (7%)	0	100	100
10	l	55/57 (96%)	51 (93%)	4 (7%)	0	100	100
11	M	164/169 (97%)	164 (100%)	0	0	100	100
11	m	164/169 (97%)	164 (100%)	0	0	100	100
12	N	129/137 (94%)	128 (99%)	1 (1%)	0	100	100
12	n	129/137 (94%)	126 (98%)	3 (2%)	0	100	100
13	O	98/116 (84%)	94 (96%)	4 (4%)	0	100	100
13	o	98/116 (84%)	94 (96%)	4 (4%)	0	100	100
14	P	112/120 (93%)	109 (97%)	3 (3%)	0	100	100
14	p	112/120 (93%)	109 (97%)	3 (3%)	0	100	100
15	Q	87/90 (97%)	79 (91%)	8 (9%)	0	100	100
15	q	87/90 (97%)	79 (91%)	8 (9%)	0	100	100
16	R	67/78 (86%)	66 (98%)	1 (2%)	0	100	100
16	r	67/78 (86%)	66 (98%)	1 (2%)	0	100	100
17	S	63/74 (85%)	63 (100%)	0	0	100	100
17	s	63/74 (85%)	63 (100%)	0	0	100	100
18	T	64/66 (97%)	64 (100%)	0	0	100	100
18	t	64/66 (97%)	64 (100%)	0	0	100	100
19	AA	522/561 (93%)	502 (96%)	20 (4%)	0	100	100
19	AB	522/561 (93%)	497 (95%)	25 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	AC	525/561 (94%)	505 (96%)	20 (4%)	0	100	100
19	BA	522/561 (93%)	501 (96%)	21 (4%)	0	100	100
19	BB	522/561 (93%)	499 (96%)	23 (4%)	0	100	100
19	BC	525/561 (94%)	506 (96%)	19 (4%)	0	100	100
20	AD	485/501 (97%)	468 (96%)	15 (3%)	2 (0%)	30	66
20	AE	485/501 (97%)	459 (95%)	25 (5%)	1 (0%)	43	77
20	AF	485/501 (97%)	467 (96%)	16 (3%)	2 (0%)	30	66
20	BD	485/501 (97%)	466 (96%)	17 (4%)	2 (0%)	30	66
20	BE	485/501 (97%)	460 (95%)	24 (5%)	1 (0%)	43	77
20	BF	485/501 (97%)	467 (96%)	16 (3%)	2 (0%)	30	66
21	AG	301/306 (98%)	294 (98%)	7 (2%)	0	100	100
21	BG	301/306 (98%)	294 (98%)	7 (2%)	0	100	100
22	AH	158/176 (90%)	148 (94%)	10 (6%)	0	100	100
22	BH	158/176 (90%)	147 (93%)	11 (7%)	0	100	100
23	AI	64/76 (84%)	60 (94%)	4 (6%)	0	100	100
23	BI	64/76 (84%)	60 (94%)	4 (6%)	0	100	100
24	AJ	168/192 (88%)	166 (99%)	2 (1%)	0	100	100
24	AK	168/192 (88%)	167 (99%)	1 (1%)	0	100	100
24	AL	168/192 (88%)	165 (98%)	3 (2%)	0	100	100
24	BJ	168/192 (88%)	165 (98%)	3 (2%)	0	100	100
24	BK	168/192 (88%)	167 (99%)	1 (1%)	0	100	100
24	BL	168/192 (88%)	165 (98%)	3 (2%)	0	100	100
25	AM	241/267 (90%)	230 (95%)	10 (4%)	1 (0%)	30	66
25	BM	241/267 (90%)	230 (95%)	10 (4%)	1 (0%)	30	66
26	AN	47/103 (46%)	46 (98%)	1 (2%)	0	100	100
26	BN	47/103 (46%)	46 (98%)	1 (2%)	0	100	100
27	AO	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
27	AP	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
27	AQ	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
27	AR	79/104 (76%)	77 (98%)	2 (2%)	0	100	100
27	AS	79/104 (76%)	77 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	AT	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
27	AU	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
27	AV	79/104 (76%)	77 (98%)	2 (2%)	0	100	100
27	AW	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
27	AX	79/104 (76%)	76 (96%)	3 (4%)	0	100	100
27	BO	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
27	BP	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
27	BQ	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
27	BR	79/104 (76%)	77 (98%)	2 (2%)	0	100	100
27	BS	79/104 (76%)	77 (98%)	2 (2%)	0	100	100
27	BT	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
27	BU	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
27	BV	79/104 (76%)	77 (98%)	2 (2%)	0	100	100
27	BW	79/104 (76%)	78 (99%)	1 (1%)	0	100	100
27	BX	79/104 (76%)	76 (96%)	3 (4%)	0	100	100
28	B	322/338 (95%)	297 (92%)	24 (8%)	1 (0%)	36	71
28	b	322/338 (95%)	299 (93%)	23 (7%)	0	100	100
29	C	155/169 (92%)	147 (95%)	8 (5%)	0	100	100
29	c	155/169 (92%)	147 (95%)	8 (5%)	0	100	100
All	All	16686/18184 (92%)	16110 (96%)	559 (3%)	17 (0%)	49	83

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	h	38	THR
20	AD	289	VAL
20	AF	289	VAL
25	AM	148	ALA
28	B	120	LYS
20	BD	289	VAL
20	BF	289	VAL
25	BM	148	ALA
6	h	37	THR
20	AD	288	ALA
20	AF	288	ALA

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Mol	Chain	Res	Type
20	BD	288	ALA
20	BF	288	ALA
6	h	331	PRO
20	AE	289	VAL
20	BE	289	VAL
6	H	331	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/427 (100%)	426 (100%)	0	100	100
1	a	426/427 (100%)	426 (100%)	0	100	100
2	D	159/160 (99%)	159 (100%)	0	100	100
2	d	159/160 (99%)	159 (100%)	0	100	100
3	E	81/82 (99%)	81 (100%)	0	100	100
3	e	81/82 (99%)	81 (100%)	0	100	100
4	F	259/259 (100%)	258 (100%)	1 (0%)	84	82
4	f	259/259 (100%)	259 (100%)	0	100	100
5	G	98/99 (99%)	98 (100%)	0	100	100
5	g	98/99 (99%)	98 (100%)	0	100	100
6	H	400/414 (97%)	400 (100%)	0	100	100
6	h	400/414 (97%)	400 (100%)	0	100	100
7	I	82/83 (99%)	82 (100%)	0	100	100
7	i	82/83 (99%)	82 (100%)	0	100	100
8	J	94/95 (99%)	94 (100%)	0	100	100
8	j	94/95 (99%)	94 (100%)	0	100	100
9	K	89/97 (92%)	89 (100%)	0	100	100
9	k	89/97 (92%)	89 (100%)	0	100	100
10	L	56/56 (100%)	56 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	l	56/56 (100%)	56 (100%)	0	100	100
11	M	137/140 (98%)	137 (100%)	0	100	100
11	m	137/140 (98%)	137 (100%)	0	100	100
12	N	114/119 (96%)	114 (100%)	0	100	100
12	n	114/119 (96%)	114 (100%)	0	100	100
13	O	90/103 (87%)	90 (100%)	0	100	100
13	o	90/103 (87%)	90 (100%)	0	100	100
14	P	96/99 (97%)	96 (100%)	0	100	100
14	p	96/99 (97%)	96 (100%)	0	100	100
15	Q	82/83 (99%)	82 (100%)	0	100	100
15	q	82/83 (99%)	82 (100%)	0	100	100
16	R	59/67 (88%)	59 (100%)	0	100	100
16	r	59/67 (88%)	59 (100%)	0	100	100
17	S	59/68 (87%)	59 (100%)	0	100	100
17	s	59/68 (87%)	59 (100%)	0	100	100
18	T	54/54 (100%)	54 (100%)	0	100	100
18	t	54/54 (100%)	54 (100%)	0	100	100
19	AA	450/474 (95%)	450 (100%)	0	100	100
19	AB	450/474 (95%)	450 (100%)	0	100	100
19	AC	452/474 (95%)	452 (100%)	0	100	100
19	BA	450/474 (95%)	450 (100%)	0	100	100
19	BB	450/474 (95%)	450 (100%)	0	100	100
19	BC	452/474 (95%)	452 (100%)	0	100	100
20	AD	397/405 (98%)	397 (100%)	0	100	100
20	AE	397/405 (98%)	397 (100%)	0	100	100
20	AF	397/405 (98%)	397 (100%)	0	100	100
20	BD	397/405 (98%)	397 (100%)	0	100	100
20	BE	397/405 (98%)	397 (100%)	0	100	100
20	BF	397/405 (98%)	397 (100%)	0	100	100
21	AG	261/264 (99%)	261 (100%)	0	100	100
21	BG	261/264 (99%)	261 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	AH	131/146 (90%)	131 (100%)	0	100	100
22	BH	131/146 (90%)	131 (100%)	0	100	100
23	AI	58/66 (88%)	58 (100%)	0	100	100
23	BI	58/66 (88%)	58 (100%)	0	100	100
24	AJ	132/151 (87%)	132 (100%)	0	100	100
24	AK	132/151 (87%)	132 (100%)	0	100	100
24	AL	132/151 (87%)	132 (100%)	0	100	100
24	BJ	132/151 (87%)	132 (100%)	0	100	100
24	BK	132/151 (87%)	132 (100%)	0	100	100
24	BL	132/151 (87%)	132 (100%)	0	100	100
25	AM	202/221 (91%)	202 (100%)	0	100	100
25	BM	202/221 (91%)	202 (100%)	0	100	100
26	AN	44/87 (51%)	44 (100%)	0	100	100
26	BN	44/87 (51%)	44 (100%)	0	100	100
27	AO	58/76 (76%)	58 (100%)	0	100	100
27	AP	58/76 (76%)	58 (100%)	0	100	100
27	AQ	58/76 (76%)	58 (100%)	0	100	100
27	AR	58/76 (76%)	58 (100%)	0	100	100
27	AS	58/76 (76%)	58 (100%)	0	100	100
27	AT	58/76 (76%)	58 (100%)	0	100	100
27	AU	58/76 (76%)	58 (100%)	0	100	100
27	AV	58/76 (76%)	58 (100%)	0	100	100
27	AW	58/76 (76%)	58 (100%)	0	100	100
27	AX	58/76 (76%)	58 (100%)	0	100	100
27	BO	58/76 (76%)	58 (100%)	0	100	100
27	BP	58/76 (76%)	58 (100%)	0	100	100
27	BQ	58/76 (76%)	58 (100%)	0	100	100
27	BR	58/76 (76%)	58 (100%)	0	100	100
27	BS	58/76 (76%)	58 (100%)	0	100	100
27	BT	58/76 (76%)	58 (100%)	0	100	100
27	BU	58/76 (76%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	BV	58/76 (76%)	58 (100%)	0	100	100
27	BW	58/76 (76%)	58 (100%)	0	100	100
27	BX	58/76 (76%)	58 (100%)	0	100	100
28	B	251/259 (97%)	251 (100%)	0	100	100
28	b	251/259 (97%)	251 (100%)	0	100	100
29	C	128/137 (93%)	128 (100%)	0	100	100
29	c	128/137 (93%)	128 (100%)	0	100	100
All	All	14058/15070 (93%)	14057 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	8	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	343	GLN
2	D	31	ASN
3	E	28	GLN
4	F	142	ASN
5	G	59	ASN
5	G	99	GLN
6	H	346	HIS
6	H	347	ASN
6	H	370	GLN
7	I	96	HIS
8	J	59	HIS
9	K	34	GLN
10	L	55	ASN
12	N	62	HIS
12	N	65	ASN
15	Q	65	ASN
15	Q	80	HIS
1	a	343	GLN
2	d	7	HIS
2	d	31	ASN
4	f	32	ASN

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Mol	Chain	Res	Type
4	f	142	ASN
5	g	59	ASN
5	g	99	GLN
6	h	346	HIS
6	h	347	ASN
6	h	370	GLN
6	h	392	HIS
8	j	44	ASN
8	j	59	HIS
10	l	55	ASN
12	n	62	HIS
12	n	65	ASN
15	q	80	HIS
19	AB	289	GLN
19	AB	512	ASN
19	AC	160	ASN
19	AC	232	HIS
19	AC	492	ASN
20	AE	188	HIS
20	AE	292	GLN
20	AE	338	HIS
20	AF	426	GLN
20	AF	443	GLN
25	AM	197	ASN
27	AR	67	GLN
27	AS	32	ASN
27	AT	32	ASN
28	B	235	ASN
19	BB	289	GLN
19	BB	512	ASN
19	BC	187	GLN
19	BC	232	HIS
20	BE	188	HIS
20	BF	426	GLN
20	BF	443	GLN
22	BH	136	HIS
25	BM	197	ASN
27	BP	35	ASN
27	BR	32	ASN
27	BR	67	GLN
27	BS	32	ASN
27	BT	32	ASN

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Mol	Chain	Res	Type
28	b	235	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 83 ligands modelled in this entry, 10 are monoatomic - leaving 73 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	$\# Z > 2$
30	CDL	P	202	-	97,97,99	0.90	8 (8%)	103,109,111	0.99	4 (3%)
32	LPP	o	202	-	22,22,43	1.43	4 (18%)	25,27,48	1.27	2 (8%)
30	CDL	a	502	-	80,80,99	0.98	8 (10%)	86,92,111	1.12	4 (4%)
32	LPP	F	301	-	23,23,43	1.40	4 (17%)	26,28,48	1.17	2 (7%)
32	LPP	f	301	-	23,23,43	1.40	5 (21%)	26,28,48	1.16	2 (7%)
34	ATP	BF	601	35	32,33,33	1.37	4 (12%)	48,52,52	1.81	11 (22%)
33	TRT	N	202	-	25,25,25	0.60	0	33,33,33	1.00	1 (3%)
33	TRT	M	203	-	25,25,25	0.56	0	33,33,33	0.94	2 (6%)
31	LMT	d	202	-	36,36,36	1.13	6 (16%)	47,47,47	0.92	1 (2%)
32	LPP	o	203	-	31,31,43	1.28	5 (16%)	34,36,48	1.02	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	TRT	AR	201	-	25,25,25	0.55	0	33,33,33	0.92	2 (6%)
33	TRT	BR	201	-	25,25,25	0.54	0	33,33,33	0.93	2 (6%)
30	CDL	A	502	-	80,80,99	0.99	8 (10%)	86,92,111	1.13	4 (4%)
33	TRT	m	202	-	25,25,25	0.58	0	33,33,33	0.68	0
32	LPP	K	201	-	30,30,43	1.28	4 (13%)	33,35,48	1.21	2 (6%)
32	LPP	k	201	-	30,30,43	1.28	4 (13%)	33,35,48	1.21	2 (6%)
30	CDL	A	505	-	84,84,99	0.97	8 (9%)	90,96,111	0.99	4 (4%)
30	CDL	M	204	-	76,76,99	1.00	8 (10%)	82,88,111	1.12	4 (4%)
33	TRT	n	203	-	25,25,25	0.52	0	33,33,33	1.05	3 (9%)
34	ATP	BB	601	35	32,33,33	1.41	4 (12%)	48,52,52	1.80	11 (22%)
34	ATP	AF	601	35	32,33,33	1.37	4 (12%)	48,52,52	1.82	11 (22%)
31	LMT	q	101	-	36,36,36	1.14	6 (16%)	47,47,47	1.01	2 (4%)
30	CDL	D	201	-	90,90,99	0.94	7 (7%)	96,102,111	1.03	4 (4%)
30	CDL	a	503	-	80,80,99	0.98	8 (10%)	85,91,111	1.08	4 (4%)
30	CDL	o	201	-	64,64,99	1.09	8 (12%)	70,76,111	1.08	4 (5%)
30	CDL	A	501	-	80,80,99	0.97	8 (10%)	86,92,111	1.09	5 (5%)
32	LPP	I	101	-	43,43,43	1.15	3 (6%)	46,48,48	1.02	2 (4%)
32	LPP	O	202	-	22,22,43	1.44	4 (18%)	25,27,48	1.25	2 (8%)
32	LPP	O	203	-	31,31,43	1.28	5 (16%)	34,36,48	1.03	2 (5%)
31	LMT	D	202	-	36,36,36	1.14	6 (16%)	47,47,47	0.92	1 (2%)
33	TRT	N	201	-	25,25,25	0.51	0	33,33,33	1.04	3 (9%)
30	CDL	e	101	-	62,62,99	1.10	8 (12%)	68,74,111	1.14	4 (5%)
33	TRT	g	202	-	25,25,25	0.52	0	33,33,33	0.81	1 (3%)
33	TRT	p	202	-	25,25,25	1.21	3 (12%)	33,33,33	4.55	9 (27%)
33	TRT	AE	600	-	25,25,25	0.67	1 (4%)	33,33,33	1.04	1 (3%)
30	CDL	E	101	-	62,62,99	1.10	8 (12%)	68,74,111	1.13	4 (5%)
34	ATP	AA	601	35	32,33,33	1.39	4 (12%)	48,52,52	1.80	10 (20%)
32	LPP	i	101	-	43,43,43	1.15	3 (6%)	46,48,48	1.02	2 (4%)
34	ATP	AC	601	35	32,33,33	1.37	4 (12%)	48,52,52	1.78	11 (22%)
33	TRT	G	202	-	25,25,25	0.61	0	33,33,33	0.82	1 (3%)
30	CDL	a	505	-	84,84,99	0.96	7 (8%)	90,96,111	0.98	4 (4%)
33	TRT	n	204	-	25,25,25	0.59	0	33,33,33	1.04	1 (3%)
33	TRT	G	201	-	25,25,25	0.52	0	33,33,33	0.81	1 (3%)
30	CDL	A	503	-	80,80,99	0.98	8 (10%)	85,91,111	1.08	4 (4%)
34	ATP	BA	601	35	32,33,33	1.38	4 (12%)	48,52,52	1.80	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	N	204	-	36,36,36	1.21	6 (16%)	47,47,47	0.97	2 (4%)
30	CDL	M	205	-	52,52,99	1.21	8 (15%)	58,64,111	1.26	4 (6%)
30	CDL	d	201	-	90,90,99	0.94	7 (7%)	96,102,111	1.03	4 (4%)
31	LMT	Q	101	-	36,36,36	1.15	6 (16%)	47,47,47	1.02	2 (4%)
33	TRT	BE	600	-	25,25,25	0.66	1 (4%)	33,33,33	1.05	1 (3%)
30	CDL	R	101	-	75,75,99	1.01	8 (10%)	81,87,111	1.15	4 (4%)
34	ATP	AB	601	35	32,33,33	1.41	4 (12%)	48,52,52	1.79	11 (22%)
33	TRT	P	203	-	25,25,25	1.23	3 (12%)	33,33,33	4.53	9 (27%)
30	CDL	P	201	-	47,47,99	1.26	8 (17%)	53,59,111	1.33	5 (9%)
34	ATP	BC	601	35	32,33,33	1.37	4 (12%)	48,52,52	1.78	11 (22%)
30	CDL	O	201	-	64,64,99	1.09	8 (12%)	70,76,111	1.07	4 (5%)
30	CDL	M	201	-	52,52,99	1.21	8 (15%)	58,64,111	1.28	4 (6%)
32	LPP	n	201	-	25,25,43	1.36	3 (12%)	28,30,48	1.28	2 (7%)
30	CDL	a	504	-	62,62,99	1.11	7 (11%)	68,74,111	1.21	4 (5%)
32	LPP	N	203	-	25,25,43	1.35	3 (12%)	28,30,48	1.28	2 (7%)
30	CDL	A	504	-	62,62,99	1.11	7 (11%)	68,74,111	1.21	4 (5%)
30	CDL	a	501	-	80,80,99	0.97	8 (10%)	86,92,111	1.10	5 (5%)
31	LMT	F	302	-	36,36,36	1.12	4 (11%)	47,47,47	0.93	2 (4%)
33	TRT	g	203	-	25,25,25	0.60	0	33,33,33	0.82	1 (3%)
33	TRT	M	202	-	25,25,25	0.58	0	33,33,33	0.68	0
33	TRT	m	203	-	25,25,25	0.55	0	33,33,33	0.92	2 (6%)
36	ADP	AD	601	35	28,29,29	1.39	4 (14%)	43,45,45	2.25	14 (32%)
31	LMT	n	202	-	36,36,36	1.18	6 (16%)	47,47,47	0.95	2 (4%)
30	CDL	p	201	-	47,47,99	1.26	8 (17%)	53,59,111	1.33	5 (9%)
31	LMT	g	201	-	36,36,36	1.12	5 (13%)	47,47,47	0.94	2 (4%)
30	CDL	m	201	-	76,76,99	1.01	8 (10%)	82,88,111	1.10	4 (4%)
36	ADP	BD	601	35	28,29,29	1.38	4 (14%)	43,45,45	2.26	14 (32%)
30	CDL	r	101	-	75,75,99	1.01	8 (10%)	81,87,111	1.15	4 (4%)

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
30	CDL	P	202	-	-	43/108/108/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LPP	o	202	-	-	7/24/24/45	-
30	CDL	a	502	-	-	28/91/91/110	-
32	LPP	F	301	-	-	8/25/25/45	-
32	LPP	f	301	-	-	8/25/25/45	-
34	ATP	BF	601	35	-	3/22/38/38	0/3/3/3
33	TRT	N	202	-	-	15/23/23/23	0/1/1/1
33	TRT	M	203	-	-	9/23/23/23	0/1/1/1
31	LMT	d	202	-	-	7/21/61/61	0/2/2/2
32	LPP	o	203	-	-	8/33/33/45	-
33	TRT	AR	201	-	-	11/23/23/23	0/1/1/1
33	TRT	BR	201	-	-	11/23/23/23	0/1/1/1
30	CDL	A	502	-	-	29/91/91/110	-
33	TRT	m	202	-	-	12/23/23/23	0/1/1/1
32	LPP	K	201	-	-	13/32/32/45	-
32	LPP	k	201	-	-	13/32/32/45	-
30	CDL	A	505	-	-	43/95/95/110	-
30	CDL	M	204	-	-	38/87/87/110	-
33	TRT	n	203	-	-	9/23/23/23	0/1/1/1
34	ATP	BB	601	35	-	2/22/38/38	0/3/3/3
34	ATP	AF	601	35	-	3/22/38/38	0/3/3/3
31	LMT	q	101	-	-	7/21/61/61	0/2/2/2
30	CDL	D	201	-	-	36/101/101/110	-
30	CDL	a	503	-	-	30/89/89/110	-
30	CDL	o	201	-	-	36/75/75/110	-
30	CDL	A	501	-	-	24/91/91/110	-
32	LPP	I	101	-	-	13/45/45/45	-
32	LPP	O	202	-	-	9/24/24/45	-
32	LPP	O	203	-	-	8/33/33/45	-
31	LMT	D	202	-	-	7/21/61/61	0/2/2/2
33	TRT	N	201	-	-	9/23/23/23	0/1/1/1
30	CDL	e	101	-	-	39/73/73/110	-
33	TRT	g	202	-	-	7/23/23/23	0/1/1/1
33	TRT	p	202	-	-	15/23/23/23	0/1/1/1
33	TRT	AE	600	-	-	10/23/23/23	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CDL	E	101	-	-	38/73/73/110	-
34	ATP	AA	601	35	-	0/22/38/38	0/3/3/3
32	LPP	i	101	-	-	13/45/45/45	-
34	ATP	AC	601	35	-	2/22/38/38	0/3/3/3
33	TRT	G	202	-	-	15/23/23/23	0/1/1/1
30	CDL	a	505	-	-	43/95/95/110	-
33	TRT	n	204	-	-	15/23/23/23	0/1/1/1
33	TRT	G	201	-	-	7/23/23/23	0/1/1/1
30	CDL	A	503	-	-	30/89/89/110	-
34	ATP	BA	601	35	-	0/22/38/38	0/3/3/3
31	LMT	N	204	-	-	10/21/61/61	0/2/2/2
30	CDL	M	205	-	-	28/63/63/110	-
30	CDL	d	201	-	-	35/101/101/110	-
31	LMT	Q	101	-	-	7/21/61/61	0/2/2/2
33	TRT	BE	600	-	-	10/23/23/23	0/1/1/1
30	CDL	R	101	-	-	33/86/86/110	-
34	ATP	AB	601	35	-	2/22/38/38	0/3/3/3
33	TRT	P	203	-	-	15/23/23/23	0/1/1/1
30	CDL	P	201	-	-	25/57/57/110	-
34	ATP	BC	601	35	-	2/22/38/38	0/3/3/3
30	CDL	O	201	-	-	34/75/75/110	-
30	CDL	M	201	-	-	28/63/63/110	-
32	LPP	n	201	-	-	15/27/27/45	-
30	CDL	a	504	-	-	26/73/73/110	-
32	LPP	N	203	-	-	15/27/27/45	-
30	CDL	A	504	-	-	27/73/73/110	-
30	CDL	a	501	-	-	25/91/91/110	-
31	LMT	F	302	-	-	9/21/61/61	0/2/2/2
33	TRT	g	203	-	-	15/23/23/23	0/1/1/1
33	TRT	M	202	-	-	12/23/23/23	0/1/1/1
33	TRT	m	203	-	-	9/23/23/23	0/1/1/1
36	ADP	AD	601	35	-	0/16/32/32	0/3/3/3
31	LMT	n	202	-	-	11/21/61/61	0/2/2/2
30	CDL	p	201	-	-	26/57/57/110	-
31	LMT	g	201	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CDL	m	201	-	-	38/87/87/110	-
36	ADP	BD	601	35	-	0/16/32/32	0/3/3/3
30	CDL	r	101	-	-	34/86/86/110	-

All (335) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	AB	601	ATP	C5-C4	4.69	1.47	1.39
34	BF	601	ATP	C5-C4	4.67	1.47	1.39
34	BB	601	ATP	C5-C4	4.66	1.47	1.39
34	AF	601	ATP	C5-C4	4.66	1.47	1.39
34	AA	601	ATP	C5-C4	4.66	1.47	1.39
34	BA	601	ATP	C5-C4	4.61	1.47	1.39
36	BD	601	ADP	C5-C4	4.56	1.47	1.39
34	AC	601	ATP	C5-C4	4.56	1.47	1.39
34	BC	601	ATP	C5-C4	4.55	1.47	1.39
36	AD	601	ADP	C5-C4	4.55	1.47	1.39
33	P	203	TRT	C6-C9	3.96	1.59	1.53
33	p	202	TRT	C6-C9	3.83	1.59	1.53
32	i	101	LPP	O9-C11	3.46	1.44	1.34
32	I	101	LPP	O9-C11	3.41	1.43	1.34
32	O	202	LPP	O9-C11	3.35	1.43	1.34
32	N	203	LPP	O9-C11	3.34	1.43	1.34
32	n	201	LPP	O9-C11	3.33	1.43	1.34
32	o	202	LPP	O9-C11	3.33	1.43	1.34
32	F	301	LPP	O9-C11	3.29	1.43	1.34
32	o	203	LPP	O9-C11	3.26	1.43	1.34
32	O	203	LPP	O9-C11	3.26	1.43	1.34
32	f	301	LPP	O9-C11	3.24	1.43	1.34
32	k	201	LPP	O9-C11	3.23	1.43	1.34
32	K	201	LPP	O9-C11	3.22	1.43	1.34
32	O	203	LPP	O27-C29	2.96	1.42	1.33
30	A	505	CDL	OB6-CB4	-2.96	1.39	1.46
32	o	203	LPP	O27-C29	2.93	1.41	1.33
32	I	101	LPP	O27-C29	2.92	1.41	1.33
30	a	505	CDL	OB6-CB4	-2.92	1.39	1.46
32	i	101	LPP	O27-C29	2.91	1.41	1.33
32	O	202	LPP	O27-C29	2.91	1.41	1.33
32	o	202	LPP	O27-C29	2.88	1.41	1.33
32	K	201	LPP	O27-C29	2.88	1.41	1.33
32	k	201	LPP	O27-C29	2.87	1.41	1.33
32	f	301	LPP	O27-C29	2.87	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	n	201	LPP	O27-C29	2.85	1.41	1.33
30	D	201	CDL	OB6-CB4	-2.83	1.39	1.46
32	F	301	LPP	O27-C29	2.83	1.41	1.33
30	d	201	CDL	OB6-CB4	-2.81	1.40	1.46
32	N	203	LPP	O27-C29	2.80	1.41	1.33
30	M	205	CDL	OB6-CB4	-2.79	1.40	1.46
30	M	201	CDL	OA6-CA4	-2.79	1.40	1.46
30	M	201	CDL	OB6-CB4	-2.78	1.40	1.46
30	a	501	CDL	OB6-CB4	-2.76	1.40	1.46
30	P	202	CDL	OB6-CB4	-2.76	1.40	1.46
30	A	501	CDL	OB6-CB4	-2.75	1.40	1.46
30	E	101	CDL	OB6-CB4	-2.73	1.40	1.46
36	AD	601	ADP	C5-C6	2.72	1.48	1.41
30	P	201	CDL	OB6-CB4	-2.72	1.40	1.46
30	m	201	CDL	OA6-CA4	-2.72	1.40	1.46
34	AB	601	ATP	C5-C6	2.71	1.48	1.41
34	BB	601	ATP	C5-C6	2.71	1.48	1.41
34	BA	601	ATP	C5-C6	2.71	1.48	1.41
36	BD	601	ADP	C5-C6	2.70	1.48	1.41
30	p	201	CDL	OB6-CB4	-2.70	1.40	1.46
34	BF	601	ATP	C5-C6	2.69	1.48	1.41
34	AA	601	ATP	C5-C6	2.69	1.48	1.41
31	n	202	LMT	O3'-C3'	-2.68	1.36	1.43
31	N	204	LMT	O3'-C3'	-2.68	1.36	1.43
30	A	503	CDL	OB6-CB4	-2.66	1.40	1.46
30	D	201	CDL	OA6-CA4	-2.66	1.40	1.46
34	AF	601	ATP	C5-C6	2.65	1.48	1.41
30	a	503	CDL	OB6-CB4	-2.65	1.40	1.46
30	e	101	CDL	OB6-CB4	-2.65	1.40	1.46
30	a	501	CDL	OA6-CA4	-2.64	1.40	1.46
30	A	501	CDL	OA6-CA4	-2.64	1.40	1.46
30	M	205	CDL	OA6-CA4	-2.64	1.40	1.46
31	D	202	LMT	O3'-C3'	-2.64	1.36	1.43
30	A	504	CDL	OA8-CA7	2.63	1.41	1.33
30	d	201	CDL	OA6-CA4	-2.63	1.40	1.46
30	a	504	CDL	OA8-CA7	2.62	1.41	1.33
30	M	204	CDL	OA6-CA4	-2.62	1.40	1.46
30	P	202	CDL	OA6-CA4	-2.62	1.40	1.46
34	BC	601	ATP	C5-C6	2.62	1.48	1.41
34	AC	601	ATP	C5-C6	2.62	1.48	1.41
30	A	502	CDL	OB6-CB4	-2.62	1.40	1.46
31	F	302	LMT	O3'-C3'	-2.62	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Q	101	LMT	O3'-C3'	-2.61	1.36	1.43
31	d	202	LMT	O3'-C3'	-2.61	1.36	1.43
30	m	201	CDL	OB6-CB4	-2.60	1.40	1.46
31	g	201	LMT	O3'-C3'	-2.60	1.36	1.43
31	q	101	LMT	O3'-C3'	-2.59	1.36	1.43
30	D	201	CDL	OB8-CB7	2.59	1.40	1.33
30	d	201	CDL	OB8-CB7	2.59	1.40	1.33
30	a	502	CDL	OB6-CB4	-2.59	1.40	1.46
30	M	204	CDL	OB6-CB4	-2.57	1.40	1.46
30	a	504	CDL	OA6-CA4	-2.56	1.40	1.46
30	a	502	CDL	OB8-CB7	2.55	1.40	1.33
30	a	504	CDL	OB6-CB4	-2.55	1.40	1.46
30	O	201	CDL	OB6-CB4	-2.55	1.40	1.46
30	r	101	CDL	OB6-CB4	-2.55	1.40	1.46
30	A	502	CDL	OB8-CB7	2.55	1.40	1.33
30	A	504	CDL	OB6-CB4	-2.54	1.40	1.46
30	R	101	CDL	OA6-CA4	-2.54	1.40	1.46
30	r	101	CDL	OA6-CA4	-2.54	1.40	1.46
30	o	201	CDL	OB6-CB4	-2.53	1.40	1.46
30	R	101	CDL	OB6-CB4	-2.52	1.40	1.46
30	O	201	CDL	OA6-CA4	-2.51	1.40	1.46
30	A	504	CDL	OA6-CA4	-2.50	1.40	1.46
30	O	201	CDL	OA8-CA7	2.48	1.40	1.33
30	E	101	CDL	OA8-CA7	2.47	1.40	1.33
30	R	101	CDL	OA8-CA7	2.47	1.40	1.33
30	o	201	CDL	OB8-CB7	2.47	1.40	1.33
30	e	101	CDL	OA8-CA7	2.46	1.40	1.33
30	P	202	CDL	OA8-CA6	-2.46	1.39	1.45
30	a	505	CDL	OA8-CA7	2.46	1.40	1.33
30	P	201	CDL	OA8-CA7	2.45	1.40	1.33
30	o	201	CDL	OA6-CA4	-2.45	1.40	1.46
30	M	201	CDL	OB8-CB7	2.45	1.40	1.33
30	p	201	CDL	OA6-CA4	-2.45	1.40	1.46
30	a	502	CDL	OA6-CA4	-2.45	1.40	1.46
30	M	205	CDL	OB8-CB7	2.45	1.40	1.33
30	p	201	CDL	OA8-CA7	2.45	1.40	1.33
30	A	505	CDL	OA8-CA7	2.45	1.40	1.33
30	O	201	CDL	OB8-CB7	2.45	1.40	1.33
30	r	101	CDL	OA8-CA7	2.44	1.40	1.33
31	D	202	LMT	O2B-C2B	-2.44	1.36	1.43
30	A	502	CDL	OA6-CA4	-2.43	1.40	1.46
30	P	201	CDL	OA6-CA4	-2.43	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	505	CDL	OA6-CA4	-2.42	1.40	1.46
30	M	205	CDL	OA8-CA7	2.42	1.40	1.33
36	AD	601	ADP	C8-N7	2.42	1.36	1.31
30	o	201	CDL	OA8-CA7	2.41	1.40	1.33
31	g	201	LMT	O2'-C2'	-2.41	1.37	1.43
31	F	302	LMT	O2'-C2'	-2.41	1.37	1.43
31	N	204	LMT	O1'-C1'	-2.41	1.36	1.40
30	E	101	CDL	OB8-CB7	2.41	1.40	1.33
30	e	101	CDL	OB8-CB7	2.40	1.40	1.33
30	a	504	CDL	OB8-CB7	2.39	1.40	1.33
30	A	501	CDL	OB8-CB7	2.39	1.40	1.33
30	P	201	CDL	OB6-CB5	2.39	1.40	1.35
30	a	505	CDL	OA6-CA4	-2.39	1.41	1.46
34	AB	601	ATP	C8-N7	2.39	1.36	1.31
31	N	204	LMT	O2'-C2'	-2.39	1.37	1.43
30	M	204	CDL	OA8-CA6	-2.38	1.39	1.45
31	g	201	LMT	O3B-C3B	-2.38	1.37	1.43
34	AA	601	ATP	C8-N7	2.38	1.36	1.31
31	d	202	LMT	O2B-C2B	-2.38	1.37	1.43
30	A	501	CDL	OA8-CA7	2.38	1.40	1.33
34	BA	601	ATP	C8-N7	2.38	1.36	1.31
30	a	505	CDL	OB8-CB7	2.38	1.40	1.33
30	p	201	CDL	OB8-CB7	2.38	1.40	1.33
30	M	201	CDL	OA8-CA7	2.37	1.40	1.33
30	P	201	CDL	OB8-CB7	2.37	1.40	1.33
30	m	201	CDL	OB8-CB7	2.37	1.40	1.33
30	a	501	CDL	OB8-CB7	2.37	1.40	1.33
30	A	504	CDL	OB8-CB7	2.37	1.40	1.33
30	A	502	CDL	OA8-CA7	2.37	1.40	1.33
30	M	204	CDL	OB8-CB7	2.36	1.40	1.33
30	a	501	CDL	OA8-CA7	2.36	1.40	1.33
30	A	505	CDL	OB8-CB7	2.36	1.40	1.33
30	R	101	CDL	OB8-CB7	2.36	1.40	1.33
33	P	203	TRT	C8-C6	2.36	1.60	1.53
30	m	201	CDL	OA8-CA6	-2.36	1.39	1.45
36	BD	601	ADP	C8-N7	2.36	1.36	1.31
30	r	101	CDL	OB8-CB7	2.36	1.40	1.33
30	p	201	CDL	OB6-CB5	2.36	1.40	1.35
30	o	201	CDL	OB6-CB5	2.35	1.40	1.34
34	AF	601	ATP	C8-N7	2.35	1.36	1.31
34	BF	601	ATP	C8-N7	2.35	1.36	1.31
30	r	101	CDL	OB6-CB5	2.35	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	F	302	LMT	O3B-C3B	-2.35	1.37	1.43
30	R	101	CDL	OB6-CB5	2.35	1.40	1.34
30	m	201	CDL	OA8-CA7	2.35	1.40	1.33
34	BB	601	ATP	C8-N7	2.34	1.36	1.31
30	A	503	CDL	OA6-CA4	-2.34	1.41	1.46
30	a	502	CDL	OA8-CA7	2.34	1.40	1.33
30	M	205	CDL	OA6-CA5	2.34	1.40	1.34
34	BC	601	ATP	C8-N7	2.34	1.36	1.31
30	a	503	CDL	OA8-CA6	-2.34	1.39	1.45
30	a	503	CDL	OB8-CB7	2.34	1.40	1.33
30	a	503	CDL	OA6-CA4	-2.33	1.41	1.46
34	BF	601	ATP	C5-N7	-2.33	1.34	1.39
31	n	202	LMT	O3B-C3B	-2.32	1.37	1.43
31	N	204	LMT	O3B-C3B	-2.32	1.37	1.43
30	d	201	CDL	OA8-CA7	2.32	1.40	1.33
30	O	201	CDL	OB6-CB5	2.32	1.40	1.34
30	A	502	CDL	OA8-CA6	-2.32	1.40	1.45
30	m	201	CDL	OB6-CB5	2.32	1.40	1.34
30	A	503	CDL	OB8-CB7	2.32	1.40	1.33
31	n	202	LMT	O1'-C1'	-2.32	1.36	1.40
33	p	202	TRT	C8-C6	2.32	1.60	1.53
30	A	504	CDL	OA6-CA5	2.32	1.40	1.34
30	A	504	CDL	OB6-CB5	2.32	1.40	1.34
30	A	503	CDL	OA8-CA6	-2.32	1.40	1.45
34	AB	601	ATP	C5-N7	-2.31	1.34	1.39
30	M	204	CDL	OA8-CA7	2.31	1.40	1.33
34	AF	601	ATP	C5-N7	-2.31	1.34	1.39
30	e	101	CDL	OA6-CA4	-2.31	1.41	1.46
30	a	502	CDL	OA8-CA6	-2.31	1.40	1.45
34	BB	601	ATP	C5-N7	-2.31	1.34	1.39
30	A	505	CDL	OB8-CB6	-2.31	1.40	1.45
34	BC	601	ATP	C5-N7	-2.30	1.34	1.39
34	AC	601	ATP	C8-N7	2.30	1.36	1.31
30	E	101	CDL	OA6-CA4	-2.30	1.41	1.46
30	a	504	CDL	OB6-CB5	2.30	1.40	1.34
30	e	101	CDL	OA6-CA5	2.30	1.40	1.34
30	E	101	CDL	OA6-CA5	2.30	1.40	1.34
30	a	504	CDL	OA6-CA5	2.30	1.40	1.34
30	P	202	CDL	OA8-CA7	2.30	1.40	1.33
30	A	502	CDL	OB6-CB5	2.30	1.40	1.34
30	D	201	CDL	OA8-CA7	2.30	1.40	1.33
30	a	505	CDL	OA6-CA5	2.30	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	P	202	CDL	OB8-CB7	2.30	1.40	1.33
31	D	202	LMT	O2'-C2'	-2.30	1.37	1.43
30	A	503	CDL	OA8-CA7	2.30	1.40	1.33
30	A	505	CDL	OA6-CA5	2.29	1.40	1.34
31	D	202	LMT	O3B-C3B	-2.29	1.37	1.43
30	D	201	CDL	OA8-CA6	-2.29	1.40	1.45
31	d	202	LMT	O2'-C2'	-2.29	1.37	1.43
34	AA	601	ATP	C5-N7	-2.28	1.34	1.39
30	A	503	CDL	OB6-CB5	2.28	1.40	1.34
30	a	503	CDL	OA8-CA7	2.28	1.40	1.33
30	M	201	CDL	OA8-CA6	-2.28	1.40	1.45
30	a	502	CDL	OB6-CB5	2.28	1.40	1.34
31	n	202	LMT	O2'-C2'	-2.28	1.37	1.43
31	d	202	LMT	O3B-C3B	-2.27	1.37	1.43
30	M	205	CDL	OA8-CA6	-2.27	1.40	1.45
34	BA	601	ATP	C5-N7	-2.27	1.34	1.39
30	d	201	CDL	OA8-CA6	-2.27	1.40	1.45
30	a	503	CDL	OB6-CB5	2.26	1.40	1.34
30	e	101	CDL	OB6-CB5	2.26	1.40	1.34
34	AC	601	ATP	C5-N7	-2.26	1.34	1.39
36	AD	601	ADP	C5-N7	-2.26	1.35	1.39
30	P	202	CDL	OB8-CB6	-2.26	1.40	1.45
30	a	505	CDL	OB8-CB6	-2.26	1.40	1.45
30	M	204	CDL	OB6-CB5	2.26	1.40	1.34
30	p	201	CDL	OA6-CA5	2.26	1.40	1.34
31	N	204	LMT	O2B-C2B	-2.25	1.37	1.43
31	Q	101	LMT	O3B-C3B	-2.25	1.37	1.43
31	Q	101	LMT	O2B-C2B	-2.25	1.37	1.43
30	D	201	CDL	OA6-CA5	2.25	1.40	1.34
30	P	201	CDL	OA8-CA6	-2.25	1.40	1.45
30	d	201	CDL	OA6-CA5	2.25	1.40	1.34
31	q	101	LMT	O3B-C3B	-2.24	1.37	1.43
30	a	503	CDL	OB8-CB6	-2.23	1.40	1.45
31	Q	101	LMT	O2'-C2'	-2.23	1.37	1.43
30	M	201	CDL	OA6-CA5	2.23	1.40	1.34
36	BD	601	ADP	C5-N7	-2.22	1.35	1.39
31	q	101	LMT	O2B-C2B	-2.22	1.37	1.43
33	p	202	TRT	C7-C6	2.22	1.59	1.53
30	R	101	CDL	OA6-CA5	2.22	1.40	1.34
30	A	505	CDL	OA8-CA6	-2.22	1.40	1.45
33	BE	600	TRT	O15-C12	2.22	1.42	1.37
30	P	201	CDL	OA6-CA5	2.21	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	r	101	CDL	OA6-CA5	2.21	1.40	1.34
30	a	501	CDL	OA8-CA6	-2.21	1.40	1.45
33	AE	600	TRT	O15-C12	2.20	1.42	1.37
30	m	201	CDL	OA6-CA5	2.20	1.40	1.34
31	n	202	LMT	O2B-C2B	-2.20	1.37	1.43
30	A	501	CDL	OA6-CA5	2.20	1.40	1.34
30	p	201	CDL	OA8-CA6	-2.19	1.40	1.45
31	q	101	LMT	O2'-C2'	-2.19	1.37	1.43
30	a	501	CDL	OA6-CA5	2.19	1.40	1.34
30	A	503	CDL	OB8-CB6	-2.18	1.40	1.45
33	P	203	TRT	C7-C6	2.18	1.59	1.53
30	o	201	CDL	OA8-CA6	-2.18	1.40	1.45
30	R	101	CDL	OB8-CB6	-2.18	1.40	1.45
30	A	501	CDL	OA8-CA6	-2.18	1.40	1.45
30	E	101	CDL	OB6-CB5	2.18	1.40	1.34
30	M	205	CDL	OB6-CB5	2.18	1.40	1.34
30	A	504	CDL	OB8-CB6	-2.18	1.40	1.45
30	o	201	CDL	OA6-CA5	2.17	1.40	1.34
30	a	503	CDL	OA6-CA5	2.17	1.40	1.34
30	P	202	CDL	OA6-CA5	2.16	1.40	1.34
30	M	201	CDL	OB6-CB5	2.16	1.40	1.34
30	a	504	CDL	OB8-CB6	-2.16	1.40	1.45
30	A	503	CDL	OA6-CA5	2.16	1.40	1.34
30	r	101	CDL	OA8-CA6	-2.16	1.40	1.45
30	O	201	CDL	OA8-CA6	-2.16	1.40	1.45
31	Q	101	LMT	O4'-C4B	-2.15	1.37	1.43
30	a	505	CDL	OA8-CA6	-2.15	1.40	1.45
30	O	201	CDL	OA6-CA5	2.15	1.40	1.34
30	a	502	CDL	OA6-CA5	2.15	1.40	1.34
30	P	201	CDL	OB8-CB6	-2.15	1.40	1.45
30	A	502	CDL	OA6-CA5	2.14	1.40	1.34
31	D	202	LMT	O1'-C1'	-2.14	1.36	1.40
30	m	201	CDL	OB8-CB6	-2.14	1.40	1.45
30	p	201	CDL	OB8-CB6	-2.14	1.40	1.45
30	r	101	CDL	OB8-CB6	-2.14	1.40	1.45
30	R	101	CDL	OA8-CA6	-2.13	1.40	1.45
30	E	101	CDL	OA8-CA6	-2.13	1.40	1.45
31	D	202	LMT	O4'-C4B	-2.13	1.37	1.43
30	e	101	CDL	OA8-CA6	-2.13	1.40	1.45
30	a	501	CDL	OB8-CB6	-2.12	1.40	1.45
30	P	202	CDL	OB6-CB5	2.12	1.40	1.34
31	d	202	LMT	O1'-C1'	-2.12	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	n	201	LPP	P1-O5	2.12	1.67	1.60
32	i	101	LPP	C12-C11	2.12	1.56	1.50
30	M	204	CDL	OA6-CA5	2.12	1.40	1.34
32	o	202	LPP	C12-C11	2.11	1.56	1.50
31	q	101	LMT	O4'-C4B	-2.11	1.37	1.43
31	F	302	LMT	O2B-C2B	-2.11	1.37	1.43
30	A	501	CDL	OB8-CB6	-2.11	1.40	1.45
30	M	201	CDL	OB8-CB6	-2.11	1.40	1.45
32	O	203	LPP	O9-C7	-2.10	1.41	1.46
31	d	202	LMT	O4'-C4B	-2.10	1.37	1.43
32	I	101	LPP	C12-C11	2.10	1.56	1.50
32	O	202	LPP	C12-C11	2.10	1.56	1.50
31	g	201	LMT	O2B-C2B	-2.09	1.37	1.43
30	M	205	CDL	OB8-CB6	-2.09	1.40	1.45
32	o	203	LPP	O9-C7	-2.09	1.41	1.46
31	N	204	LMT	O4'-C4B	-2.09	1.37	1.43
32	N	203	LPP	P1-O5	2.09	1.66	1.60
30	e	101	CDL	OB8-CB6	-2.09	1.40	1.45
30	d	201	CDL	OB6-CB5	2.09	1.40	1.34
32	F	301	LPP	O9-C7	-2.09	1.41	1.46
30	M	204	CDL	OB8-CB6	-2.08	1.40	1.45
32	k	201	LPP	C12-C11	2.08	1.56	1.50
32	k	201	LPP	O9-C7	-2.08	1.41	1.46
32	f	301	LPP	P1-O5	2.07	1.66	1.60
32	K	201	LPP	C12-C11	2.07	1.56	1.50
32	F	301	LPP	P1-O5	2.07	1.66	1.60
30	O	201	CDL	OB8-CB6	-2.07	1.40	1.45
31	n	202	LMT	O4'-C4B	-2.06	1.37	1.43
32	f	301	LPP	O9-C7	-2.06	1.41	1.46
30	E	101	CDL	OB8-CB6	-2.06	1.40	1.45
31	Q	101	LMT	O1'-C1'	-2.06	1.36	1.40
32	K	201	LPP	O9-C7	-2.06	1.41	1.46
30	D	201	CDL	OB6-CB5	2.06	1.40	1.34
32	o	203	LPP	P1-O5	2.05	1.66	1.60
30	a	502	CDL	OB8-CB6	-2.05	1.40	1.45
30	o	201	CDL	OB8-CB6	-2.05	1.40	1.45
31	g	201	LMT	O4'-C4B	-2.05	1.37	1.43
30	A	502	CDL	OB8-CB6	-2.04	1.40	1.45
31	q	101	LMT	O1'-C1'	-2.04	1.36	1.40
32	o	202	LPP	P1-O5	2.03	1.66	1.60
32	O	202	LPP	P1-O5	2.03	1.66	1.60
32	O	203	LPP	C12-C11	2.02	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	o	203	LPP	C12-C11	2.02	1.56	1.50
30	A	505	CDL	OB6-CB5	2.02	1.40	1.34
32	f	301	LPP	C12-C11	2.01	1.56	1.50
32	O	203	LPP	P1-O5	2.01	1.66	1.60
30	A	501	CDL	OB6-CB5	2.01	1.39	1.34
30	a	501	CDL	OB6-CB5	2.00	1.39	1.34

All (296) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	P	203	TRT	C7-C6-C8	14.23	150.20	107.26
33	p	202	TRT	C7-C6-C8	13.71	148.64	107.26
33	p	202	TRT	C5-C6-C9	13.47	143.47	112.00
33	P	203	TRT	C5-C6-C9	12.60	141.46	112.00
33	P	203	TRT	C8-C6-C9	-11.32	81.58	110.18
33	p	202	TRT	C8-C6-C9	-11.21	81.84	110.18
33	p	202	TRT	C7-C6-C9	-10.88	82.69	110.18
33	P	203	TRT	C7-C6-C9	-10.81	82.85	110.18
36	BD	601	ADP	O4'-C1'-N9	6.93	121.40	108.09
36	AD	601	ADP	O4'-C1'-N9	6.91	121.36	108.09
34	AB	601	ATP	C5-C4-N3	-5.97	118.49	126.72
34	BB	601	ATP	C5-C4-N3	-5.96	118.52	126.72
34	BA	601	ATP	C5-C4-N3	-5.88	118.62	126.72
34	AA	601	ATP	C5-C4-N3	-5.87	118.63	126.72
34	AF	601	ATP	C5-C4-N3	-5.85	118.66	126.72
34	BF	601	ATP	C5-C4-N3	-5.84	118.68	126.72
36	BD	601	ADP	C5-C4-N3	-5.74	118.81	126.72
34	BC	601	ATP	C5-C4-N3	-5.73	118.82	126.72
36	AD	601	ADP	C5-C4-N3	-5.70	118.87	126.72
34	AC	601	ATP	C5-C4-N3	-5.70	118.87	126.72
30	p	201	CDL	OB6-CB5-C51	5.07	120.13	111.09
30	P	201	CDL	OB6-CB5-C51	5.04	120.07	111.09
34	BB	601	ATP	N3-C4-N9	4.82	135.37	127.17
34	AB	601	ATP	N3-C4-N9	4.81	135.34	127.17
34	AF	601	ATP	N3-C4-N9	4.76	135.26	127.17
34	BF	601	ATP	N3-C4-N9	4.74	135.23	127.17
34	AA	601	ATP	N3-C4-N9	4.73	135.21	127.17
34	BA	601	ATP	N3-C4-N9	4.73	135.21	127.17
34	BC	601	ATP	N3-C4-N9	4.68	135.13	127.17
30	M	205	CDL	OA6-CA5-C11	4.65	121.54	111.48
34	AC	601	ATP	N3-C4-N9	4.63	135.05	127.17
30	a	504	CDL	OA6-CA5-C11	4.61	121.46	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BD	601	ADP	N3-C4-N9	4.59	134.98	127.17
36	AD	601	ADP	N3-C4-N9	4.56	134.92	127.17
30	A	504	CDL	OA6-CA5-C11	4.56	121.34	111.48
30	M	201	CDL	OA6-CA5-C11	4.47	121.15	111.48
33	P	203	TRT	C8-C6-C5	-4.44	87.51	109.11
33	p	202	TRT	C8-C6-C5	-4.43	87.58	109.11
32	k	201	LPP	O9-C11-C12	4.29	120.77	111.48
30	E	101	CDL	OA6-CA5-C11	4.27	120.72	111.48
30	e	101	CDL	OA6-CA5-C11	4.26	120.70	111.48
32	K	201	LPP	O9-C11-C12	4.24	120.66	111.48
30	a	502	CDL	OB6-CB5-C51	4.21	120.60	111.48
30	A	502	CDL	OB6-CB5-C51	4.20	120.56	111.48
30	R	101	CDL	OA6-CA5-C11	4.19	120.56	111.48
33	p	202	TRT	C7-C6-C5	-4.17	88.84	109.11
30	r	101	CDL	OA6-CA5-C11	4.16	120.48	111.48
33	P	203	TRT	C7-C6-C5	-4.13	89.04	109.11
30	A	503	CDL	OA6-CA5-C11	4.10	120.36	111.48
30	a	503	CDL	OA6-CA5-C11	4.07	120.30	111.48
32	N	203	LPP	O9-C11-C12	4.07	120.28	111.48
32	n	201	LPP	O9-C11-C12	4.06	120.27	111.48
30	R	101	CDL	OB6-CB5-C51	4.05	120.25	111.48
30	r	101	CDL	OB6-CB5-C51	4.05	120.25	111.48
30	o	201	CDL	OB6-CB5-C51	4.03	120.21	111.48
30	O	201	CDL	OB6-CB5-C51	4.03	120.19	111.48
30	A	501	CDL	OA6-CA5-C11	4.01	120.17	111.48
30	M	201	CDL	OB6-CB5-C51	4.00	120.13	111.48
30	a	501	CDL	OA6-CA5-C11	3.99	120.12	111.48
30	d	201	CDL	OA6-CA5-C11	3.96	120.05	111.48
30	D	201	CDL	OA6-CA5-C11	3.92	119.96	111.48
34	BA	601	ATP	C2-N3-C4	3.89	121.33	111.83
34	AB	601	ATP	C2-N3-C4	3.89	121.33	111.83
32	o	202	LPP	O9-C11-C12	3.89	119.89	111.48
34	AA	601	ATP	C2-N3-C4	3.89	121.32	111.83
34	BB	601	ATP	C2-N3-C4	3.88	121.31	111.83
30	a	503	CDL	OB6-CB5-C51	3.87	119.86	111.48
30	M	205	CDL	OB6-CB5-C51	3.86	119.84	111.48
36	BD	601	ADP	C2-N3-C4	3.86	121.25	111.83
34	AF	601	ATP	C2-N3-C4	3.84	121.20	111.83
36	AD	601	ADP	C2-N3-C4	3.83	121.19	111.83
34	BF	601	ATP	C2-N3-C4	3.83	121.19	111.83
34	BC	601	ATP	C2-N3-C4	3.81	121.14	111.83
34	AC	601	ATP	C2-N3-C4	3.80	121.10	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	O	202	LPP	O9-C11-C12	3.79	119.68	111.48
30	A	503	CDL	OB6-CB5-C51	3.76	119.61	111.48
30	M	204	CDL	OA6-CA5-C11	3.74	119.56	111.48
36	BD	601	ADP	N3-C2-N1	-3.73	122.93	128.58
36	AD	601	ADP	N3-C2-N1	-3.71	122.97	128.58
34	AA	601	ATP	N3-C2-N1	-3.71	122.97	128.58
34	BA	601	ATP	N3-C2-N1	-3.70	122.98	128.58
33	BE	600	TRT	C7-C6-C9	-3.69	100.86	110.18
30	A	504	CDL	OB6-CB5-C51	3.68	119.43	111.48
30	a	504	CDL	OB6-CB5-C51	3.67	119.41	111.48
34	AC	601	ATP	N3-C2-N1	-3.66	123.03	128.58
33	AE	600	TRT	C7-C6-C9	-3.65	100.94	110.18
34	AF	601	ATP	N3-C2-N1	-3.65	123.06	128.58
34	BC	601	ATP	N3-C2-N1	-3.64	123.07	128.58
34	BF	601	ATP	N3-C2-N1	-3.64	123.07	128.58
30	M	204	CDL	OB6-CB5-C51	3.64	119.35	111.48
34	BB	601	ATP	N3-C2-N1	-3.64	123.08	128.58
34	AB	601	ATP	N3-C2-N1	-3.62	123.11	128.58
30	m	201	CDL	OB6-CB5-C51	3.60	119.28	111.48
33	n	204	TRT	C7-C6-C9	-3.57	101.16	110.18
30	e	101	CDL	OB6-CB5-C51	3.55	119.15	111.48
30	A	504	CDL	OA8-CA7-C31	3.54	122.64	111.83
30	a	504	CDL	OA8-CA7-C31	3.53	122.61	111.83
30	m	201	CDL	OA6-CA5-C11	3.51	119.08	111.48
34	AA	601	ATP	C4-C5-N7	-3.50	106.58	110.58
36	BD	601	ADP	C4-C5-N7	-3.50	106.58	110.58
34	BA	601	ATP	C4-C5-N7	-3.48	106.60	110.58
30	P	202	CDL	OB6-CB5-C51	3.48	119.01	111.48
36	AD	601	ADP	C4-C5-N7	-3.48	106.60	110.58
34	AB	601	ATP	C4-C5-N7	-3.47	106.61	110.58
32	f	301	LPP	O9-C11-C12	3.47	118.99	111.48
34	AF	601	ATP	C4-C5-N7	-3.45	106.64	110.58
30	M	204	CDL	OA8-CA7-C31	3.45	122.35	111.83
30	A	502	CDL	OA6-CA5-C11	3.45	118.93	111.48
32	F	301	LPP	O9-C11-C12	3.44	118.93	111.48
30	d	201	CDL	OB6-CB5-C51	3.44	118.93	111.48
34	BF	601	ATP	C4-C5-N7	-3.43	106.66	110.58
32	O	203	LPP	O9-C11-C12	3.43	118.90	111.48
34	BB	601	ATP	C4-C5-N7	-3.42	106.67	110.58
32	I	101	LPP	O9-C11-C12	3.41	118.87	111.48
32	o	203	LPP	O9-C11-C12	3.41	118.86	111.48
30	m	201	CDL	OA8-CA7-C31	3.40	122.21	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AC	601	ATP	C4-C5-N7	-3.40	106.70	110.58
32	i	101	LPP	O9-C11-C12	3.39	118.83	111.48
30	D	201	CDL	OB6-CB5-C51	3.39	118.81	111.48
30	R	101	CDL	OA8-CA7-C31	3.38	122.14	111.83
30	E	101	CDL	OB6-CB5-C51	3.38	118.79	111.48
30	a	502	CDL	OA6-CA5-C11	3.38	118.79	111.48
33	N	202	TRT	C7-C6-C9	-3.37	101.66	110.18
34	BC	601	ATP	C4-C5-N7	-3.36	106.74	110.58
30	r	101	CDL	OA8-CA7-C31	3.32	121.97	111.83
30	a	501	CDL	OB6-CB5-C51	3.32	118.66	111.48
33	p	202	TRT	C1-C5-C6	-3.31	110.97	123.78
33	P	203	TRT	C1-C5-C6	-3.28	111.07	123.78
30	o	201	CDL	OA6-CA5-C11	3.27	118.55	111.48
30	A	501	CDL	OB6-CB5-C51	3.26	118.54	111.48
30	P	202	CDL	OA6-CA5-C11	3.21	118.43	111.48
30	a	505	CDL	OB6-CB5-C51	3.21	118.43	111.48
30	O	201	CDL	OA6-CA5-C11	3.20	118.40	111.48
30	M	205	CDL	OA8-CA7-C31	3.16	121.46	111.83
30	P	201	CDL	OA6-CA5-C11	3.15	118.29	111.48
30	A	505	CDL	OB6-CB5-C51	3.13	118.25	111.48
30	M	201	CDL	OA8-CA7-C31	3.11	121.30	111.83
30	D	201	CDL	OA8-CA7-C31	3.10	121.30	111.83
30	P	202	CDL	OB8-CB7-C71	3.08	121.23	111.83
30	a	501	CDL	CB4-OB6-CB5	-3.08	110.42	117.80
30	p	201	CDL	OA6-CA5-C11	3.08	118.14	111.48
30	p	201	CDL	OA8-CA7-C31	3.08	121.21	111.83
30	P	201	CDL	OA8-CA7-C31	3.07	121.18	111.83
34	AC	601	ATP	C4-N9-C8	3.06	108.95	105.74
30	A	501	CDL	CB4-OB6-CB5	-3.06	110.48	117.80
34	BC	601	ATP	C4-N9-C8	3.05	108.94	105.74
30	d	201	CDL	OA8-CA7-C31	3.05	121.12	111.83
30	A	505	CDL	OA6-CA5-C11	3.04	118.05	111.48
33	G	202	TRT	C8-C6-C9	-3.03	102.53	110.18
36	BD	601	ADP	C3'-C2'-C1'	3.02	107.17	101.46
30	a	501	CDL	OA8-CA7-C31	3.01	121.01	111.83
36	AD	601	ADP	C4-N9-C8	3.00	108.89	105.74
30	o	201	CDL	OA8-CA7-C31	2.99	120.24	111.15
33	g	203	TRT	C8-C6-C9	-2.98	102.64	110.18
30	a	502	CDL	OA8-CA7-C31	2.98	120.92	111.83
30	A	502	CDL	OA8-CA7-C31	2.97	120.90	111.83
36	BD	601	ADP	C4-N9-C8	2.97	108.86	105.74
30	a	505	CDL	OA6-CA5-C11	2.96	117.88	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AA	601	ATP	C4-N9-C8	2.93	108.82	105.74
34	BA	601	ATP	C4-N9-C8	2.93	108.81	105.74
36	AD	601	ADP	C3'-C2'-C1'	2.92	106.99	101.46
30	O	201	CDL	OA8-CA7-C31	2.91	119.99	111.15
30	a	503	CDL	OB8-CB7-C71	2.91	120.70	111.83
34	AF	601	ATP	C4-N9-C8	2.90	108.78	105.74
34	BF	601	ATP	C4-N9-C8	2.87	108.75	105.74
30	A	501	CDL	OA8-CA7-C31	2.87	120.58	111.83
34	BB	601	ATP	C4-N9-C8	2.87	108.75	105.74
33	p	202	TRT	C14-C9-C6	2.87	126.70	121.52
30	A	503	CDL	OB8-CB7-C71	2.85	120.52	111.83
30	E	101	CDL	OB8-CB7-C71	2.84	120.50	111.83
30	e	101	CDL	OB8-CB7-C71	2.84	120.49	111.83
34	AB	601	ATP	C4-N9-C8	2.83	108.71	105.74
33	n	203	TRT	C7-C6-C9	-2.82	103.06	110.18
32	n	201	LPP	O27-C29-C30	2.81	120.40	111.83
30	m	201	CDL	OB8-CB7-C71	2.80	120.38	111.83
33	P	203	TRT	C14-C9-C6	2.80	126.58	121.52
32	N	203	LPP	O27-C29-C30	2.80	120.36	111.83
30	a	504	CDL	OB8-CB7-C71	2.80	120.36	111.83
30	A	504	CDL	OB8-CB7-C71	2.79	120.35	111.83
30	M	204	CDL	OB8-CB7-C71	2.79	120.34	111.83
33	BR	201	TRT	C7-C6-C9	-2.78	103.15	110.18
34	AA	601	ATP	C5-N7-C8	2.77	107.80	103.45
33	n	203	TRT	C5-C6-C9	-2.75	105.56	112.00
33	N	201	TRT	C7-C6-C9	-2.75	103.22	110.18
36	BD	601	ADP	C4'-O4'-C1'	-2.75	103.40	109.47
34	BA	601	ATP	C5-N7-C8	2.74	107.75	103.45
36	AD	601	ADP	C5'-C4'-C3'	2.73	125.04	115.21
36	BD	601	ADP	C5-N7-C8	2.72	107.73	103.45
33	M	203	TRT	C7-C6-C9	-2.72	103.29	110.18
36	AD	601	ADP	C5-N7-C8	2.71	107.71	103.45
30	r	101	CDL	OB8-CB7-C71	2.70	120.05	111.83
36	AD	601	ADP	C4'-O4'-C1'	-2.69	103.52	109.47
30	P	202	CDL	OA8-CA7-C31	2.69	120.03	111.83
30	R	101	CDL	OB8-CB7-C71	2.68	120.02	111.83
30	p	201	CDL	OB8-CB7-C71	2.67	119.99	111.83
30	P	201	CDL	OB8-CB7-C71	2.67	119.98	111.83
33	N	201	TRT	C5-C6-C9	-2.67	105.76	112.00
30	A	502	CDL	OB8-CB7-C71	2.67	119.97	111.83
34	BC	601	ATP	C5-N7-C8	2.67	107.64	103.45
30	a	502	CDL	OB8-CB7-C71	2.66	119.94	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AC	601	ATP	C5-N7-C8	2.66	107.63	103.45
32	F	301	LPP	O27-C29-C30	2.65	119.91	111.83
34	AB	601	ATP	C5-N7-C8	2.65	107.61	103.45
30	M	201	CDL	OB8-CB7-C71	2.64	119.88	111.83
33	AR	201	TRT	C5-C6-C9	-2.64	105.83	112.00
34	BB	601	ATP	C5-N7-C8	2.64	107.59	103.45
36	BD	601	ADP	C5'-C4'-C3'	2.62	124.66	115.21
30	O	201	CDL	OB8-CB7-C71	2.60	119.76	111.83
32	o	202	LPP	O27-C29-C30	2.60	119.76	111.83
30	M	205	CDL	OB8-CB7-C71	2.60	119.76	111.83
30	p	201	CDL	CB4-OB6-CB5	-2.59	113.27	117.85
33	AR	201	TRT	C7-C6-C9	-2.59	103.62	110.18
30	P	201	CDL	CB4-OB6-CB5	-2.58	113.28	117.85
32	f	301	LPP	O27-C29-C30	2.58	119.71	111.83
32	O	202	LPP	O27-C29-C30	2.58	119.70	111.83
34	AF	601	ATP	C5-N7-C8	2.58	107.50	103.45
30	o	201	CDL	OB8-CB7-C71	2.57	119.67	111.83
33	m	203	TRT	C7-C6-C9	-2.57	103.69	110.18
33	M	203	TRT	C5-C6-C9	-2.57	106.00	112.00
34	BF	601	ATP	C5-N7-C8	2.56	107.47	103.45
30	A	505	CDL	OB8-CB7-C71	2.56	119.63	111.83
33	m	203	TRT	C5-C6-C9	-2.55	106.04	112.00
30	a	505	CDL	OB8-CB7-C71	2.54	119.58	111.83
30	A	505	CDL	OA8-CA7-C31	2.53	119.56	111.83
30	A	503	CDL	OA8-CA7-C31	2.53	119.55	111.83
30	a	501	CDL	OB8-CB7-C71	2.53	119.54	111.83
30	D	201	CDL	OB8-CB7-C71	2.51	119.49	111.83
30	d	201	CDL	OB8-CB7-C71	2.51	119.49	111.83
30	a	503	CDL	OA8-CA7-C31	2.50	119.45	111.83
30	A	501	CDL	OB8-CB7-C71	2.47	119.36	111.83
33	BR	201	TRT	C5-C6-C9	-2.46	106.24	112.00
32	O	203	LPP	O27-C29-C30	2.45	119.32	111.83
31	Q	101	LMT	C3B-C4B-C5B	-2.45	105.78	110.23
30	E	101	CDL	OA8-CA7-C31	2.44	119.27	111.83
30	a	505	CDL	OA8-CA7-C31	2.43	119.25	111.83
31	q	101	LMT	C3B-C4B-C5B	-2.42	105.84	110.23
30	e	101	CDL	OA8-CA7-C31	2.42	119.22	111.83
31	q	101	LMT	C3'-C4'-C5'	-2.40	105.61	110.93
32	K	201	LPP	O27-C29-C30	2.39	119.13	111.83
32	k	201	LPP	O27-C29-C30	2.39	119.12	111.83
31	Q	101	LMT	C3'-C4'-C5'	-2.39	105.64	110.93
31	n	202	LMT	C3'-C4'-C5'	-2.38	105.65	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	G	201	TRT	C5-C6-C9	-2.38	106.44	112.00
36	AD	601	ADP	N9-C8-N7	-2.35	110.60	113.94
34	AC	601	ATP	O4'-C1'-N9	2.35	112.60	108.09
32	o	203	LPP	O27-C29-C30	2.34	118.98	111.83
31	N	204	LMT	C3'-C4'-C5'	-2.34	105.73	110.93
36	BD	601	ADP	N9-C8-N7	-2.34	110.61	113.94
34	BC	601	ATP	N9-C8-N7	-2.33	110.63	113.94
34	AA	601	ATP	N9-C8-N7	-2.32	110.64	113.94
34	AC	601	ATP	N9-C8-N7	-2.32	110.64	113.94
33	N	201	TRT	C16-O15-C12	-2.32	111.90	117.93
33	g	202	TRT	C5-C6-C9	-2.32	106.58	112.00
34	BA	601	ATP	N9-C8-N7	-2.31	110.66	113.94
34	BC	601	ATP	O4'-C1'-N9	2.30	112.51	108.09
33	n	203	TRT	C16-O15-C12	-2.27	112.04	117.93
31	g	201	LMT	C3B-C4B-C5B	-2.24	106.17	110.23
32	i	101	LPP	O27-C29-C30	2.24	118.66	111.83
34	BB	601	ATP	O4'-C1'-N9	2.22	112.36	108.09
32	I	101	LPP	O27-C29-C30	2.22	118.59	111.83
33	p	202	TRT	C10-C9-C6	-2.21	117.53	121.52
31	F	302	LMT	C3B-C4B-C5B	-2.21	106.23	110.23
34	AF	601	ATP	O4'-C1'-N9	2.20	112.31	108.09
36	AD	601	ADP	C6-C5-N7	2.19	136.31	132.09
34	BF	601	ATP	O4'-C1'-N9	2.18	112.28	108.09
36	BD	601	ADP	C6-C5-N7	2.18	136.29	132.09
34	AB	601	ATP	O4'-C1'-N9	2.17	112.25	108.09
31	g	201	LMT	C3'-C4'-C5'	-2.17	106.13	110.93
31	F	302	LMT	C3'-C4'-C5'	-2.16	106.15	110.93
34	BB	601	ATP	N9-C8-N7	-2.16	110.88	113.94
34	AA	601	ATP	C6-C5-N7	2.15	136.24	132.09
34	AB	601	ATP	N9-C8-N7	-2.14	110.90	113.94
34	BA	601	ATP	C6-C5-N7	2.14	136.21	132.09
36	AD	601	ADP	C2-N1-C6	2.13	122.23	118.73
36	BD	601	ADP	C2-N1-C6	2.13	122.23	118.73
34	BF	601	ATP	C2-N1-C6	2.11	122.19	118.73
34	AC	601	ATP	C2-N1-C6	2.10	122.17	118.73
34	AC	601	ATP	C6-C5-N7	2.09	136.13	132.09
34	AF	601	ATP	C2-N1-C6	2.08	122.14	118.73
34	AF	601	ATP	N9-C8-N7	-2.07	111.00	113.94
34	BF	601	ATP	C6-C5-N7	2.07	136.08	132.09
34	AF	601	ATP	C6-C5-N7	2.07	136.07	132.09
34	AA	601	ATP	C2-N1-C6	2.06	122.12	118.73
34	BC	601	ATP	C6-C5-N7	2.06	136.06	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AB	601	ATP	C6-C5-N7	2.06	136.06	132.09
34	BB	601	ATP	C2-N1-C6	2.06	122.11	118.73
33	P	203	TRT	C10-C9-C6	-2.06	117.81	121.52
31	N	204	LMT	C3B-C4B-C5B	-2.05	106.51	110.23
34	BF	601	ATP	N9-C8-N7	-2.05	111.03	113.94
34	AB	601	ATP	C2-N1-C6	2.04	122.08	118.73
31	d	202	LMT	C3'-C4'-C5'	-2.04	106.41	110.93
34	BC	601	ATP	C2-N1-C6	2.03	122.07	118.73
34	BA	601	ATP	C2-N1-C6	2.03	122.06	118.73
31	n	202	LMT	C3B-C4B-C5B	-2.03	106.56	110.23
34	BB	601	ATP	C6-C5-N7	2.02	135.98	132.09
31	D	202	LMT	C3'-C4'-C5'	-2.00	106.49	110.93

There are no chirality outliers.

All (1234) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	A	501	CDL	CB2-OB2-PB2-OB3
30	A	501	CDL	C51-CB5-OB6-CB4
30	A	502	CDL	CB2-OB2-PB2-OB3
30	A	502	CDL	CB3-OB5-PB2-OB2
30	A	502	CDL	CB3-OB5-PB2-OB3
30	A	502	CDL	OB7-CB5-OB6-CB4
30	A	503	CDL	CB2-C1-CA2-OA2
30	A	503	CDL	CA2-OA2-PA1-OA3
30	A	503	CDL	CA3-OA5-PA1-OA2
30	A	503	CDL	CA3-OA5-PA1-OA3
30	A	503	CDL	CA3-OA5-PA1-OA4
30	A	503	CDL	CB3-OB5-PB2-OB2
30	A	503	CDL	CB3-OB5-PB2-OB3
30	A	504	CDL	O1-C1-CB2-OB2
30	A	504	CDL	CA2-C1-CB2-OB2
30	A	504	CDL	OA6-CA4-CA6-OA8
30	A	504	CDL	OA7-CA5-OA6-CA4
30	A	504	CDL	CB3-OB5-PB2-OB2
30	A	504	CDL	CB3-OB5-PB2-OB4
30	A	505	CDL	O1-C1-CA2-OA2
30	A	505	CDL	CA2-OA2-PA1-OA3
30	A	505	CDL	CA2-OA2-PA1-OA5
30	A	505	CDL	CA3-OA5-PA1-OA2
30	A	505	CDL	CA3-OA5-PA1-OA3
30	A	505	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
30	A	505	CDL	CB2-OB2-PB2-OB3
30	A	505	CDL	CB2-OB2-PB2-OB5
30	A	505	CDL	CB3-OB5-PB2-OB2
30	A	505	CDL	CB3-OB5-PB2-OB4
30	A	505	CDL	C51-CB5-OB6-CB4
30	D	201	CDL	CA2-OA2-PA1-OA3
30	D	201	CDL	CA2-OA2-PA1-OA4
30	D	201	CDL	CA3-OA5-PA1-OA2
30	D	201	CDL	CA3-OA5-PA1-OA4
30	D	201	CDL	CB2-OB2-PB2-OB3
30	D	201	CDL	CB2-OB2-PB2-OB5
30	E	101	CDL	O1-C1-CB2-OB2
30	E	101	CDL	CA2-OA2-PA1-OA4
30	E	101	CDL	CA3-OA5-PA1-OA2
30	E	101	CDL	CA3-OA5-PA1-OA3
30	E	101	CDL	CA3-OA5-PA1-OA4
30	E	101	CDL	CB2-OB2-PB2-OB3
30	E	101	CDL	CB2-OB2-PB2-OB5
30	M	201	CDL	CA2-OA2-PA1-OA5
30	M	201	CDL	CB2-OB2-PB2-OB3
30	M	204	CDL	CA2-OA2-PA1-OA3
30	M	204	CDL	CA2-OA2-PA1-OA4
30	M	204	CDL	CA2-OA2-PA1-OA5
30	M	205	CDL	CA2-OA2-PA1-OA5
30	M	205	CDL	CB2-OB2-PB2-OB3
30	O	201	CDL	CA2-OA2-PA1-OA4
30	O	201	CDL	CA2-OA2-PA1-OA5
30	O	201	CDL	CA3-OA5-PA1-OA2
30	O	201	CDL	CA3-OA5-PA1-OA3
30	O	201	CDL	CA3-OA5-PA1-OA4
30	O	201	CDL	CB2-OB2-PB2-OB3
30	O	201	CDL	CB2-OB2-PB2-OB5
30	O	201	CDL	CB3-OB5-PB2-OB2
30	O	201	CDL	CB3-OB5-PB2-OB3
30	O	201	CDL	CB3-OB5-PB2-OB4
30	P	201	CDL	CA2-OA2-PA1-OA3
30	P	201	CDL	CA2-OA2-PA1-OA5
30	P	201	CDL	CA3-OA5-PA1-OA2
30	P	201	CDL	CA3-OA5-PA1-OA3
30	P	201	CDL	CB2-OB2-PB2-OB3
30	P	201	CDL	CB2-OB2-PB2-OB5
30	P	201	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
30	P	202	CDL	OA5-CA3-CA4-OA6
30	P	202	CDL	CB2-OB2-PB2-OB4
30	P	202	CDL	CB2-OB2-PB2-OB5
30	P	202	CDL	CB3-OB5-PB2-OB2
30	P	202	CDL	CB3-OB5-PB2-OB3
30	P	202	CDL	CB3-OB5-PB2-OB4
30	R	101	CDL	CB2-OB2-PB2-OB5
30	a	501	CDL	CB2-OB2-PB2-OB3
30	a	501	CDL	C51-CB5-OB6-CB4
30	a	502	CDL	OA7-CA5-OA6-CA4
30	a	502	CDL	C11-CA5-OA6-CA4
30	a	502	CDL	CB2-OB2-PB2-OB3
30	a	502	CDL	CB3-OB5-PB2-OB2
30	a	502	CDL	CB3-OB5-PB2-OB3
30	a	502	CDL	OB7-CB5-OB6-CB4
30	a	503	CDL	CB2-C1-CA2-OA2
30	a	503	CDL	CA2-OA2-PA1-OA3
30	a	503	CDL	CA3-OA5-PA1-OA2
30	a	503	CDL	CA3-OA5-PA1-OA3
30	a	503	CDL	CA3-OA5-PA1-OA4
30	a	503	CDL	CB3-OB5-PB2-OB2
30	a	503	CDL	CB3-OB5-PB2-OB3
30	a	504	CDL	O1-C1-CB2-OB2
30	a	504	CDL	CA2-C1-CB2-OB2
30	a	504	CDL	OA6-CA4-CA6-OA8
30	a	504	CDL	OA7-CA5-OA6-CA4
30	a	504	CDL	CB3-OB5-PB2-OB2
30	a	504	CDL	CB3-OB5-PB2-OB4
30	a	505	CDL	O1-C1-CA2-OA2
30	a	505	CDL	CA2-OA2-PA1-OA3
30	a	505	CDL	CA2-OA2-PA1-OA5
30	a	505	CDL	CA3-OA5-PA1-OA2
30	a	505	CDL	CA3-OA5-PA1-OA3
30	a	505	CDL	CA3-OA5-PA1-OA4
30	a	505	CDL	CB2-OB2-PB2-OB3
30	a	505	CDL	CB2-OB2-PB2-OB5
30	a	505	CDL	CB3-OB5-PB2-OB2
30	a	505	CDL	CB3-OB5-PB2-OB4
30	a	505	CDL	C51-CB5-OB6-CB4
30	d	201	CDL	CA2-OA2-PA1-OA3
30	d	201	CDL	CA2-OA2-PA1-OA4
30	d	201	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
30	d	201	CDL	CA3-OA5-PA1-OA4
30	d	201	CDL	CB2-OB2-PB2-OB3
30	d	201	CDL	CB2-OB2-PB2-OB5
30	e	101	CDL	O1-C1-CB2-OB2
30	e	101	CDL	CA3-OA5-PA1-OA2
30	e	101	CDL	CA3-OA5-PA1-OA3
30	e	101	CDL	CA3-OA5-PA1-OA4
30	e	101	CDL	CB2-OB2-PB2-OB3
30	e	101	CDL	CB2-OB2-PB2-OB5
30	m	201	CDL	CA2-OA2-PA1-OA3
30	m	201	CDL	CA2-OA2-PA1-OA4
30	m	201	CDL	CA2-OA2-PA1-OA5
30	m	201	CDL	OA5-CA3-CA4-OA6
30	o	201	CDL	CA2-OA2-PA1-OA4
30	o	201	CDL	CA2-OA2-PA1-OA5
30	o	201	CDL	CA3-OA5-PA1-OA2
30	o	201	CDL	CA3-OA5-PA1-OA3
30	o	201	CDL	CA3-OA5-PA1-OA4
30	o	201	CDL	CB2-OB2-PB2-OB3
30	o	201	CDL	CB2-OB2-PB2-OB5
30	o	201	CDL	CB3-OB5-PB2-OB2
30	o	201	CDL	CB3-OB5-PB2-OB3
30	o	201	CDL	CB3-OB5-PB2-OB4
30	p	201	CDL	CA2-OA2-PA1-OA3
30	p	201	CDL	CA2-OA2-PA1-OA5
30	p	201	CDL	CA3-OA5-PA1-OA2
30	p	201	CDL	CA3-OA5-PA1-OA3
30	p	201	CDL	CB2-OB2-PB2-OB3
30	p	201	CDL	CB2-OB2-PB2-OB5
30	p	201	CDL	C51-CB5-OB6-CB4
30	r	101	CDL	CB2-OB2-PB2-OB5
32	I	101	LPP	C6-O5-P1-O2
32	I	101	LPP	C6-O5-P1-O4
32	K	201	LPP	O10-C11-O9-C7
32	N	203	LPP	C6-O5-P1-O2
32	N	203	LPP	C6-O5-P1-O3
32	N	203	LPP	C6-O5-P1-O4
32	O	202	LPP	C6-O5-P1-O2
32	O	202	LPP	C6-O5-P1-O3
32	O	202	LPP	C6-O5-P1-O4
32	i	101	LPP	C6-O5-P1-O2
32	i	101	LPP	C6-O5-P1-O3

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Mol	Chain	Res	Type	Atoms
32	i	101	LPP	C6-O5-P1-O4
32	k	201	LPP	O10-C11-O9-C7
32	n	201	LPP	C6-O5-P1-O2
32	n	201	LPP	C6-O5-P1-O3
32	n	201	LPP	C6-O5-P1-O4
32	o	202	LPP	C6-O5-P1-O2
32	o	202	LPP	C6-O5-P1-O3
32	o	202	LPP	C6-O5-P1-O4
34	AF	601	ATP	C5'-O5'-PA-O1A
34	AF	601	ATP	C5'-O5'-PA-O3A
34	BF	601	ATP	C5'-O5'-PA-O1A
34	BF	601	ATP	C5'-O5'-PA-O3A
30	P	201	CDL	OB7-CB5-OB6-CB4
30	p	201	CDL	OB7-CB5-OB6-CB4
30	P	201	CDL	OA9-CA7-OA8-CA6
32	K	201	LPP	O28-C29-O27-C8
32	k	201	LPP	O28-C29-O27-C8
30	M	201	CDL	C31-CA7-OA8-CA6
30	M	205	CDL	C31-CA7-OA8-CA6
30	d	201	CDL	C31-CA7-OA8-CA6
30	p	201	CDL	C31-CA7-OA8-CA6
30	A	501	CDL	OA9-CA7-OA8-CA6
30	D	201	CDL	OA9-CA7-OA8-CA6
30	M	201	CDL	OA9-CA7-OA8-CA6
30	M	204	CDL	OA9-CA7-OA8-CA6
30	M	205	CDL	OA9-CA7-OA8-CA6
30	P	202	CDL	OB9-CB7-OB8-CB6
30	a	501	CDL	OA9-CA7-OA8-CA6
30	d	201	CDL	OA9-CA7-OA8-CA6
30	m	201	CDL	OA9-CA7-OA8-CA6
30	p	201	CDL	OA9-CA7-OA8-CA6
30	A	501	CDL	OB7-CB5-OB6-CB4
30	A	502	CDL	OA7-CA5-OA6-CA4
30	A	505	CDL	OB7-CB5-OB6-CB4
30	a	501	CDL	OB7-CB5-OB6-CB4
30	a	505	CDL	OB7-CB5-OB6-CB4
30	A	501	CDL	C31-CA7-OA8-CA6
30	D	201	CDL	C31-CA7-OA8-CA6
30	M	204	CDL	C31-CA7-OA8-CA6
30	P	201	CDL	C31-CA7-OA8-CA6
30	P	202	CDL	C71-CB7-OB8-CB6
30	a	501	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
30	m	201	CDL	C31-CA7-OA8-CA6
32	K	201	LPP	C30-C29-O27-C8
32	k	201	LPP	C30-C29-O27-C8
30	A	502	CDL	C11-CA5-OA6-CA4
30	A	502	CDL	C51-CB5-OB6-CB4
30	A	504	CDL	C11-CA5-OA6-CA4
30	a	502	CDL	C51-CB5-OB6-CB4
30	a	504	CDL	C11-CA5-OA6-CA4
32	K	201	LPP	C12-C11-O9-C7
32	k	201	LPP	C12-C11-O9-C7
30	P	201	CDL	C71-CB7-OB8-CB6
30	p	201	CDL	C71-CB7-OB8-CB6
31	g	201	LMT	C4B-C5B-C6B-O6B
30	P	201	CDL	OB9-CB7-OB8-CB6
30	P	202	CDL	OA9-CA7-OA8-CA6
30	p	201	CDL	OB9-CB7-OB8-CB6
32	N	203	LPP	O28-C29-O27-C8
32	n	201	LPP	O28-C29-O27-C8
31	d	202	LMT	O5B-C5B-C6B-O6B
31	F	302	LMT	C4B-C5B-C6B-O6B
30	A	503	CDL	O1-C1-CA2-OA2
30	O	201	CDL	O1-C1-CA2-OA2
30	a	503	CDL	O1-C1-CA2-OA2
30	o	201	CDL	O1-C1-CA2-OA2
30	R	101	CDL	C31-CA7-OA8-CA6
33	P	203	TRT	C4-C1-C5-C6
33	p	202	TRT	C4-C1-C5-C6
31	D	202	LMT	O5B-C5B-C6B-O6B
30	M	204	CDL	C11-CA5-OA6-CA4
31	Q	101	LMT	C4B-C5B-C6B-O6B
30	P	202	CDL	C31-CA7-OA8-CA6
30	r	101	CDL	C31-CA7-OA8-CA6
32	N	203	LPP	C30-C29-O27-C8
32	n	201	LPP	C30-C29-O27-C8
31	N	204	LMT	C4'-C5'-C6'-O6'
33	P	203	TRT	O15-C16-C17-O18
33	p	202	TRT	O15-C16-C17-O18
33	AR	201	TRT	C13-C12-O15-C16
33	BR	201	TRT	C13-C12-O15-C16
33	p	202	TRT	O21-C22-C23-O24
30	R	101	CDL	OA9-CA7-OA8-CA6
31	N	204	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
31	n	202	LMT	O5'-C1'-O1'-C1
33	G	202	TRT	O21-C22-C23-O24
33	P	203	TRT	O21-C22-C23-O24
33	g	203	TRT	O21-C22-C23-O24
31	N	204	LMT	O5'-C5'-C6'-O6'
31	q	101	LMT	C4B-C5B-C6B-O6B
33	AR	201	TRT	C11-C12-O15-C16
33	BR	201	TRT	C11-C12-O15-C16
31	g	201	LMT	O5B-C5B-C6B-O6B
33	P	203	TRT	C2-C1-C5-C6
33	P	203	TRT	C3-C1-C5-C6
33	p	202	TRT	C2-C1-C5-C6
33	p	202	TRT	C3-C1-C5-C6
30	r	101	CDL	OA9-CA7-OA8-CA6
31	F	302	LMT	O5B-C5B-C6B-O6B
30	m	201	CDL	C11-CA5-OA6-CA4
33	N	201	TRT	C13-C12-O15-C16
33	n	203	TRT	C13-C12-O15-C16
31	n	202	LMT	O5B-C5B-C6B-O6B
30	A	502	CDL	C74-C75-C76-C77
30	a	502	CDL	C74-C75-C76-C77
33	N	201	TRT	C11-C12-O15-C16
33	n	203	TRT	C11-C12-O15-C16
30	A	505	CDL	CB2-C1-CA2-OA2
30	a	505	CDL	CB2-C1-CA2-OA2
30	A	503	CDL	C71-CB7-OB8-CB6
30	A	505	CDL	C71-CB7-OB8-CB6
30	E	101	CDL	C71-CB7-OB8-CB6
30	a	503	CDL	C71-CB7-OB8-CB6
30	a	505	CDL	C71-CB7-OB8-CB6
30	e	101	CDL	C71-CB7-OB8-CB6
32	K	201	LPP	C37-C38-C39-C40
32	k	201	LPP	C37-C38-C39-C40
33	G	201	TRT	O18-C19-C20-O21
33	g	202	TRT	O18-C19-C20-O21
30	M	205	CDL	C71-C72-C73-C74
31	N	204	LMT	O5B-C5B-C6B-O6B
33	P	203	TRT	C13-C12-O15-C16
33	p	202	TRT	C13-C12-O15-C16
31	N	204	LMT	C2'-C1'-O1'-C1
31	n	202	LMT	C2'-C1'-O1'-C1
30	M	201	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
33	AR	201	TRT	O21-C22-C23-O24
33	BR	201	TRT	O21-C22-C23-O24
30	A	502	CDL	O1-C1-CB2-OB2
30	E	101	CDL	OB9-CB7-OB8-CB6
30	e	101	CDL	OB9-CB7-OB8-CB6
30	a	505	CDL	C75-C76-C77-C78
33	P	203	TRT	C11-C12-O15-C16
33	p	202	TRT	C11-C12-O15-C16
30	A	505	CDL	C75-C76-C77-C78
33	g	202	TRT	C11-C12-O15-C16
30	A	504	CDL	CB5-C51-C52-C53
30	A	505	CDL	OB9-CB7-OB8-CB6
30	a	505	CDL	OB9-CB7-OB8-CB6
31	d	202	LMT	C4B-C5B-C6B-O6B
33	G	201	TRT	C11-C12-O15-C16
30	M	204	CDL	OA5-CA3-CA4-OA6
30	E	101	CDL	OB6-CB4-CB6-OB8
30	e	101	CDL	OB6-CB4-CB6-OB8
30	a	504	CDL	CB5-C51-C52-C53
33	G	201	TRT	C13-C12-O15-C16
33	g	202	TRT	C13-C12-O15-C16
33	AE	600	TRT	O15-C16-C17-O18
33	BE	600	TRT	O15-C16-C17-O18
30	P	202	CDL	CB5-C51-C52-C53
33	P	203	TRT	C1-C5-C6-C7
33	p	202	TRT	C1-C5-C6-C7
33	BR	201	TRT	C1-C5-C6-C8
31	Q	101	LMT	O5B-C5B-C6B-O6B
31	D	202	LMT	C4B-C5B-C6B-O6B
31	n	202	LMT	C4'-C5'-C6'-O6'
30	A	502	CDL	C31-CA7-OA8-CA6
30	P	202	CDL	C57-C58-C59-C60
31	q	101	LMT	O5B-C5B-C6B-O6B
30	A	504	CDL	CA5-C11-C12-C13
30	M	204	CDL	OA7-CA5-OA6-CA4
33	G	202	TRT	C11-C12-O15-C16
33	g	203	TRT	C11-C12-O15-C16
30	A	503	CDL	CB5-C51-C52-C53
30	a	503	CDL	CB5-C51-C52-C53
32	N	203	LPP	C29-C30-C31-C32
32	n	201	LPP	C29-C30-C31-C32
30	A	503	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
30	A	503	CDL	C31-CA7-OA8-CA6
33	G	202	TRT	C13-C12-O15-C16
33	g	203	TRT	C13-C12-O15-C16
33	AR	201	TRT	O18-C19-C20-O21
33	BR	201	TRT	O18-C19-C20-O21
30	a	503	CDL	C31-CA7-OA8-CA6
30	a	503	CDL	OB9-CB7-OB8-CB6
30	P	202	CDL	CA5-C11-C12-C13
30	m	201	CDL	OA7-CA5-OA6-CA4
30	a	501	CDL	C72-C73-C74-C75
30	A	504	CDL	CA7-C31-C32-C33
30	a	504	CDL	CA7-C31-C32-C33
30	A	501	CDL	C72-C73-C74-C75
33	N	202	TRT	O18-C19-C20-O21
33	n	204	TRT	O18-C19-C20-O21
31	Q	101	LMT	O5'-C5'-C6'-O6'
33	P	203	TRT	C1-C5-C6-C8
33	p	202	TRT	C1-C5-C6-C8
33	AR	201	TRT	C1-C5-C6-C8
30	a	502	CDL	C31-CA7-OA8-CA6
30	R	101	CDL	CA5-C11-C12-C13
30	E	101	CDL	CA2-C1-CB2-OB2
30	e	101	CDL	CA2-C1-CB2-OB2
31	d	202	LMT	O5'-C5'-C6'-O6'
30	a	505	CDL	C78-C79-C80-C81
31	q	101	LMT	O5'-C5'-C6'-O6'
30	A	505	CDL	C78-C79-C80-C81
33	P	203	TRT	C5-C6-C9-C14
33	p	202	TRT	C5-C6-C9-C14
31	g	201	LMT	O1'-C1-C2-C3
30	a	502	CDL	O1-C1-CB2-OB2
30	m	201	CDL	O1-C1-CB2-OB2
31	F	302	LMT	O1'-C1-C2-C3
31	n	202	LMT	C4B-C5B-C6B-O6B
30	A	503	CDL	OA9-CA7-OA8-CA6
33	N	202	TRT	C13-C12-O15-C16
33	n	204	TRT	C13-C12-O15-C16
30	r	101	CDL	CA5-C11-C12-C13
30	A	502	CDL	OA9-CA7-OA8-CA6
30	a	503	CDL	OA9-CA7-OA8-CA6
30	R	101	CDL	OB7-CB5-OB6-CB4
30	R	101	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
30	r	101	CDL	C51-CB5-OB6-CB4
33	N	202	TRT	C11-C12-O15-C16
33	M	202	TRT	O15-C16-C17-O18
33	m	202	TRT	O15-C16-C17-O18
33	m	203	TRT	C13-C12-O15-C16
33	M	203	TRT	C13-C12-O15-C16
33	n	204	TRT	C11-C12-O15-C16
30	A	502	CDL	C13-C14-C15-C16
30	M	204	CDL	C13-C14-C15-C16
30	m	201	CDL	C13-C14-C15-C16
32	O	203	LPP	C17-C18-C19-C20
32	o	203	LPP	C17-C18-C19-C20
30	A	503	CDL	C72-C73-C74-C75
30	D	201	CDL	C17-C18-C19-C20
30	E	101	CDL	C72-C73-C74-C75
30	M	204	CDL	C71-C72-C73-C74
30	a	502	CDL	C13-C14-C15-C16
30	d	201	CDL	C17-C18-C19-C20
30	m	201	CDL	C71-C72-C73-C74
30	M	204	CDL	C73-C74-C75-C76
30	m	201	CDL	C32-C33-C34-C35
30	a	502	CDL	OA9-CA7-OA8-CA6
30	A	501	CDL	C17-C18-C19-C20
30	A	503	CDL	C74-C75-C76-C77
30	a	503	CDL	C74-C75-C76-C77
30	m	201	CDL	C73-C74-C75-C76
30	r	101	CDL	C55-C56-C57-C58
32	i	101	LPP	C21-C22-C23-C24
30	P	201	CDL	OA7-CA5-OA6-CA4
30	r	101	CDL	OB7-CB5-OB6-CB4
30	M	204	CDL	C32-C33-C34-C35
30	e	101	CDL	C72-C73-C74-C75
32	I	101	LPP	C21-C22-C23-C24
30	A	505	CDL	CA5-C11-C12-C13
33	P	203	TRT	C5-C6-C9-C10
33	p	202	TRT	C5-C6-C9-C10
30	R	101	CDL	C55-C56-C57-C58
30	a	501	CDL	C17-C18-C19-C20
32	O	203	LPP	C18-C19-C20-C21
32	o	203	LPP	C18-C19-C20-C21
30	D	201	CDL	C11-CA5-OA6-CA4
30	D	201	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
30	P	201	CDL	C11-CA5-OA6-CA4
30	d	201	CDL	C11-CA5-OA6-CA4
30	d	201	CDL	C51-CB5-OB6-CB4
30	e	101	CDL	C11-CA5-OA6-CA4
30	p	201	CDL	C11-CA5-OA6-CA4
33	G	201	TRT	O21-C22-C23-O24
33	g	202	TRT	O21-C22-C23-O24
31	n	202	LMT	C11-C10-C9-C8
32	I	101	LPP	C35-C36-C37-C38
32	i	101	LPP	C35-C36-C37-C38
30	M	204	CDL	O1-C1-CB2-OB2
33	m	203	TRT	C11-C12-O15-C16
30	A	505	CDL	C72-C73-C74-C75
30	D	201	CDL	C42-C43-C44-C45
30	a	502	CDL	C60-C61-C62-C63
30	a	505	CDL	C72-C73-C74-C75
31	N	204	LMT	C11-C10-C9-C8
30	A	502	CDL	C60-C61-C62-C63
30	A	505	CDL	C37-C38-C39-C40
30	P	202	CDL	C18-C19-C20-C21
30	d	201	CDL	C42-C43-C44-C45
30	a	503	CDL	C72-C73-C74-C75
30	a	505	CDL	C37-C38-C39-C40
30	a	504	CDL	CA5-C11-C12-C13
33	M	203	TRT	C11-C12-O15-C16
30	a	501	CDL	CB7-C71-C72-C73
30	m	201	CDL	C79-C80-C81-C82
31	N	204	LMT	C4B-C5B-C6B-O6B
30	e	101	CDL	OA7-CA5-OA6-CA4
30	A	505	CDL	C77-C78-C79-C80
30	M	204	CDL	C79-C80-C81-C82
30	a	505	CDL	C77-C78-C79-C80
31	n	202	LMT	O5'-C5'-C6'-O6'
30	A	502	CDL	C72-C73-C74-C75
30	a	502	CDL	C72-C73-C74-C75
33	M	202	TRT	C5-C6-C9-C10
33	m	202	TRT	C5-C6-C9-C10
30	e	101	CDL	C71-C72-C73-C74
30	P	202	CDL	C31-C32-C33-C34
32	K	201	LPP	C30-C31-C32-C33
32	k	201	LPP	C30-C31-C32-C33
30	A	501	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
30	M	201	CDL	CA5-C11-C12-C13
30	M	205	CDL	CA5-C11-C12-C13
30	a	505	CDL	CA5-C11-C12-C13
30	P	202	CDL	C55-C56-C57-C58
30	E	101	CDL	C11-CA5-OA6-CA4
30	M	201	CDL	C11-CA5-OA6-CA4
30	M	204	CDL	C51-CB5-OB6-CB4
30	P	202	CDL	C51-CB5-OB6-CB4
30	m	201	CDL	C51-CB5-OB6-CB4
30	P	201	CDL	C72-C73-C74-C75
30	R	101	CDL	C57-C58-C59-C60
30	r	101	CDL	C57-C58-C59-C60
30	O	201	CDL	C71-C72-C73-C74
30	p	201	CDL	C72-C73-C74-C75
30	r	101	CDL	C36-C37-C38-C39
31	n	202	LMT	C3-C4-C5-C6
30	P	202	CDL	C15-C16-C17-C18
30	D	201	CDL	OA7-CA5-OA6-CA4
30	E	101	CDL	OA7-CA5-OA6-CA4
30	d	201	CDL	OA7-CA5-OA6-CA4
30	d	201	CDL	OB7-CB5-OB6-CB4
30	p	201	CDL	OA7-CA5-OA6-CA4
30	E	101	CDL	C71-C72-C73-C74
30	R	101	CDL	C36-C37-C38-C39
30	o	201	CDL	C71-C72-C73-C74
31	N	204	LMT	C3-C4-C5-C6
32	K	201	LPP	C32-C33-C34-C35
32	O	203	LPP	C19-C20-C21-C22
32	k	201	LPP	C32-C33-C34-C35
32	o	203	LPP	C19-C20-C21-C22
31	D	202	LMT	C3-C4-C5-C6
31	d	202	LMT	C3-C4-C5-C6
30	A	505	CDL	C74-C75-C76-C77
33	g	203	TRT	C5-C6-C9-C10
30	a	505	CDL	C74-C75-C76-C77
30	D	201	CDL	O1-C1-CB2-OB2
30	d	201	CDL	O1-C1-CB2-OB2
30	A	505	CDL	C34-C35-C36-C37
30	a	505	CDL	C34-C35-C36-C37
30	A	503	CDL	C11-CA5-OA6-CA4
30	A	503	CDL	C51-CB5-OB6-CB4
30	A	505	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
30	M	201	CDL	C51-CB5-OB6-CB4
30	M	205	CDL	C11-CA5-OA6-CA4
30	M	205	CDL	C51-CB5-OB6-CB4
30	O	201	CDL	C51-CB5-OB6-CB4
30	a	503	CDL	C11-CA5-OA6-CA4
30	a	503	CDL	C51-CB5-OB6-CB4
30	a	505	CDL	C11-CA5-OA6-CA4
30	o	201	CDL	C51-CB5-OB6-CB4
32	N	203	LPP	C12-C11-O9-C7
32	n	201	LPP	C12-C11-O9-C7
30	m	201	CDL	CB7-C71-C72-C73
30	A	503	CDL	OA7-CA5-OA6-CA4
30	A	503	CDL	OB7-CB5-OB6-CB4
30	a	503	CDL	OA7-CA5-OA6-CA4
30	a	503	CDL	OB7-CB5-OB6-CB4
30	o	201	CDL	OB7-CB5-OB6-CB4
30	a	503	CDL	C21-C22-C23-C24
30	M	204	CDL	C82-C83-C84-C85
30	m	201	CDL	C82-C83-C84-C85
30	A	503	CDL	C21-C22-C23-C24
30	M	204	CDL	CB7-C71-C72-C73
30	a	503	CDL	C33-C34-C35-C36
30	A	503	CDL	C33-C34-C35-C36
33	M	202	TRT	C5-C6-C9-C14
33	m	202	TRT	C5-C6-C9-C14
31	Q	101	LMT	C1-C2-C3-C4
31	q	101	LMT	C1-C2-C3-C4
30	D	201	CDL	CB5-C51-C52-C53
30	d	201	CDL	CB5-C51-C52-C53
30	A	505	CDL	OA7-CA5-OA6-CA4
30	D	201	CDL	OB7-CB5-OB6-CB4
30	M	205	CDL	OB7-CB5-OB6-CB4
30	O	201	CDL	OB7-CB5-OB6-CB4
30	M	204	CDL	C77-C78-C79-C80
30	m	201	CDL	C77-C78-C79-C80
30	A	503	CDL	C31-C32-C33-C34
30	a	503	CDL	C31-C32-C33-C34
33	G	202	TRT	C5-C6-C9-C10
33	n	204	TRT	C5-C6-C9-C10
30	M	205	CDL	C1-CA2-OA2-PA1
30	R	101	CDL	C62-C63-C64-C65
30	M	205	CDL	C53-C54-C55-C56

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Mol	Chain	Res	Type	Atoms
30	r	101	CDL	C62-C63-C64-C65
30	A	504	CDL	C74-C75-C76-C77
32	k	201	LPP	C36-C37-C38-C39
30	R	101	CDL	C74-C75-C76-C77
30	a	504	CDL	C74-C75-C76-C77
32	K	201	LPP	C36-C37-C38-C39
30	E	101	CDL	C56-C57-C58-C59
30	a	502	CDL	C11-C12-C13-C14
31	D	202	LMT	O5'-C5'-C6'-O6'
30	r	101	CDL	C74-C75-C76-C77
33	g	203	TRT	C5-C6-C9-C14
33	n	204	TRT	C5-C6-C9-C14
30	M	204	CDL	C74-C75-C76-C77
30	m	201	CDL	C74-C75-C76-C77
30	A	503	CDL	OB5-CB3-CB4-CB6
30	A	505	CDL	OA5-CA3-CA4-CA6
30	E	101	CDL	OA5-CA3-CA4-CA6
30	P	202	CDL	OA5-CA3-CA4-CA6
30	a	503	CDL	OB5-CB3-CB4-CB6
30	a	505	CDL	OA5-CA3-CA4-CA6
30	e	101	CDL	OA5-CA3-CA4-CA6
30	a	505	CDL	OA7-CA5-OA6-CA4
30	A	502	CDL	C11-C12-C13-C14
30	A	502	CDL	C23-C24-C25-C26
30	a	502	CDL	C23-C24-C25-C26
30	e	101	CDL	C56-C57-C58-C59
32	I	101	LPP	C30-C29-O27-C8
32	i	101	LPP	C30-C29-O27-C8
31	d	202	LMT	O1'-C1-C2-C3
33	G	202	TRT	C5-C6-C9-C14
33	N	202	TRT	C5-C6-C9-C14
33	N	202	TRT	C5-C6-C9-C10
30	M	201	CDL	OB7-CB5-OB6-CB4
30	M	204	CDL	OB7-CB5-OB6-CB4
30	M	205	CDL	OA7-CA5-OA6-CA4
30	P	202	CDL	OB7-CB5-OB6-CB4
30	m	201	CDL	OB7-CB5-OB6-CB4
31	D	202	LMT	O1'-C1-C2-C3
30	a	501	CDL	C34-C35-C36-C37
30	e	101	CDL	CB3-CB4-CB6-OB8
30	E	101	CDL	C63-C64-C65-C66
30	M	201	CDL	C53-C54-C55-C56

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Mol	Chain	Res	Type	Atoms
30	A	501	CDL	C34-C35-C36-C37
30	e	101	CDL	C63-C64-C65-C66
30	o	201	CDL	C55-C56-C57-C58
30	O	201	CDL	C55-C56-C57-C58
30	M	201	CDL	C1-CA2-OA2-PA1
32	k	201	LPP	C34-C35-C36-C37
32	f	301	LPP	C6-O5-P1-O3
32	K	201	LPP	C34-C35-C36-C37
32	K	201	LPP	C11-C12-C13-C14
30	M	205	CDL	C73-C74-C75-C76
30	P	201	CDL	CA6-CA4-OA6-CA5
30	p	201	CDL	CA6-CA4-OA6-CA5
30	A	502	CDL	C20-C21-C22-C23
30	a	502	CDL	C20-C21-C22-C23
32	k	201	LPP	C11-C12-C13-C14
30	A	502	CDL	C75-C76-C77-C78
30	a	502	CDL	C75-C76-C77-C78
30	M	204	CDL	OB5-CB3-CB4-OB6
30	m	201	CDL	OB5-CB3-CB4-OB6
30	M	204	CDL	C71-CB7-OB8-CB6
30	m	201	CDL	C71-CB7-OB8-CB6
30	M	201	CDL	C73-C74-C75-C76
30	P	202	CDL	C41-C42-C43-C44
30	R	101	CDL	OB6-CB4-CB6-OB8
30	o	201	CDL	OA6-CA4-CA6-OA8
30	r	101	CDL	OB6-CB4-CB6-OB8
30	A	501	CDL	C55-C56-C57-C58
30	M	205	CDL	C51-C52-C53-C54
30	O	201	CDL	C15-C16-C17-C18
30	P	202	CDL	C37-C38-C39-C40
30	a	501	CDL	C55-C56-C57-C58
32	I	101	LPP	O28-C29-O27-C8
30	E	101	CDL	C53-C54-C55-C56
30	O	201	CDL	C20-C21-C22-C23
30	P	202	CDL	C79-C80-C81-C82
30	o	201	CDL	C20-C21-C22-C23
30	a	505	CDL	C43-C44-C45-C46
30	o	201	CDL	C15-C16-C17-C18
31	F	302	LMT	C5-C6-C7-C8
32	i	101	LPP	O28-C29-O27-C8
30	A	505	CDL	C43-C44-C45-C46
31	g	201	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
34	AB	601	ATP	PG-O3B-PB-O1B
34	AC	601	ATP	PG-O3B-PB-O1B
34	BB	601	ATP	PG-O3B-PB-O1B
34	BC	601	ATP	PG-O3B-PB-O1B
30	P	202	CDL	C81-C82-C83-C84
32	K	201	LPP	C38-C39-C40-C41
32	k	201	LPP	C38-C39-C40-C41
32	N	203	LPP	C32-C33-C34-C35
33	g	202	TRT	O15-C16-C17-O18
32	n	201	LPP	C32-C33-C34-C35
33	G	201	TRT	O15-C16-C17-O18
30	D	201	CDL	C71-CB7-OB8-CB6
30	d	201	CDL	C71-CB7-OB8-CB6
30	M	201	CDL	OA7-CA5-OA6-CA4
32	N	203	LPP	O10-C11-O9-C7
32	n	201	LPP	O10-C11-O9-C7
30	e	101	CDL	C53-C54-C55-C56
30	m	201	CDL	C72-C73-C74-C75
30	a	503	CDL	C52-C53-C54-C55
30	A	502	CDL	C73-C74-C75-C76
30	M	204	CDL	C72-C73-C74-C75
30	D	201	CDL	OB5-CB3-CB4-CB6
30	M	204	CDL	OA5-CA3-CA4-CA6
30	P	201	CDL	OA5-CA3-CA4-CA6
30	d	201	CDL	OB5-CB3-CB4-CB6
30	m	201	CDL	OA5-CA3-CA4-CA6
30	a	502	CDL	C73-C74-C75-C76
33	M	202	TRT	O18-C19-C20-O21
33	m	202	TRT	O18-C19-C20-O21
32	N	203	LPP	C13-C14-C15-C16
32	n	201	LPP	C13-C14-C15-C16
30	r	101	CDL	C59-C60-C61-C62
30	P	202	CDL	CA7-C31-C32-C33
30	R	101	CDL	C59-C60-C61-C62
30	E	101	CDL	CB3-CB4-CB6-OB8
30	M	201	CDL	CB3-CB4-CB6-OB8
30	M	205	CDL	CB3-CB4-CB6-OB8
30	R	101	CDL	CA3-CA4-CA6-OA8
30	R	101	CDL	CB3-CB4-CB6-OB8
30	r	101	CDL	CA3-CA4-CA6-OA8
30	r	101	CDL	CB3-CB4-CB6-OB8
33	P	203	TRT	C17-C16-O15-C12

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Mol	Chain	Res	Type	Atoms
30	P	202	CDL	C59-C60-C61-C62
30	A	503	CDL	C52-C53-C54-C55
30	E	101	CDL	OB5-CB3-CB4-OB6
30	d	201	CDL	OA5-CA3-CA4-OA6
30	e	101	CDL	OB5-CB3-CB4-OB6
30	A	502	CDL	C31-C32-C33-C34
33	p	202	TRT	C17-C16-O15-C12
33	AR	201	TRT	O15-C16-C17-O18
30	A	504	CDL	CA4-CA3-OA5-PA1
30	a	504	CDL	CA4-CA3-OA5-PA1
30	o	201	CDL	C1-CB2-OB2-PB2
33	BR	201	TRT	O15-C16-C17-O18
30	M	205	CDL	OB6-CB4-CB6-OB8
30	O	201	CDL	OA6-CA4-CA6-OA8
30	P	202	CDL	OB6-CB4-CB6-OB8
32	F	301	LPP	O9-C7-C8-O27
32	f	301	LPP	O9-C7-C8-O27
33	AR	201	TRT	C22-C23-O24-C25
33	BR	201	TRT	C22-C23-O24-C25
30	A	503	CDL	C71-C72-C73-C74
30	a	502	CDL	C31-C32-C33-C34
30	M	204	CDL	OB9-CB7-OB8-CB6
33	P	203	TRT	C22-C23-O24-C25
33	p	202	TRT	C22-C23-O24-C25
32	F	301	LPP	C12-C13-C14-C15
32	f	301	LPP	C12-C13-C14-C15
30	A	501	CDL	C15-C16-C17-C18
30	e	101	CDL	C51-C52-C53-C54
30	a	503	CDL	C71-C72-C73-C74
30	m	201	CDL	OB9-CB7-OB8-CB6
31	D	202	LMT	C6-C7-C8-C9
33	M	203	TRT	C1-C5-C6-C8
33	m	203	TRT	C1-C5-C6-C8
33	BE	600	TRT	C1-C5-C6-C8
30	O	201	CDL	CB2-C1-CA2-OA2
30	o	201	CDL	CB2-C1-CA2-OA2
30	A	505	CDL	C53-C54-C55-C56
30	D	201	CDL	C12-C13-C14-C15
30	P	202	CDL	C38-C39-C40-C41
30	e	101	CDL	C62-C63-C64-C65
31	d	202	LMT	C6-C7-C8-C9
30	d	201	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
30	E	101	CDL	C62-C63-C64-C65
30	A	501	CDL	OB5-CB3-CB4-CB6
30	o	201	CDL	OB5-CB3-CB4-CB6
30	p	201	CDL	OA5-CA3-CA4-CA6
30	P	202	CDL	C72-C73-C74-C75
31	q	101	LMT	C3-C4-C5-C6
30	a	505	CDL	C53-C54-C55-C56
31	Q	101	LMT	C3-C4-C5-C6
30	d	201	CDL	OB9-CB7-OB8-CB6
33	N	202	TRT	C22-C23-O24-C25
33	n	204	TRT	C22-C23-O24-C25
30	E	101	CDL	C12-C11-CA5-OA6
30	e	101	CDL	C12-C11-CA5-OA6
30	D	201	CDL	OB9-CB7-OB8-CB6
30	A	504	CDL	C53-C54-C55-C56
30	p	201	CDL	C32-C33-C34-C35
33	m	203	TRT	O18-C19-C20-O21
30	a	505	CDL	CA6-CA4-OA6-CA5
31	g	201	LMT	O5'-C5'-C6'-O6'
33	M	203	TRT	O18-C19-C20-O21
30	a	501	CDL	C15-C16-C17-C18
33	AE	600	TRT	C1-C5-C6-C8
33	G	201	TRT	C16-C17-O18-C19
33	g	202	TRT	C16-C17-O18-C19
30	a	504	CDL	C53-C54-C55-C56
30	A	505	CDL	OA5-CA3-CA4-OA6
30	D	201	CDL	OA5-CA3-CA4-OA6
30	D	201	CDL	OB5-CB3-CB4-OB6
30	a	505	CDL	OA5-CA3-CA4-OA6
30	d	201	CDL	OB5-CB3-CB4-OB6
30	e	101	CDL	OA5-CA3-CA4-OA6
30	o	201	CDL	OB5-CB3-CB4-OB6
32	N	203	LPP	O5-C6-C7-O9
32	n	201	LPP	O5-C6-C7-O9
33	N	202	TRT	C16-C17-O18-C19
33	n	204	TRT	C16-C17-O18-C19
30	A	505	CDL	C13-C14-C15-C16
30	A	504	CDL	CA3-CA4-CA6-OA8
30	P	202	CDL	CB3-CB4-CB6-OB8
30	a	504	CDL	CA3-CA4-CA6-OA8
30	o	201	CDL	CA3-CA4-CA6-OA8
32	f	301	LPP	C6-C7-C8-O27

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Mol	Chain	Res	Type	Atoms
33	AE	600	TRT	C5-C6-C9-C10
33	BE	600	TRT	C5-C6-C9-C10
30	A	501	CDL	C11-CA5-OA6-CA4
30	a	501	CDL	C11-CA5-OA6-CA4
30	E	101	CDL	C51-C52-C53-C54
30	R	101	CDL	C75-C76-C77-C78
30	a	505	CDL	C39-C40-C41-C42
30	r	101	CDL	C75-C76-C77-C78
31	F	302	LMT	C11-C10-C9-C8
31	g	201	LMT	C11-C10-C9-C8
30	A	505	CDL	C39-C40-C41-C42
30	a	505	CDL	C13-C14-C15-C16
30	r	101	CDL	C72-C73-C74-C75
30	R	101	CDL	OA6-CA4-CA6-OA8
30	r	101	CDL	OA6-CA4-CA6-OA8
33	M	203	TRT	C16-C17-O18-C19
33	m	203	TRT	C16-C17-O18-C19
30	R	101	CDL	C31-C32-C33-C34
30	R	101	CDL	C72-C73-C74-C75
30	D	201	CDL	C11-C12-C13-C14
30	M	201	CDL	C51-C52-C53-C54
30	P	202	CDL	C74-C75-C76-C77
30	r	101	CDL	CA7-C31-C32-C33
30	d	201	CDL	C11-C12-C13-C14
30	r	101	CDL	C31-C32-C33-C34
32	k	201	LPP	C35-C36-C37-C38
30	P	202	CDL	C20-C21-C22-C23
32	K	201	LPP	C35-C36-C37-C38
30	A	502	CDL	CA2-C1-CB2-OB2
30	A	502	CDL	C76-C77-C78-C79
30	a	501	CDL	C51-C52-C53-C54
30	P	201	CDL	C32-C33-C34-C35
30	A	501	CDL	C51-C52-C53-C54
30	e	101	CDL	CA7-C31-C32-C33
30	A	503	CDL	C18-C19-C20-C21
30	A	505	CDL	C31-C32-C33-C34
33	g	203	TRT	C17-C16-O15-C12
33	AR	201	TRT	C17-C16-O15-C12
33	AR	201	TRT	C1-C5-C6-C9
33	BR	201	TRT	C1-C5-C6-C9
30	a	501	CDL	C58-C59-C60-C61
33	G	202	TRT	C17-C16-O15-C12

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Mol	Chain	Res	Type	Atoms
30	O	201	CDL	OB5-CB3-CB4-CB6
30	a	501	CDL	OB5-CB3-CB4-CB6
30	m	201	CDL	OB5-CB3-CB4-CB6
32	N	203	LPP	O5-C6-C7-C8
32	n	201	LPP	O5-C6-C7-C8
30	A	501	CDL	OA7-CA5-OA6-CA4
30	A	501	CDL	C58-C59-C60-C61
30	a	502	CDL	C76-C77-C78-C79
30	d	201	CDL	C53-C54-C55-C56
30	m	201	CDL	C17-C18-C19-C20
33	N	201	TRT	O21-C22-C23-O24
30	a	503	CDL	C18-C19-C20-C21
30	a	501	CDL	CA7-C31-C32-C33
30	A	505	CDL	C1-CA2-OA2-PA1
30	a	501	CDL	CB4-CB3-OB5-PB2
30	o	201	CDL	C1-CA2-OA2-PA1
30	M	204	CDL	C81-C82-C83-C84
33	n	203	TRT	O21-C22-C23-O24
30	a	501	CDL	OA7-CA5-OA6-CA4
30	A	503	CDL	OB5-CB3-CB4-OB6
30	E	101	CDL	OA5-CA3-CA4-OA6
30	O	201	CDL	OB5-CB3-CB4-OB6
30	a	503	CDL	OB5-CB3-CB4-OB6
32	O	202	LPP	C13-C14-C15-C16
30	P	202	CDL	C53-C54-C55-C56
30	r	101	CDL	C63-C64-C65-C66
33	n	203	TRT	C1-C5-C6-C8
30	A	501	CDL	CA7-C31-C32-C33
30	M	204	CDL	C17-C18-C19-C20
30	D	201	CDL	C53-C54-C55-C56
33	AE	600	TRT	C5-C6-C9-C14
30	R	101	CDL	C63-C64-C65-C66
30	M	201	CDL	OB6-CB4-CB6-OB8
30	a	505	CDL	OA6-CA4-CA6-OA8
30	m	201	CDL	C81-C82-C83-C84
33	n	203	TRT	C17-C16-O15-C12
30	A	505	CDL	CB3-CB4-CB6-OB8
30	a	505	CDL	CB3-CB4-CB6-OB8
32	F	301	LPP	C6-C7-C8-O27
32	o	202	LPP	C13-C14-C15-C16
30	M	205	CDL	C12-C11-CA5-OA6
30	m	201	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
33	BE	600	TRT	C5-C6-C9-C14
30	M	204	CDL	C80-C81-C82-C83
30	M	204	CDL	C16-C17-C18-C19
30	R	101	CDL	CA7-C31-C32-C33
33	N	201	TRT	C1-C5-C6-C8
30	a	505	CDL	C31-C32-C33-C34
32	o	203	LPP	C12-C13-C14-C15
30	O	201	CDL	C72-C71-CB7-OB8
33	AE	600	TRT	C1-C5-C6-C9
33	BE	600	TRT	C1-C5-C6-C9
32	O	203	LPP	C12-C13-C14-C15
30	A	501	CDL	CB3-OB5-PB2-OB3
30	A	502	CDL	CA3-OA5-PA1-OA2
30	A	502	CDL	CA3-OA5-PA1-OA3
30	A	502	CDL	CA3-OA5-PA1-OA4
30	A	504	CDL	CB2-OB2-PB2-OB3
30	D	201	CDL	CA2-OA2-PA1-OA5
30	D	201	CDL	CB2-OB2-PB2-OB4
30	E	101	CDL	CA2-OA2-PA1-OA3
30	E	101	CDL	CA2-OA2-PA1-OA5
30	E	101	CDL	CB2-OB2-PB2-OB4
30	E	101	CDL	CB3-OB5-PB2-OB4
30	M	201	CDL	CA2-OA2-PA1-OA3
30	M	201	CDL	CA3-OA5-PA1-OA2
30	M	201	CDL	CA3-OA5-PA1-OA3
30	M	201	CDL	CA3-OA5-PA1-OA4
30	M	201	CDL	CB3-OB5-PB2-OB2
30	M	201	CDL	CB3-OB5-PB2-OB3
30	M	201	CDL	CB3-OB5-PB2-OB4
30	M	204	CDL	CB2-OB2-PB2-OB3
30	M	205	CDL	CA2-OA2-PA1-OA3
30	M	205	CDL	CA3-OA5-PA1-OA2
30	M	205	CDL	CA3-OA5-PA1-OA3
30	M	205	CDL	CA3-OA5-PA1-OA4
30	M	205	CDL	CB3-OB5-PB2-OB2
30	M	205	CDL	CB3-OB5-PB2-OB3
30	M	205	CDL	CB3-OB5-PB2-OB4
30	O	201	CDL	CB2-OB2-PB2-OB4
30	P	201	CDL	CA2-OA2-PA1-OA4
30	P	201	CDL	CB2-OB2-PB2-OB4
30	P	202	CDL	CA3-OA5-PA1-OA2
30	P	202	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
30	a	501	CDL	CB3-OB5-PB2-OB3
30	a	502	CDL	CA3-OA5-PA1-OA2
30	a	502	CDL	CA3-OA5-PA1-OA3
30	a	502	CDL	CA3-OA5-PA1-OA4
30	a	504	CDL	CB2-OB2-PB2-OB3
30	d	201	CDL	CA2-OA2-PA1-OA5
30	d	201	CDL	CB2-OB2-PB2-OB4
30	e	101	CDL	CA2-OA2-PA1-OA3
30	e	101	CDL	CA2-OA2-PA1-OA4
30	e	101	CDL	CA2-OA2-PA1-OA5
30	e	101	CDL	CB2-OB2-PB2-OB4
30	m	201	CDL	CB2-OB2-PB2-OB3
30	o	201	CDL	CB2-OB2-PB2-OB4
30	p	201	CDL	CA2-OA2-PA1-OA4
30	p	201	CDL	CB2-OB2-PB2-OB4
34	AF	601	ATP	C5'-O5'-PA-O2A
34	BF	601	ATP	C5'-O5'-PA-O2A
30	P	202	CDL	C76-C77-C78-C79
30	A	501	CDL	CB4-CB3-OB5-PB2
30	A	505	CDL	CB4-CB3-OB5-PB2
30	M	201	CDL	CB4-CB3-OB5-PB2
30	M	205	CDL	CB4-CB3-OB5-PB2
30	O	201	CDL	C1-CA2-OA2-PA1
30	O	201	CDL	C1-CB2-OB2-PB2
30	P	202	CDL	C1-CA2-OA2-PA1
30	a	504	CDL	C1-CA2-OA2-PA1
30	a	505	CDL	C1-CA2-OA2-PA1
30	a	505	CDL	CB4-CB3-OB5-PB2
30	E	101	CDL	C73-C74-C75-C76
32	I	101	LPP	C18-C19-C20-C21
31	n	202	LMT	C5'-C4'-O1B-C1B
30	o	201	CDL	C72-C71-CB7-OB8
32	F	301	LPP	C6-O5-P1-O3
31	q	101	LMT	C7-C8-C9-C10
33	AE	600	TRT	C7-C6-C9-C10
30	m	201	CDL	C21-C22-C23-C24
31	Q	101	LMT	C7-C8-C9-C10
33	BE	600	TRT	C7-C6-C9-C10
30	M	204	CDL	C21-C22-C23-C24
30	A	502	CDL	CA6-CA4-OA6-CA5
30	A	503	CDL	CA6-CA4-OA6-CA5
30	A	505	CDL	CA6-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
30	E	101	CDL	CA6-CA4-OA6-CA5
30	a	502	CDL	CA6-CA4-OA6-CA5
30	a	503	CDL	CA6-CA4-OA6-CA5
30	e	101	CDL	CA6-CA4-OA6-CA5
30	E	101	CDL	CA7-C31-C32-C33
32	I	101	LPP	C31-C32-C33-C34
32	i	101	LPP	C31-C32-C33-C34
31	N	204	LMT	C5'-C4'-O1B-C1B
32	i	101	LPP	C18-C19-C20-C21
30	M	204	CDL	OB5-CB3-CB4-CB6
30	e	101	CDL	C73-C74-C75-C76
30	P	201	CDL	C71-C72-C73-C74
30	A	501	CDL	OB5-CB3-CB4-OB6
30	p	201	CDL	OA5-CA3-CA4-OA6
30	m	201	CDL	C80-C81-C82-C83
30	A	503	CDL	C55-C56-C57-C58
30	a	503	CDL	C55-C56-C57-C58
30	a	501	CDL	C20-C21-C22-C23
30	a	501	CDL	C12-C11-CA5-OA6
30	a	505	CDL	C73-C74-C75-C76
30	E	101	CDL	C32-C33-C34-C35
33	AE	600	TRT	C7-C6-C9-C14
33	M	203	TRT	C1-C5-C6-C9
33	m	203	TRT	C1-C5-C6-C9
30	A	501	CDL	C13-C14-C15-C16
30	A	503	CDL	C51-C52-C53-C54
30	A	501	CDL	C12-C11-CA5-OA6
30	M	201	CDL	C12-C11-CA5-OA6
32	I	101	LPP	C39-C40-C41-C42
32	i	101	LPP	C39-C40-C41-C42
30	o	201	CDL	C17-C18-C19-C20
33	N	201	TRT	C17-C16-O15-C12
33	BE	600	TRT	C7-C6-C9-C14
30	A	504	CDL	C32-C31-CA7-OA8
32	N	203	LPP	O9-C11-C12-C13
32	n	201	LPP	O9-C11-C12-C13
30	O	201	CDL	C17-C18-C19-C20
33	m	202	TRT	C20-C19-O18-C17
30	e	101	CDL	C32-C33-C34-C35
34	AB	601	ATP	PG-O3B-PB-O2B
34	AC	601	ATP	PG-O3B-PB-O2B
34	BB	601	ATP	PG-O3B-PB-O2B

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Mol	Chain	Res	Type	Atoms
34	BC	601	ATP	PG-O3B-PB-O2B
33	n	203	TRT	O15-C16-C17-O18
30	m	201	CDL	C75-C76-C77-C78
30	A	504	CDL	C75-C76-C77-C78
30	a	504	CDL	C75-C76-C77-C78
33	N	201	TRT	O15-C16-C17-O18
30	A	505	CDL	C32-C31-CA7-OA8
32	K	201	LPP	C39-C40-C41-C42
30	a	505	CDL	C81-C82-C83-C84
32	k	201	LPP	C39-C40-C41-C42
30	a	504	CDL	C32-C31-CA7-OA8
31	F	302	LMT	C2-C1-O1'-C1'
31	g	201	LMT	C2-C1-O1'-C1'
30	A	504	CDL	C1-CA2-OA2-PA1
33	G	202	TRT	O15-C16-C17-O18
30	a	502	CDL	C32-C33-C34-C35
33	g	203	TRT	O15-C16-C17-O18
30	A	505	CDL	C81-C82-C83-C84
33	N	201	TRT	C1-C5-C6-C9
33	n	203	TRT	C1-C5-C6-C9
33	BE	600	TRT	O21-C22-C23-O24
30	M	204	CDL	C75-C76-C77-C78
31	N	204	LMT	C2-C3-C4-C5
31	n	202	LMT	C2-C3-C4-C5
33	AE	600	TRT	O21-C22-C23-O24
30	A	505	CDL	C73-C74-C75-C76
33	m	203	TRT	O21-C22-C23-O24
30	a	501	CDL	C13-C14-C15-C16
33	M	203	TRT	O21-C22-C23-O24
31	g	201	LMT	C4'-C5'-C6'-O6'
33	BR	201	TRT	C1-C5-C6-C7
30	a	504	CDL	C54-C55-C56-C57
31	F	302	LMT	O5'-C5'-C6'-O6'
32	I	101	LPP	C12-C13-C14-C15
32	i	101	LPP	C12-C13-C14-C15
30	A	504	CDL	C54-C55-C56-C57
32	o	203	LPP	C23-C24-C25-C26
30	a	501	CDL	C40-C41-C42-C43
30	a	503	CDL	C51-C52-C53-C54
33	G	201	TRT	C1-C5-C6-C9
33	N	202	TRT	C1-C5-C6-C9
33	g	202	TRT	C1-C5-C6-C9

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Mol	Chain	Res	Type	Atoms
33	n	204	TRT	C1-C5-C6-C9
32	O	203	LPP	C23-C24-C25-C26
33	BR	201	TRT	C17-C16-O15-C12
30	O	201	CDL	CA3-CA4-OA6-CA5
32	N	203	LPP	C8-C7-O9-C11
32	n	201	LPP	C8-C7-O9-C11
30	A	501	CDL	C40-C41-C42-C43
33	M	202	TRT	C20-C19-O18-C17
33	M	202	TRT	C11-C12-O15-C16
30	A	502	CDL	C24-C25-C26-C27
30	P	202	CDL	C73-C74-C75-C76
30	a	502	CDL	C24-C25-C26-C27
30	O	201	CDL	C18-C19-C20-C21
30	M	201	CDL	C1-CB2-OB2-PB2
30	a	505	CDL	C15-C16-C17-C18
30	d	201	CDL	OA5-CA3-CA4-CA6
30	o	201	CDL	C18-C19-C20-C21
30	A	505	CDL	OA6-CA4-CA6-OA8
30	O	201	CDL	C52-C51-CB5-OB6
30	a	505	CDL	C32-C31-CA7-OA8
32	i	101	LPP	C23-C24-C25-C26
33	m	203	TRT	C23-C22-O21-C20
30	a	504	CDL	C71-C72-C73-C74
32	I	101	LPP	C23-C24-C25-C26
30	d	201	CDL	CB2-C1-CA2-OA2
30	A	505	CDL	C40-C41-C42-C43
30	P	202	CDL	C42-C43-C44-C45
33	AR	201	TRT	C1-C5-C6-C7
33	N	202	TRT	C7-C6-C9-C10
33	P	203	TRT	C1-C5-C6-C9
33	p	202	TRT	C1-C5-C6-C9
30	o	201	CDL	C52-C51-CB5-OB6
30	a	505	CDL	C40-C41-C42-C43
30	P	202	CDL	C83-C84-C85-C86
30	d	201	CDL	C34-C35-C36-C37
30	D	201	CDL	C55-C56-C57-C58
30	A	505	CDL	C15-C16-C17-C18
33	M	202	TRT	C13-C12-O15-C16
33	BR	201	TRT	C23-C22-O21-C20
30	M	205	CDL	C1-CB2-OB2-PB2
30	r	101	CDL	C1-CB2-OB2-PB2
33	n	204	TRT	C1-C5-C6-C8

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Mol	Chain	Res	Type	Atoms
30	O	201	CDL	CA3-CA4-CA6-OA8
30	R	101	CDL	C13-C14-C15-C16
33	m	202	TRT	C13-C12-O15-C16
30	d	201	CDL	C55-C56-C57-C58
30	A	504	CDL	C71-C72-C73-C74
33	m	202	TRT	C11-C12-O15-C16
31	F	302	LMT	C1-C2-C3-C4
31	g	201	LMT	C1-C2-C3-C4
30	D	201	CDL	C34-C35-C36-C37
30	P	201	CDL	OA5-CA3-CA4-OA6
30	a	501	CDL	OB5-CB3-CB4-OB6
33	n	204	TRT	C7-C6-C9-C10
30	R	101	CDL	C60-C61-C62-C63
30	r	101	CDL	C60-C61-C62-C63
30	D	201	CDL	CB2-C1-CA2-OA2
30	E	101	CDL	C72-C71-CB7-OB8
30	E	101	CDL	C60-C61-C62-C63
30	e	101	CDL	C60-C61-C62-C63
30	D	201	CDL	OA5-CA3-CA4-CA6
30	E	101	CDL	OB5-CB3-CB4-CB6
32	O	202	LPP	O5-C6-C7-C8
30	p	201	CDL	OA6-CA4-CA6-OA8
30	P	201	CDL	CA4-CA3-OA5-PA1
30	R	101	CDL	C1-CB2-OB2-PB2
30	p	201	CDL	CA4-CA3-OA5-PA1
32	n	201	LPP	C31-C32-C33-C34
33	M	203	TRT	C23-C22-O21-C20
32	N	203	LPP	C31-C32-C33-C34
31	g	201	LMT	C7-C8-C9-C10
30	R	101	CDL	C37-C38-C39-C40
30	e	101	CDL	C72-C71-CB7-OB8
33	g	203	TRT	O18-C19-C20-O21
32	I	101	LPP	C6-O5-P1-O3
31	F	302	LMT	C7-C8-C9-C10
33	G	202	TRT	O18-C19-C20-O21
31	D	202	LMT	C1-C2-C3-C4
31	d	202	LMT	C1-C2-C3-C4
32	F	301	LPP	C29-C30-C31-C32
32	f	301	LPP	C29-C30-C31-C32
30	o	201	CDL	CA3-CA4-OA6-CA5
30	p	201	CDL	C71-C72-C73-C74
32	O	203	LPP	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
33	G	202	TRT	C4-C1-C5-C6
32	o	202	LPP	C30-C29-O27-C8
33	G	202	TRT	C1-C5-C6-C9
33	g	203	TRT	C1-C5-C6-C9
33	N	201	TRT	C16-C17-O18-C19
30	P	202	CDL	C61-C62-C63-C64
32	o	203	LPP	C21-C22-C23-C24
32	O	202	LPP	O5-C6-C7-O9
33	g	203	TRT	C23-C22-O21-C20
33	n	203	TRT	C16-C17-O18-C19
30	e	101	CDL	C31-CA7-OA8-CA6
32	O	202	LPP	C30-C29-O27-C8
32	O	202	LPP	O28-C29-O27-C8
32	o	202	LPP	O28-C29-O27-C8
33	N	202	TRT	C7-C6-C9-C14
33	n	204	TRT	C7-C6-C9-C14
30	A	504	CDL	C31-CA7-OA8-CA6
33	g	203	TRT	C4-C1-C5-C6
33	G	202	TRT	C7-C6-C9-C14
30	r	101	CDL	C35-C36-C37-C38
32	O	203	LPP	C15-C16-C17-C18
33	N	202	TRT	C1-C5-C6-C8
30	m	201	CDL	C72-C71-CB7-OB8
30	d	201	CDL	C40-C41-C42-C43
30	E	101	CDL	C12-C11-CA5-OA7
30	a	505	CDL	OB6-CB4-CB6-OB8
33	g	203	TRT	C7-C6-C9-C14
30	M	204	CDL	C72-C71-CB7-OB8
30	R	101	CDL	C32-C31-CA7-OA8
30	e	101	CDL	OB5-CB3-CB4-CB6
30	r	101	CDL	C13-C14-C15-C16
30	a	504	CDL	C73-C74-C75-C76
33	P	203	TRT	O18-C19-C20-O21
33	p	202	TRT	O18-C19-C20-O21
32	o	203	LPP	C15-C16-C17-C18
30	a	504	CDL	OB9-CB7-OB8-CB6
30	e	101	CDL	C12-C11-CA5-OA7
30	A	504	CDL	C73-C74-C75-C76
30	r	101	CDL	C32-C33-C34-C35
30	e	101	CDL	OA9-CA7-OA8-CA6
33	M	202	TRT	C7-C6-C9-C10
33	N	202	TRT	C8-C6-C9-C10

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Mol	Chain	Res	Type	Atoms
33	n	204	TRT	C8-C6-C9-C10
33	m	202	TRT	C7-C6-C9-C10
30	d	201	CDL	C33-C34-C35-C36
30	M	204	CDL	C33-C34-C35-C36
31	Q	101	LMT	C4'-C5'-C6'-O6'
30	A	504	CDL	OB9-CB7-OB8-CB6
30	A	502	CDL	C32-C33-C34-C35
33	M	202	TRT	C8-C6-C9-C10
30	r	101	CDL	C32-C31-CA7-OA8
33	G	202	TRT	C7-C6-C9-C10
33	m	202	TRT	C8-C6-C9-C10
33	M	202	TRT	O21-C22-C23-O24
33	m	202	TRT	O21-C22-C23-O24
30	r	101	CDL	C77-C78-C79-C80
33	N	202	TRT	C8-C6-C9-C14
33	n	204	TRT	C8-C6-C9-C14
30	M	201	CDL	C52-C51-CB5-OB6
30	R	101	CDL	C77-C78-C79-C80
30	M	205	CDL	C52-C51-CB5-OB6
33	n	203	TRT	O18-C19-C20-O21
33	G	202	TRT	C23-C22-O21-C20
33	N	201	TRT	O18-C19-C20-O21
32	o	203	LPP	C14-C15-C16-C17
30	A	504	CDL	C60-C61-C62-C63
30	a	504	CDL	C72-C73-C74-C75
30	m	201	CDL	C33-C34-C35-C36
30	O	201	CDL	C13-C14-C15-C16
32	O	203	LPP	C14-C15-C16-C17
30	o	201	CDL	C13-C14-C15-C16
33	g	203	TRT	C7-C6-C9-C10
30	A	504	CDL	C72-C73-C74-C75
30	D	201	CDL	C33-C34-C35-C36
32	f	301	LPP	O28-C29-O27-C8
33	m	203	TRT	O15-C16-C17-O18
30	D	201	CDL	C40-C41-C42-C43
30	o	201	CDL	OA9-CA7-OA8-CA6
33	M	203	TRT	O15-C16-C17-O18
32	o	202	LPP	C14-C15-C16-C17
33	M	202	TRT	C7-C6-C9-C14
33	m	202	TRT	C7-C6-C9-C14
30	d	201	CDL	C59-C60-C61-C62
32	F	301	LPP	O28-C29-O27-C8

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Mol	Chain	Res	Type	Atoms
32	O	202	LPP	C14-C15-C16-C17
30	D	201	CDL	C59-C60-C61-C62
30	a	504	CDL	C60-C61-C62-C63
30	R	101	CDL	C53-C54-C55-C56
30	A	501	CDL	C54-C55-C56-C57
30	r	101	CDL	C53-C54-C55-C56
30	o	201	CDL	C72-C73-C74-C75
30	m	201	CDL	C72-C71-CB7-OB9
33	M	202	TRT	C8-C6-C9-C14
30	P	202	CDL	OA7-CA5-OA6-CA4
30	R	101	CDL	C35-C36-C37-C38
30	D	201	CDL	C22-C23-C24-C25
33	G	202	TRT	C2-C1-C5-C6
30	O	201	CDL	C12-C13-C14-C15
30	D	201	CDL	CB7-C71-C72-C73
30	a	501	CDL	C54-C55-C56-C57
30	O	201	CDL	C72-C73-C74-C75
30	d	201	CDL	CA7-C31-C32-C33
30	d	201	CDL	C22-C23-C24-C25
30	E	101	CDL	C59-C60-C61-C62
30	M	204	CDL	C72-C71-CB7-OB9
33	g	203	TRT	C2-C1-C5-C6
30	e	101	CDL	C59-C60-C61-C62
30	o	201	CDL	C31-CA7-OA8-CA6
33	m	202	TRT	C8-C6-C9-C14
30	R	101	CDL	C76-C77-C78-C79
30	m	201	CDL	C12-C13-C14-C15
30	r	101	CDL	C52-C51-CB5-OB6
33	BE	600	TRT	C1-C5-C6-C7
30	R	101	CDL	C51-C52-C53-C54
31	q	101	LMT	C4'-C5'-C6'-O6'
33	g	203	TRT	C8-C6-C9-C14
30	R	101	CDL	C52-C51-CB5-OB6
30	p	201	CDL	C11-C12-C13-C14
32	F	301	LPP	C30-C29-O27-C8
32	f	301	LPP	C30-C29-O27-C8
30	o	201	CDL	C12-C13-C14-C15
30	M	201	CDL	C52-C51-CB5-OB7
30	M	205	CDL	C52-C51-CB5-OB7
30	O	201	CDL	C72-C71-CB7-OB9
30	A	505	CDL	OB6-CB4-CB6-OB8
30	P	201	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
30	r	101	CDL	C32-C31-CA7-OA9
30	A	504	CDL	C52-C51-CB5-OB6
30	P	201	CDL	C72-C71-CB7-OB8
30	P	202	CDL	C52-C53-C54-C55
30	r	101	CDL	C51-C52-C53-C54
30	r	101	CDL	C76-C77-C78-C79
30	A	502	CDL	CA3-CA4-CA6-OA8
30	a	502	CDL	CA3-CA4-CA6-OA8
30	R	101	CDL	C32-C31-CA7-OA9
30	o	201	CDL	C72-C71-CB7-OB9
30	a	504	CDL	C52-C51-CB5-OB6
33	G	202	TRT	C8-C6-C9-C14
33	n	204	TRT	O21-C22-C23-O24
33	N	202	TRT	O21-C22-C23-O24
33	N	202	TRT	O15-C16-C17-O18
32	f	301	LPP	C14-C15-C16-C17
33	AE	600	TRT	C8-C6-C9-C14
33	n	204	TRT	O15-C16-C17-O18
30	M	204	CDL	C12-C13-C14-C15
30	r	101	CDL	C33-C34-C35-C36
30	D	201	CDL	CA7-C31-C32-C33
30	M	204	CDL	C52-C51-CB5-OB6
30	p	201	CDL	C72-C71-CB7-OB8
32	i	101	LPP	O9-C11-C12-C13
30	A	504	CDL	C52-C51-CB5-OB7
32	F	301	LPP	C14-C15-C16-C17
33	BE	600	TRT	C8-C6-C9-C14
33	AE	600	TRT	C1-C5-C6-C7
33	AR	201	TRT	C23-C22-O21-C20
30	m	201	CDL	C52-C51-CB5-OB6
32	I	101	LPP	O9-C11-C12-C13
30	a	504	CDL	C52-C51-CB5-OB7
31	n	202	LMT	C3'-C4'-O1B-C1B

There are no ring outliers.

42 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	P	202	CDL	1	0
30	a	502	CDL	5	0
34	BF	601	ATP	2	0
33	N	202	TRT	1	0

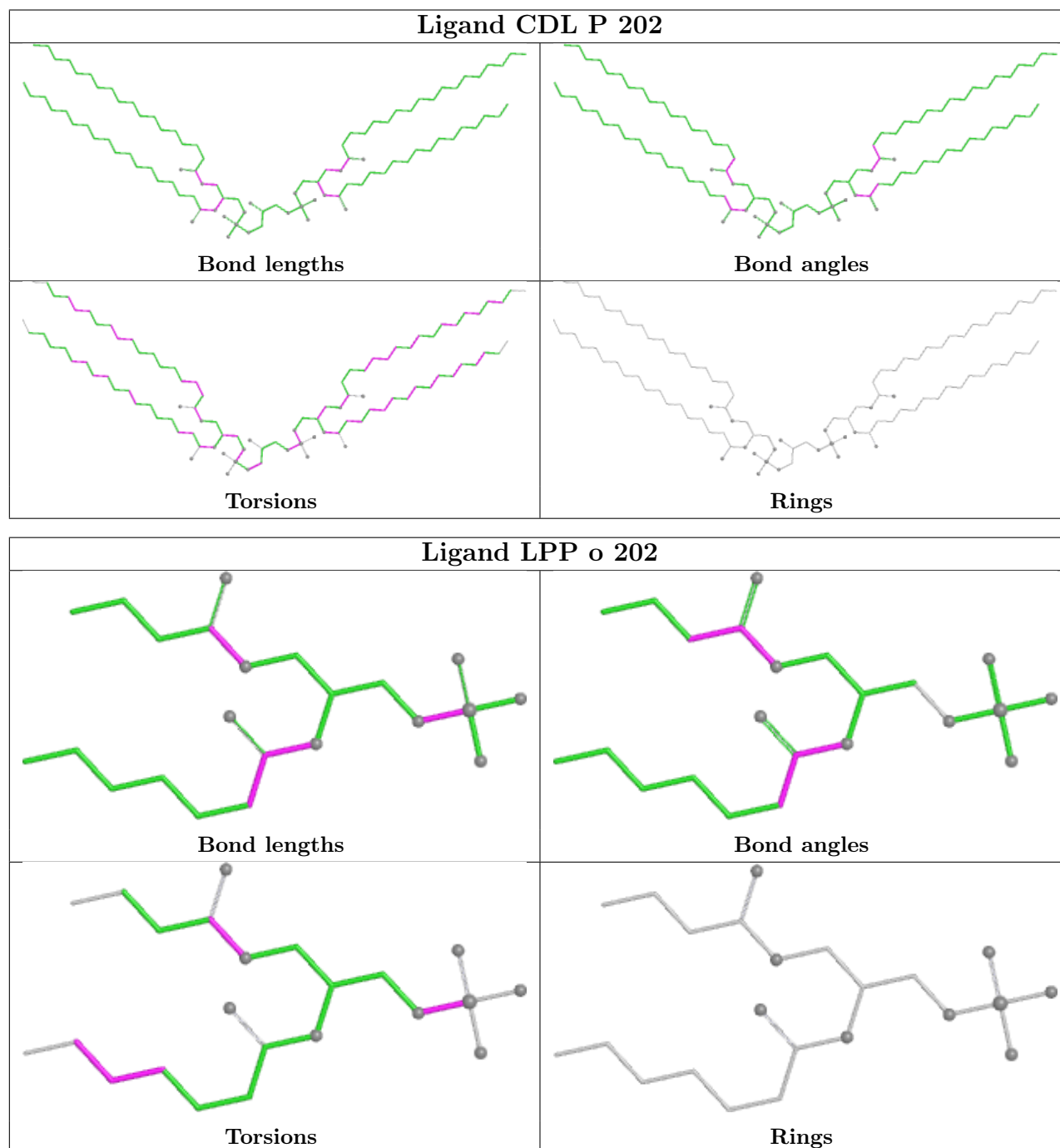
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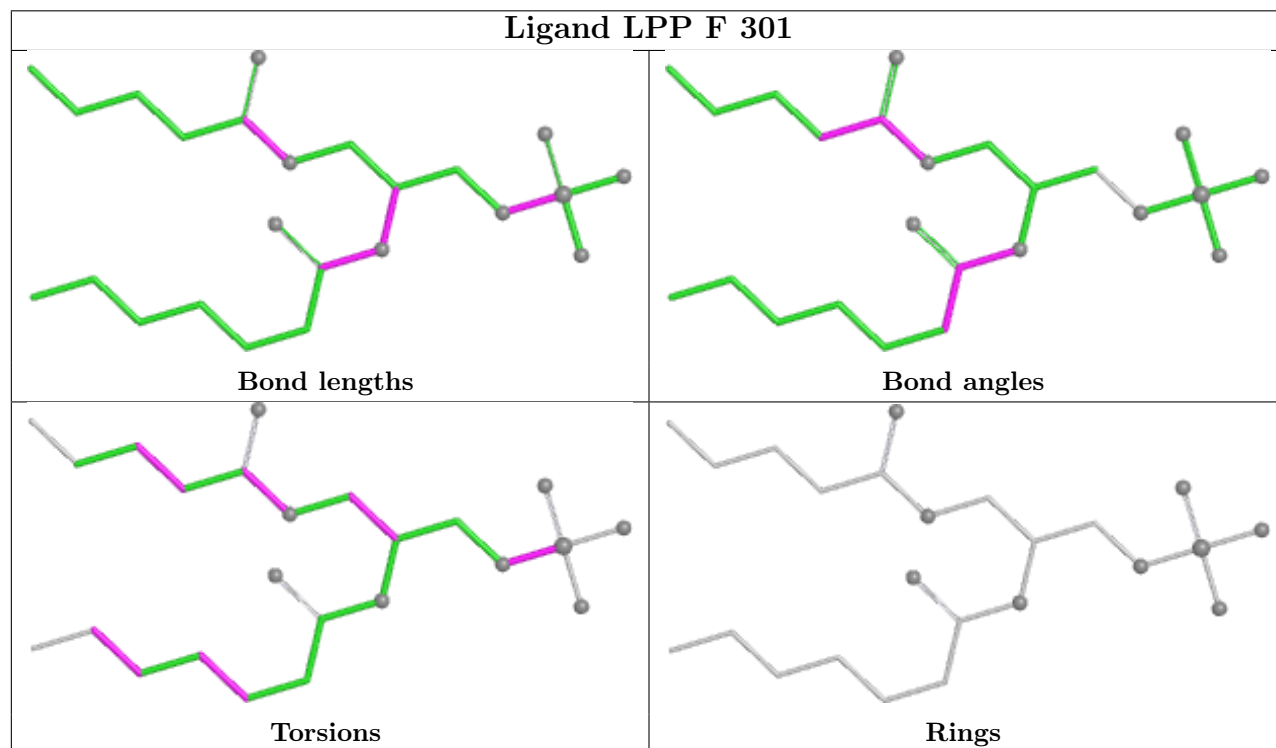
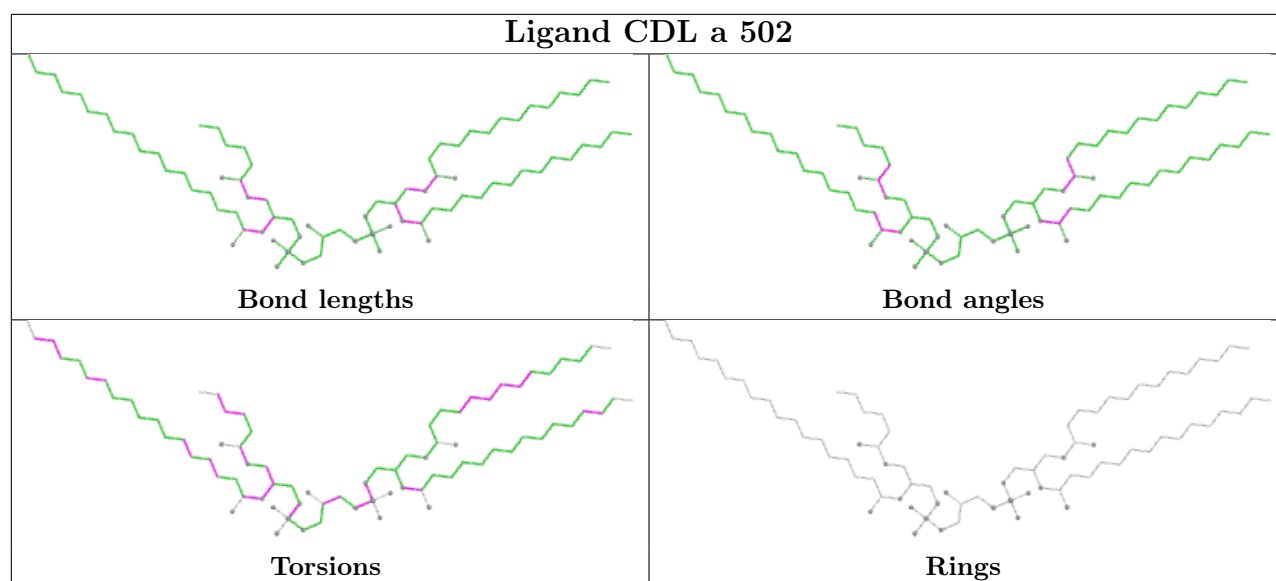
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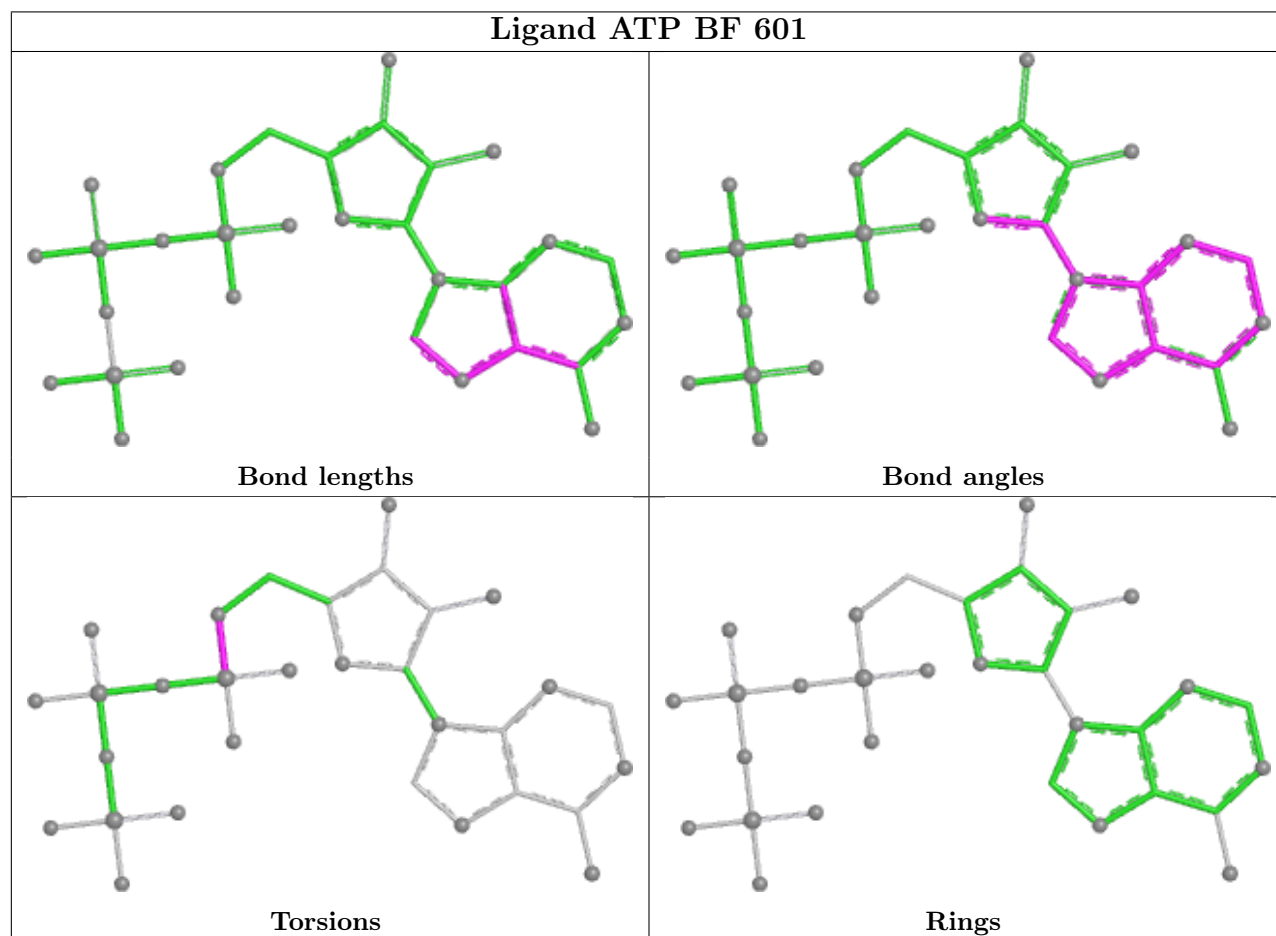
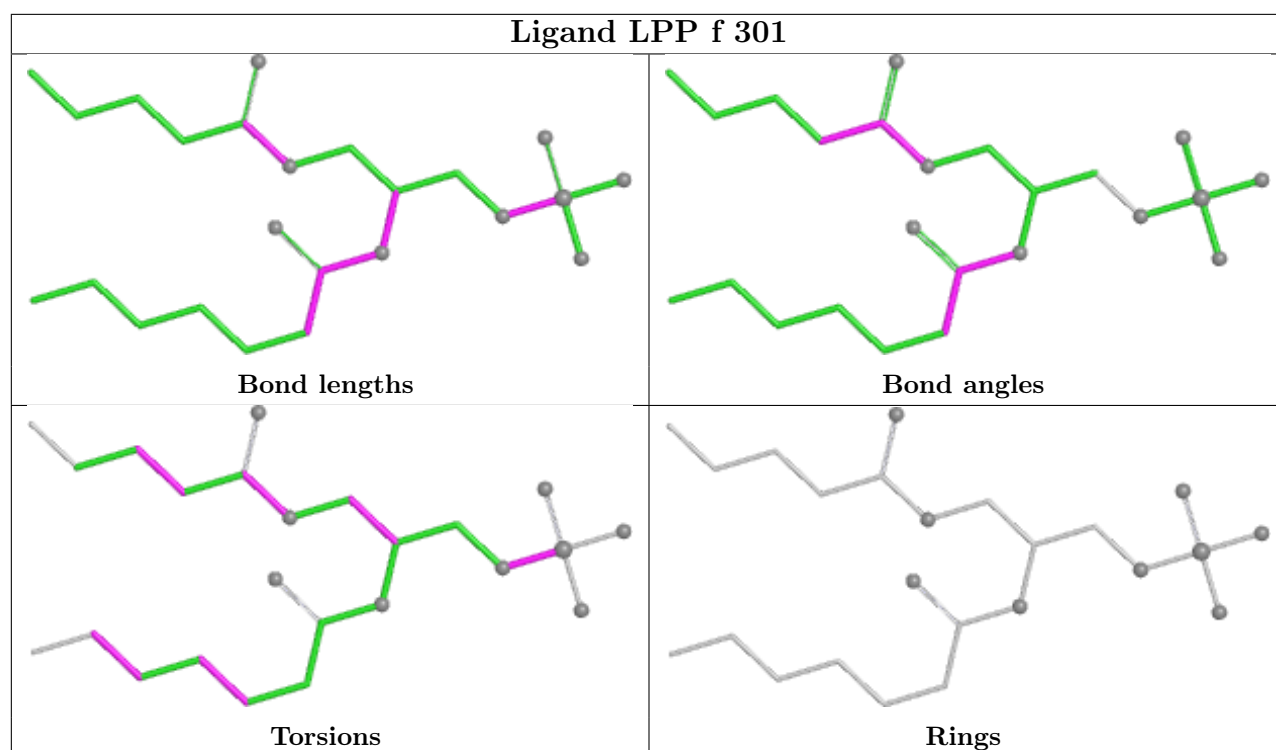
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	A	502	CDL	4	0
32	K	201	LPP	1	0
32	k	201	LPP	2	0
30	A	505	CDL	4	0
30	M	204	CDL	1	0
33	n	203	TRT	1	0
34	BB	601	ATP	2	0
34	AF	601	ATP	2	0
31	q	101	LMT	1	0
30	D	201	CDL	2	0
30	a	503	CDL	4	0
30	o	201	CDL	3	0
30	A	501	CDL	1	0
33	N	201	TRT	1	0
30	e	101	CDL	6	0
33	g	202	TRT	1	0
30	E	101	CDL	6	0
34	AC	601	ATP	1	0
30	a	505	CDL	5	0
33	n	204	TRT	1	0
33	G	201	TRT	1	0
30	A	503	CDL	3	0
30	M	205	CDL	3	0
30	d	201	CDL	2	0
31	Q	101	LMT	1	0
30	R	101	CDL	2	0
34	AB	601	ATP	1	0
30	P	201	CDL	1	0
30	O	201	CDL	2	0
30	M	201	CDL	2	0
30	a	504	CDL	1	0
30	A	504	CDL	1	0
30	a	501	CDL	1	0
31	F	302	LMT	2	0
30	p	201	CDL	1	0
31	g	201	LMT	3	0
30	m	201	CDL	2	0
30	r	101	CDL	3	0

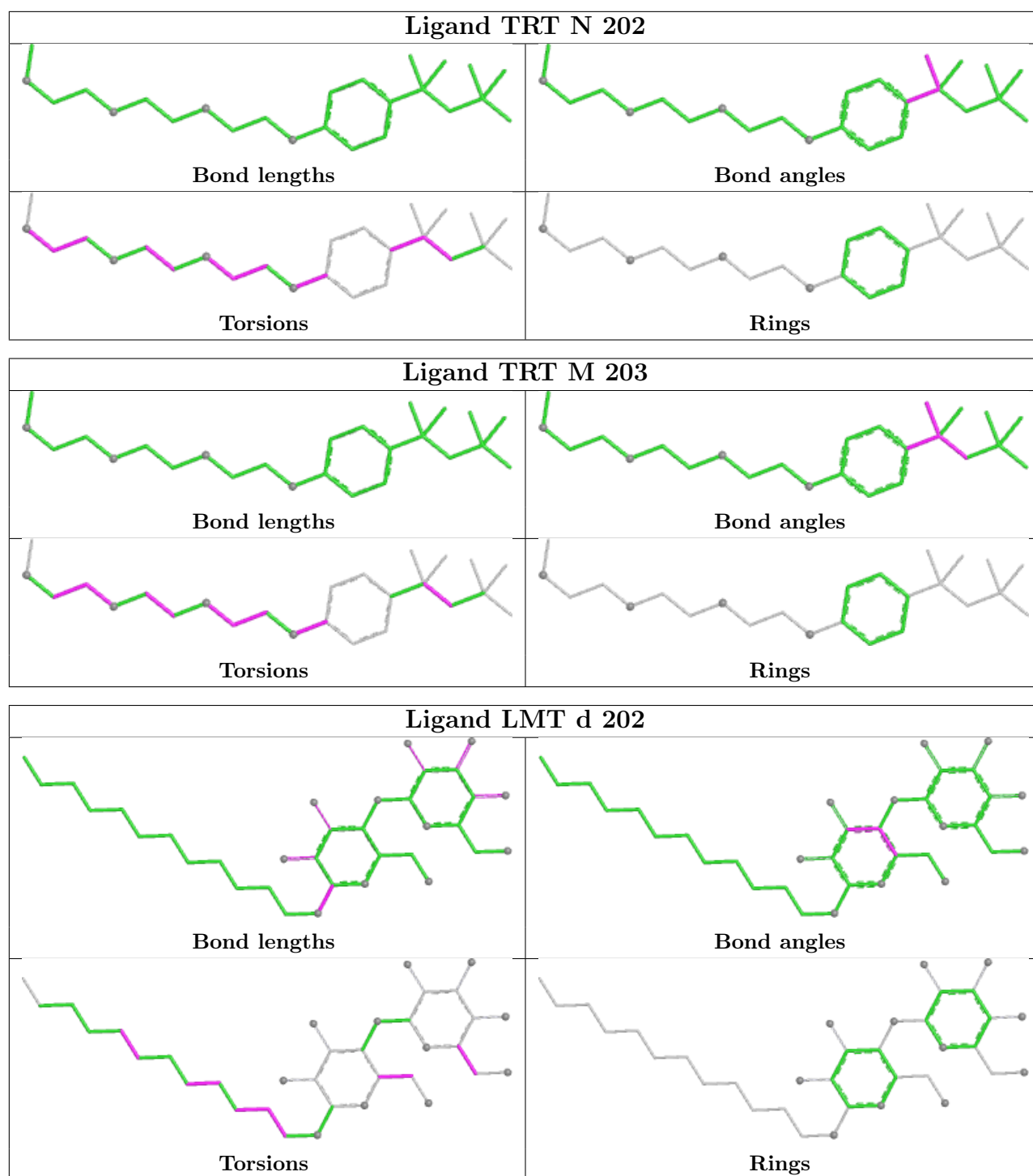
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

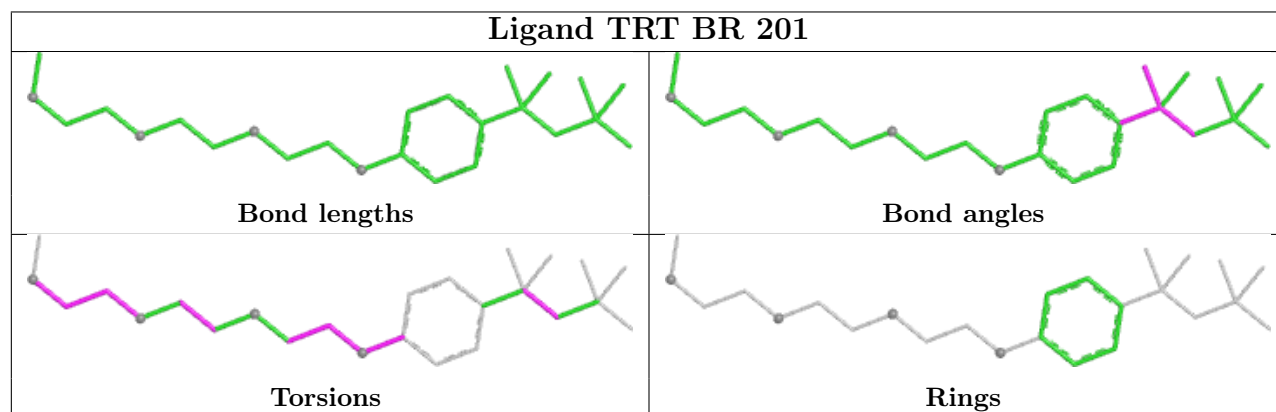
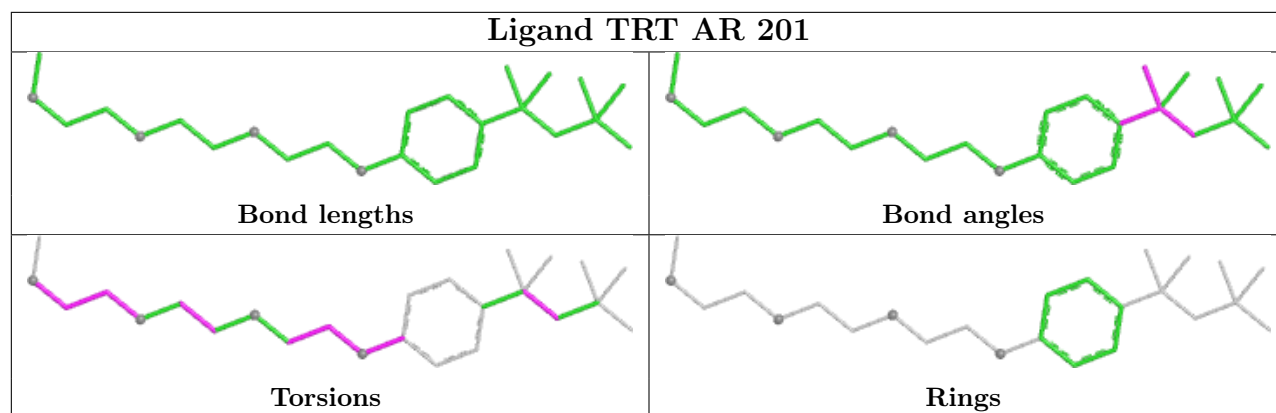
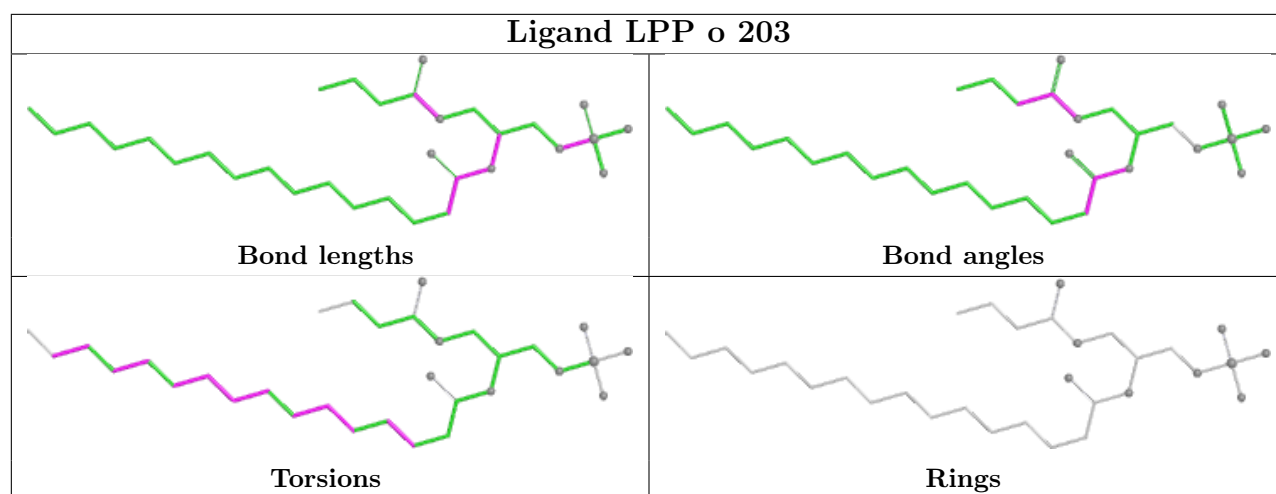
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

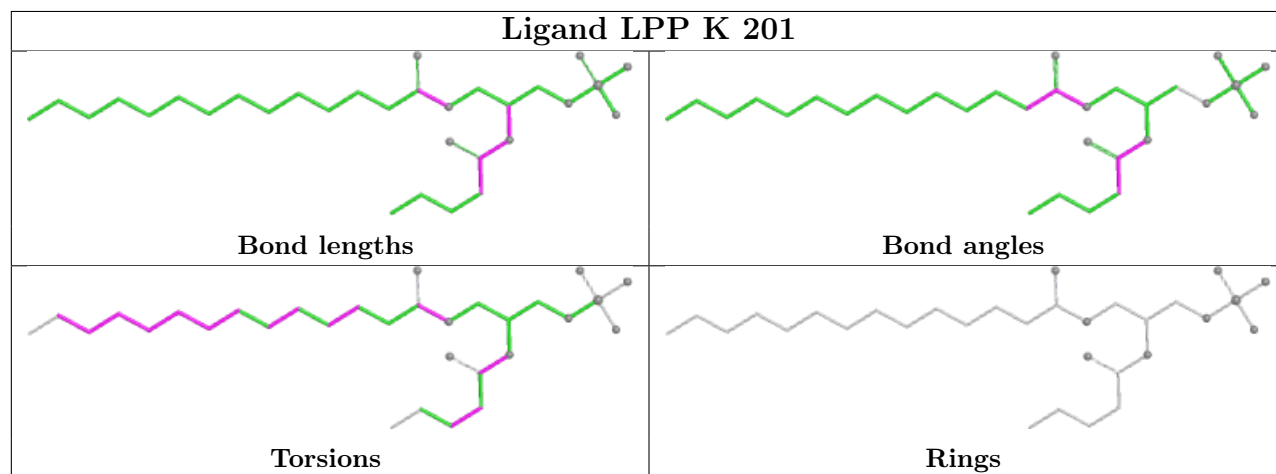
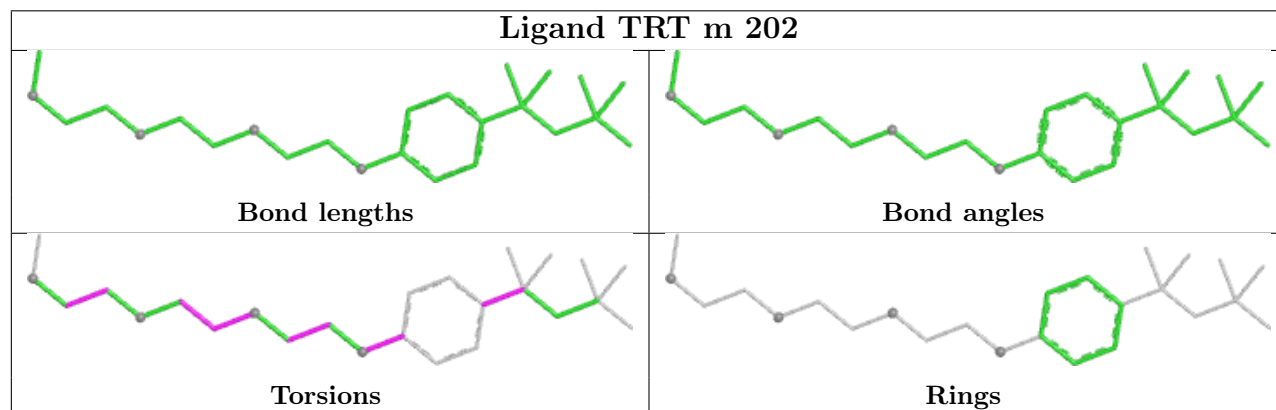
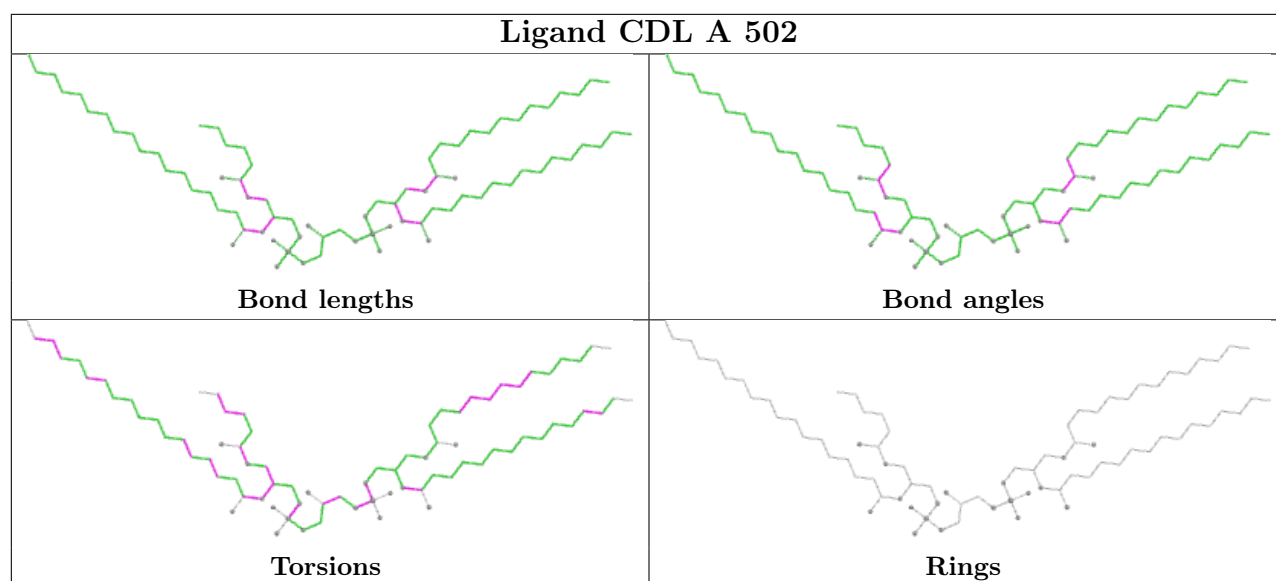


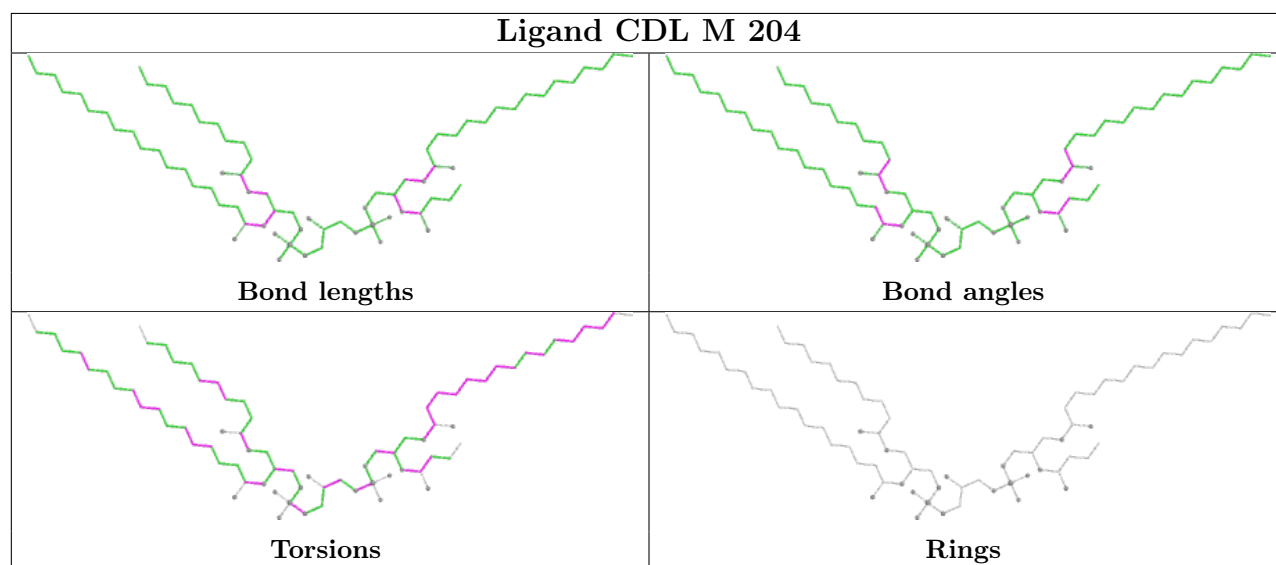
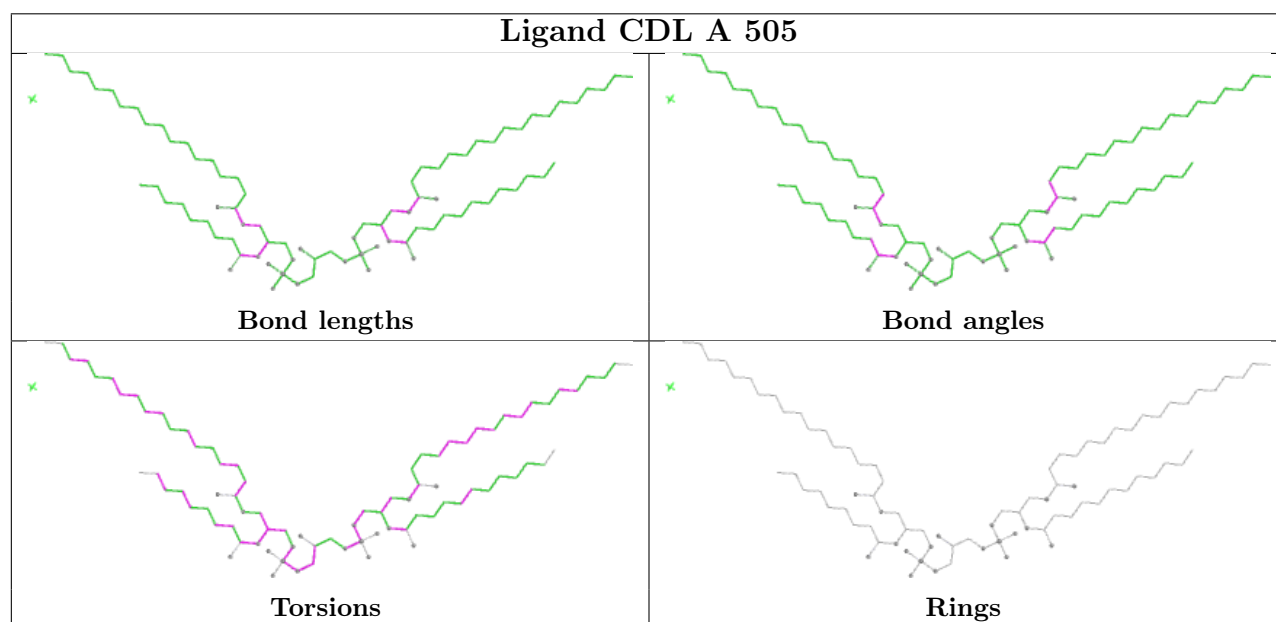
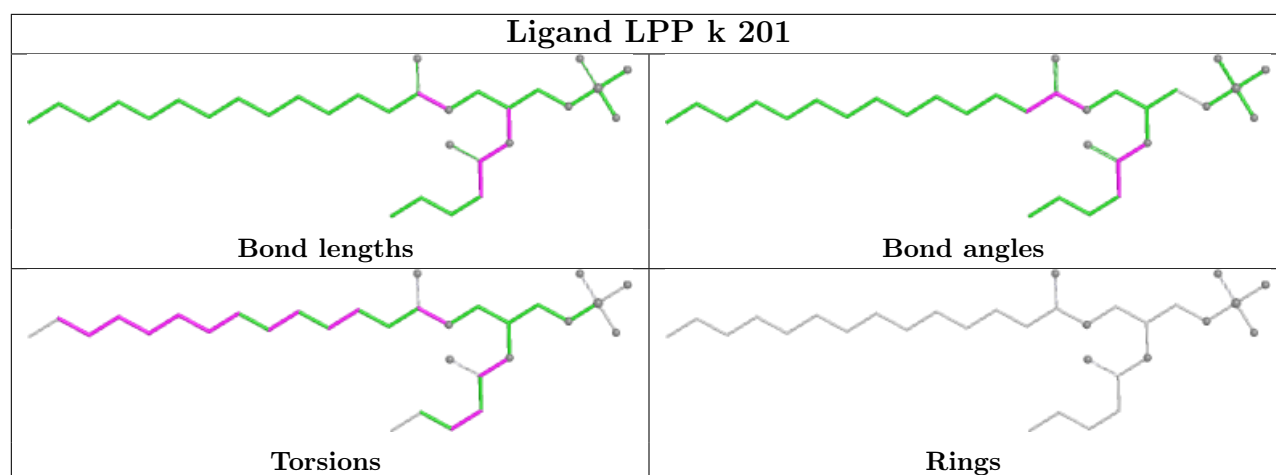


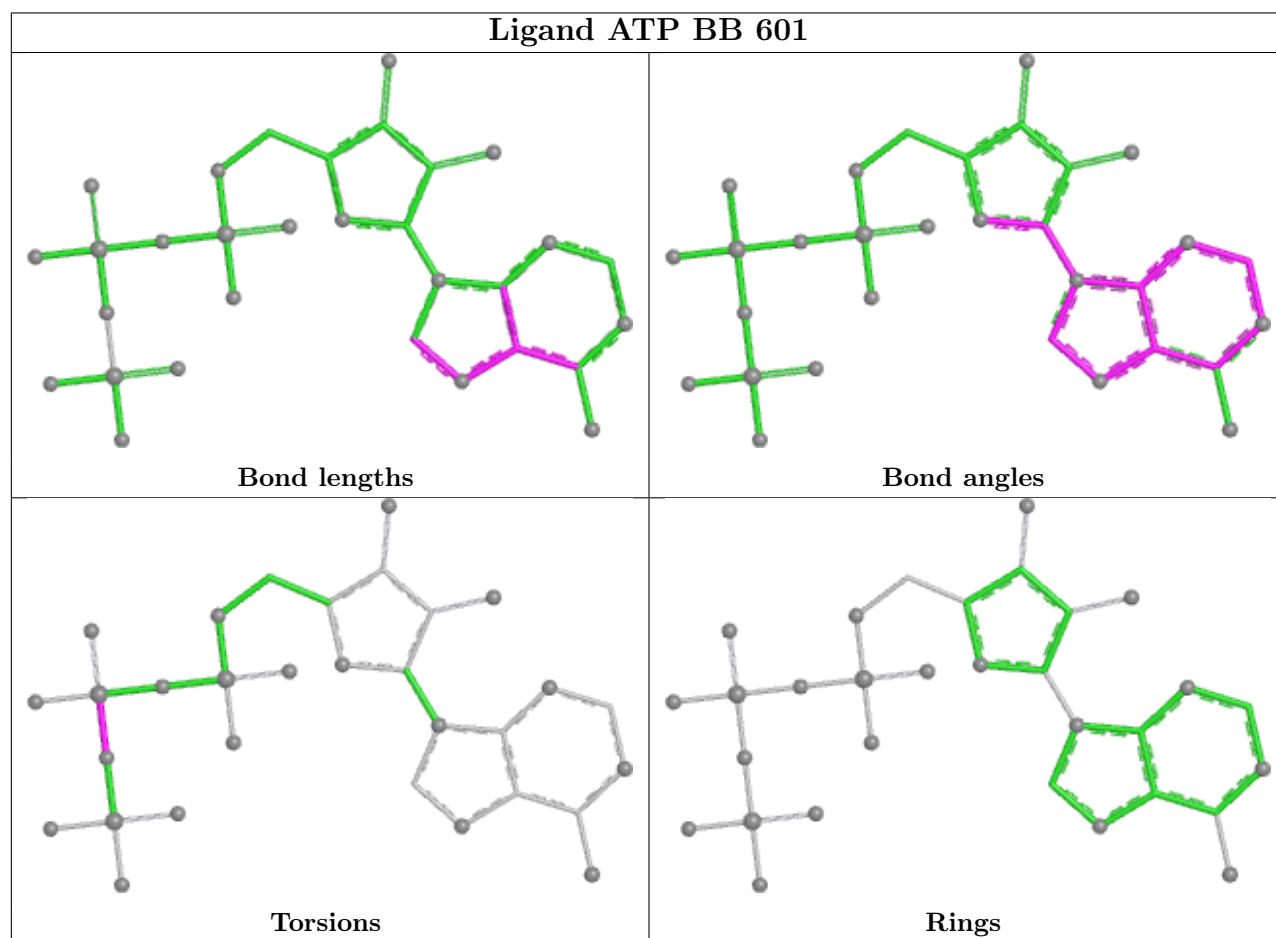
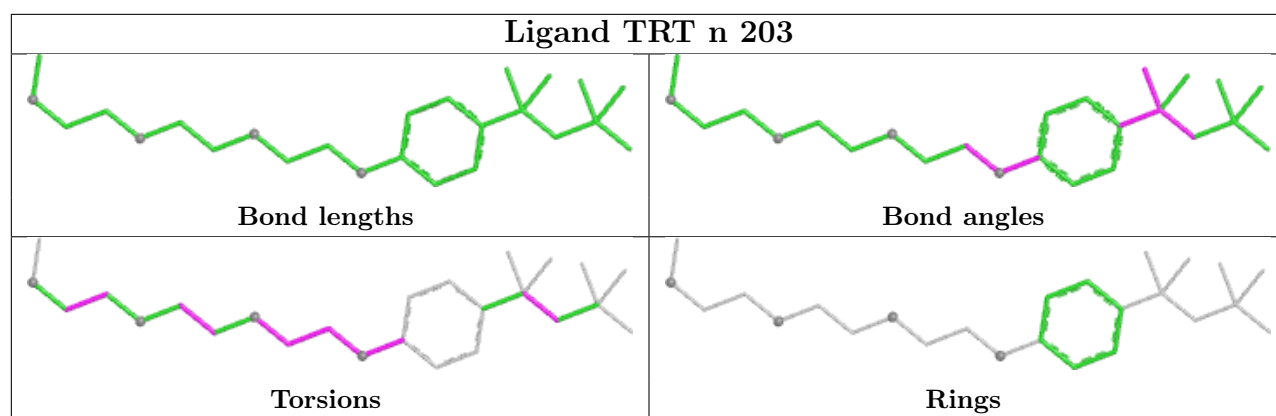


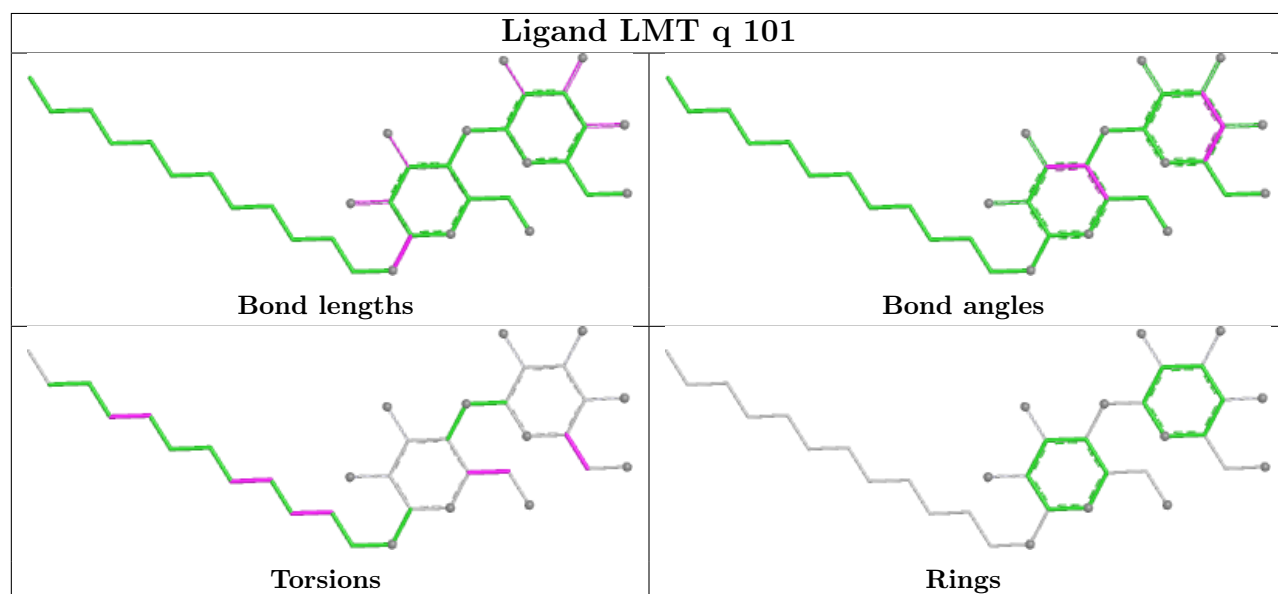
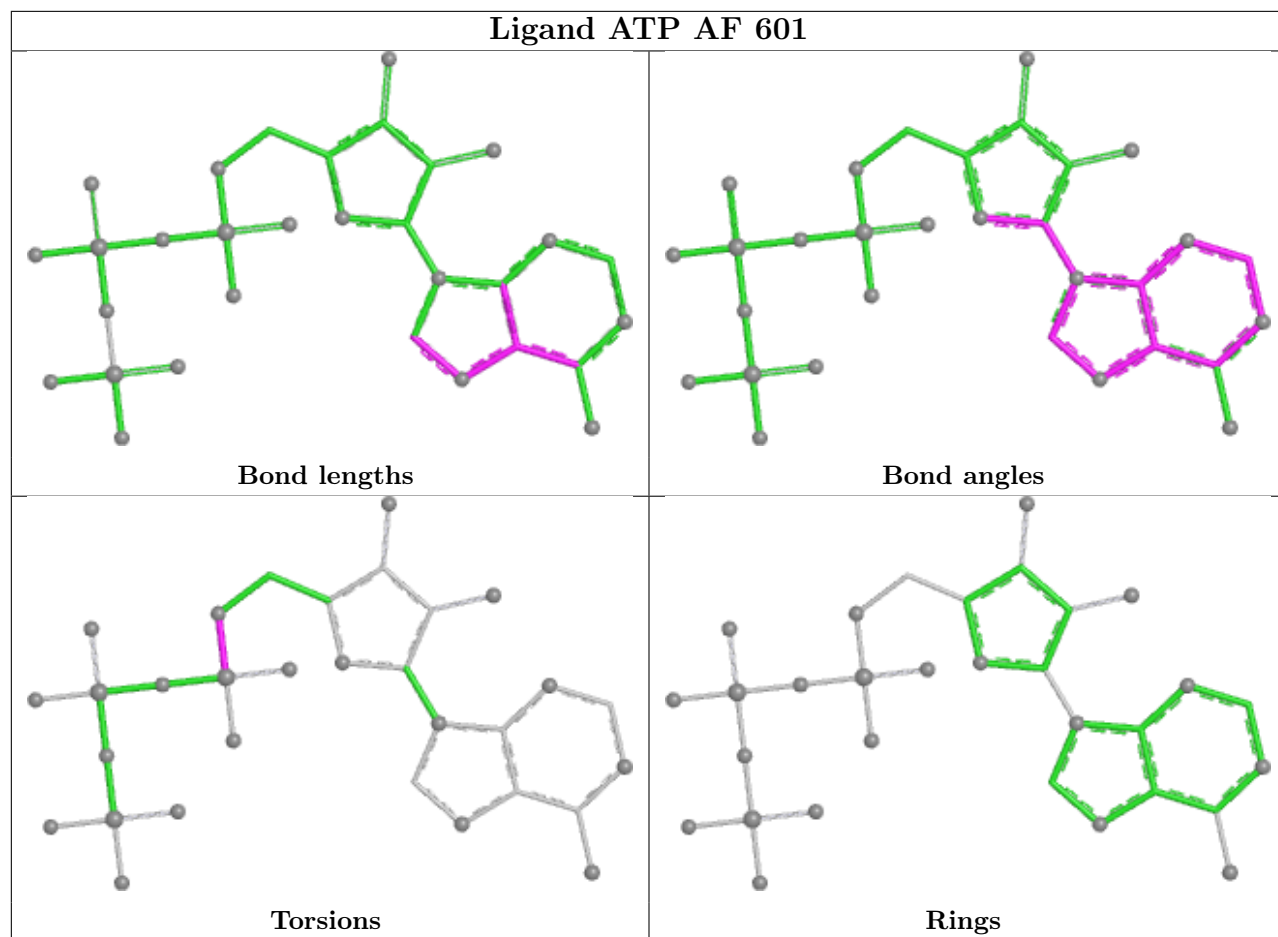


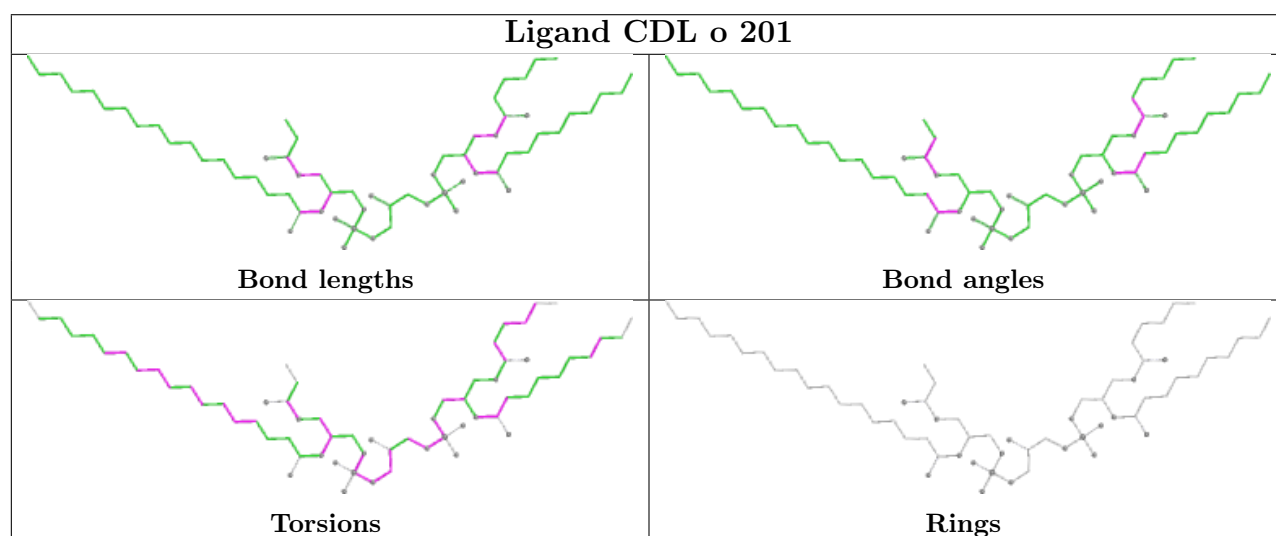
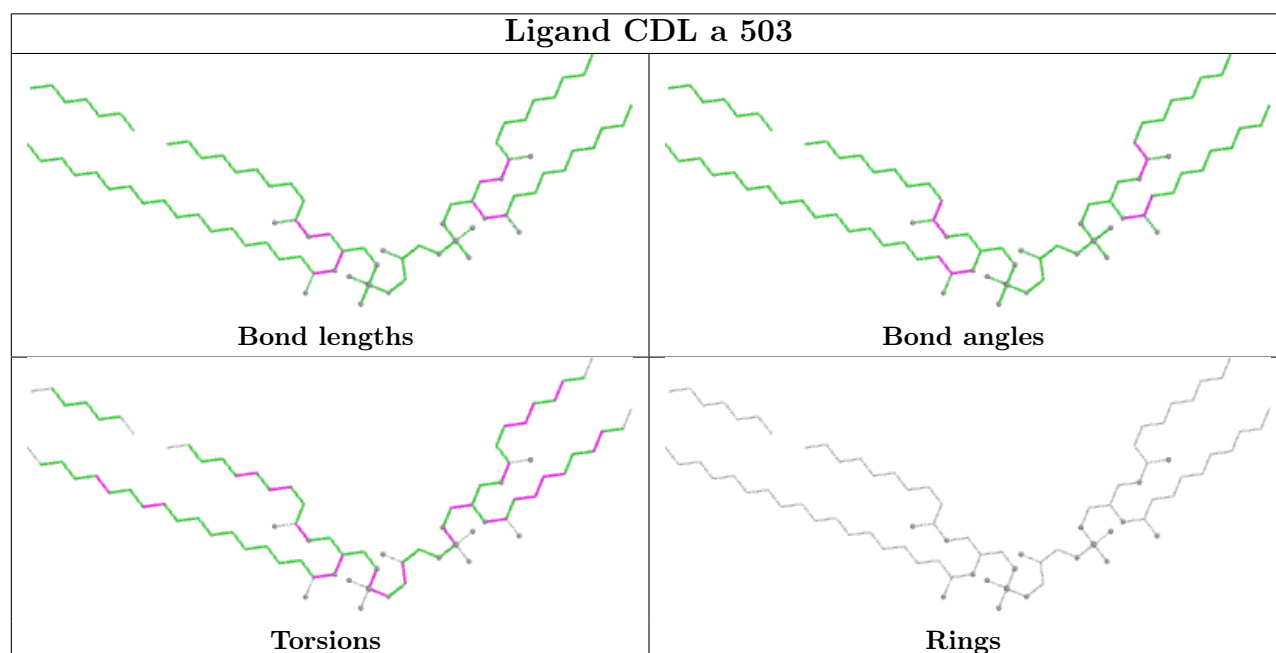
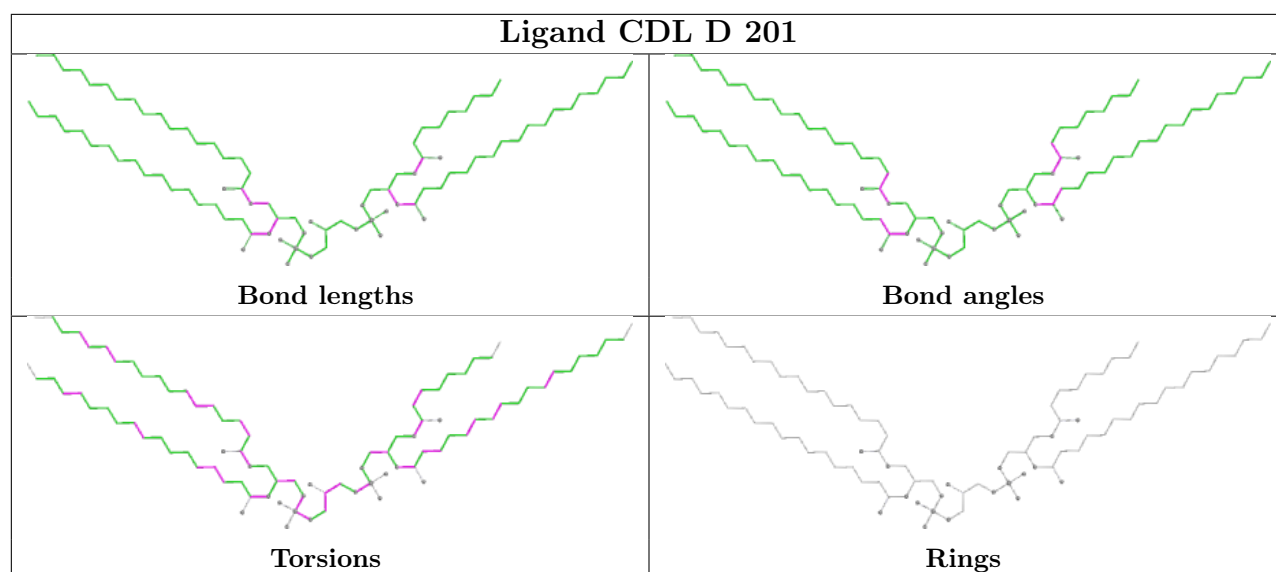


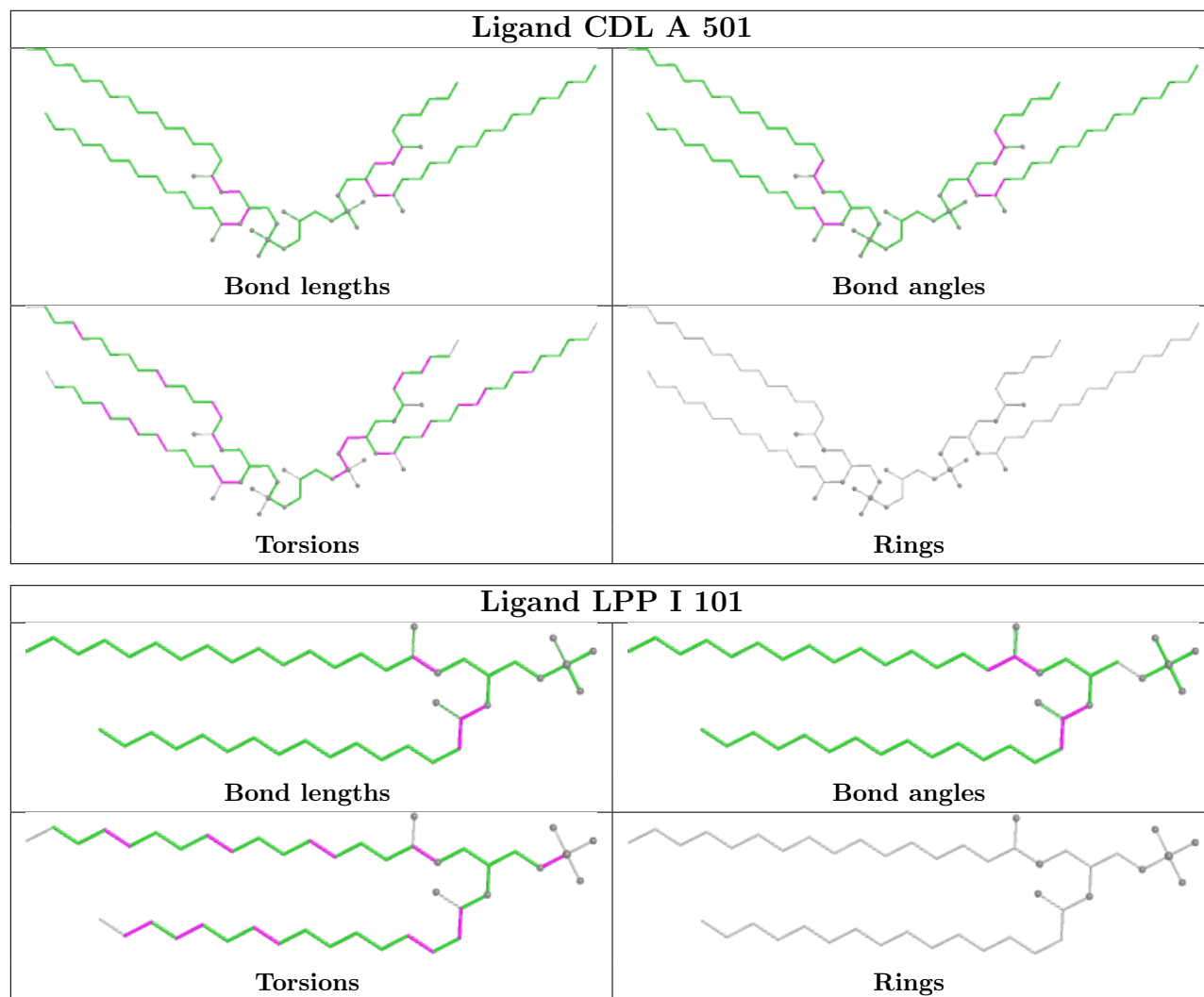




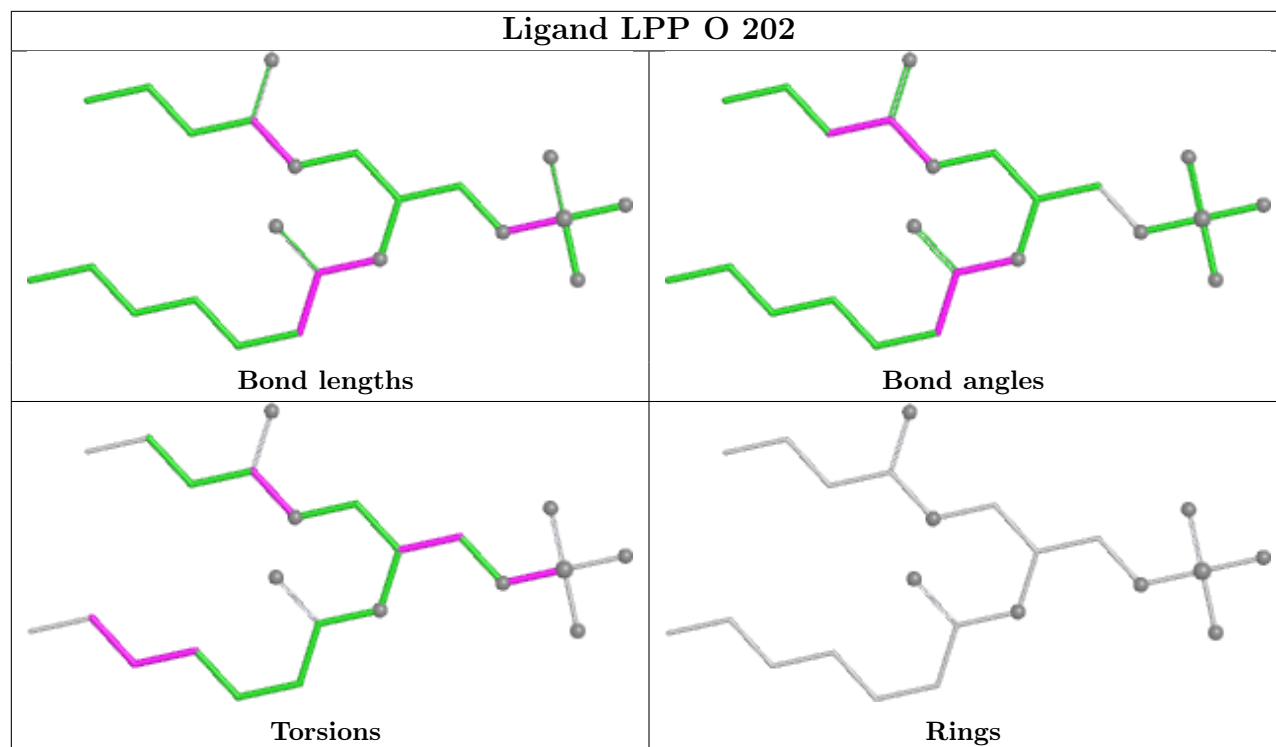




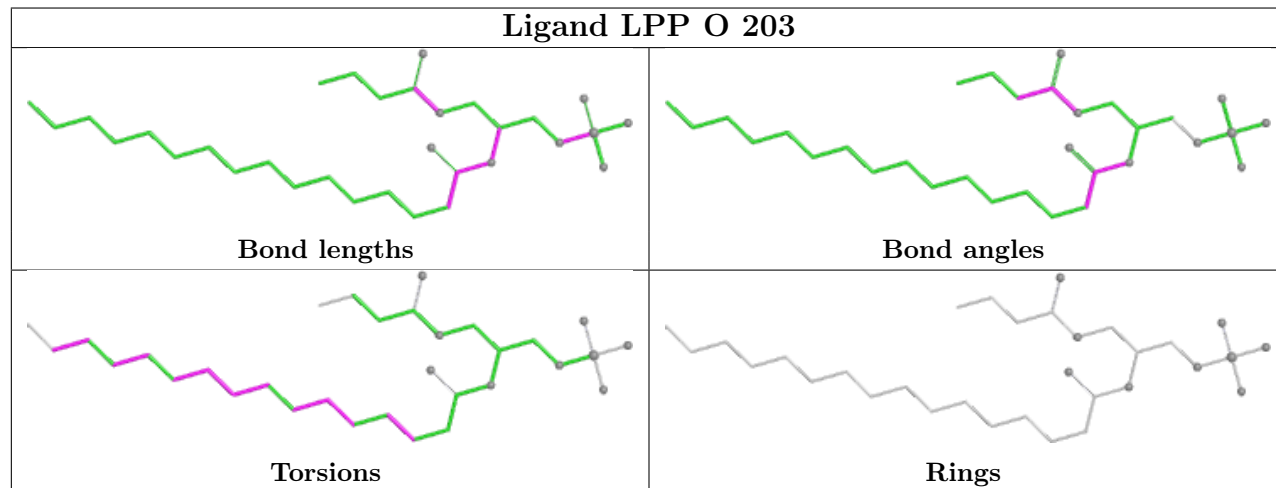


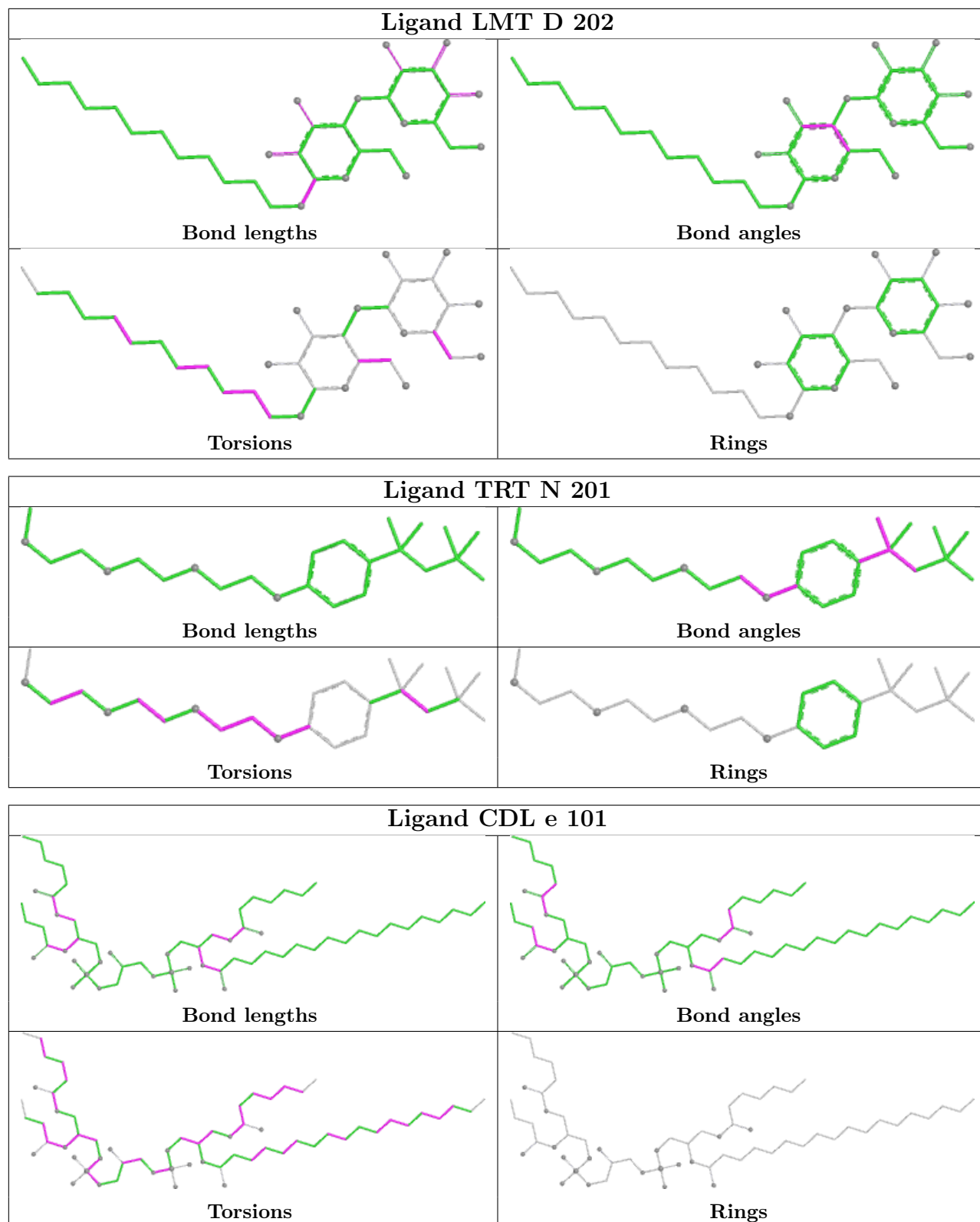


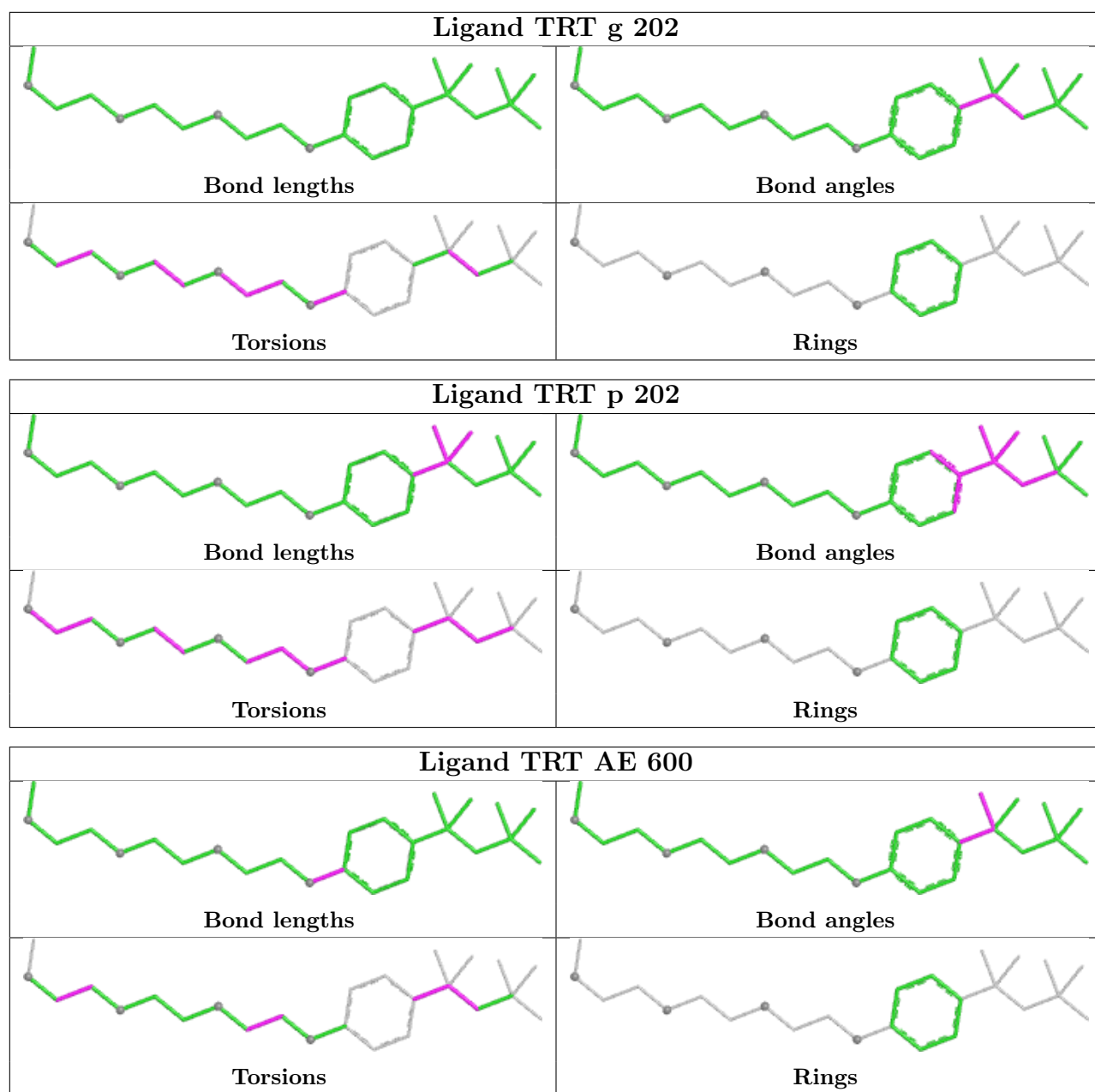
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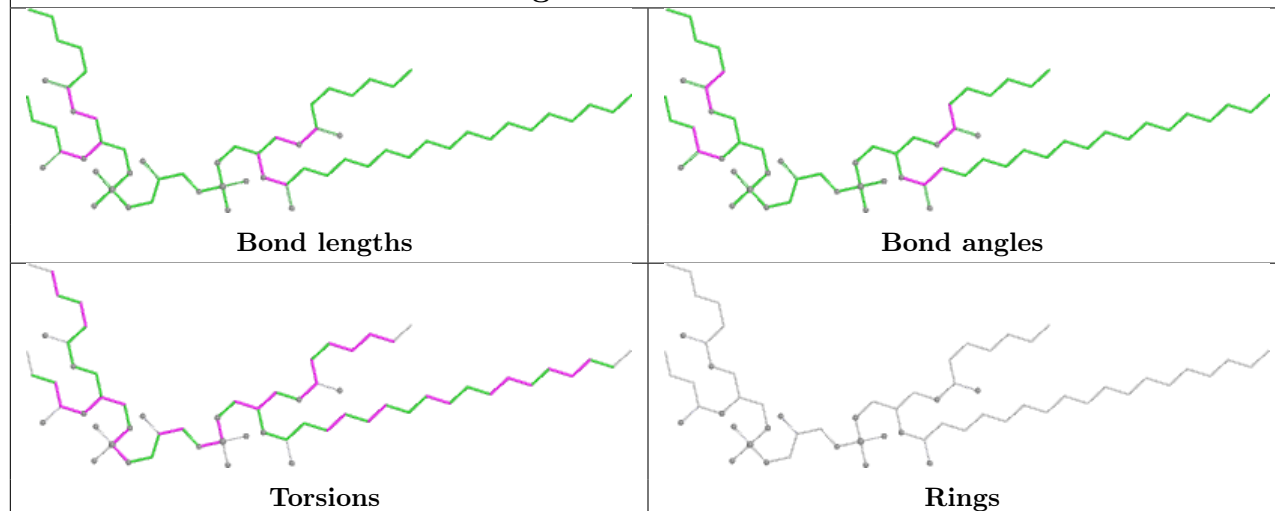
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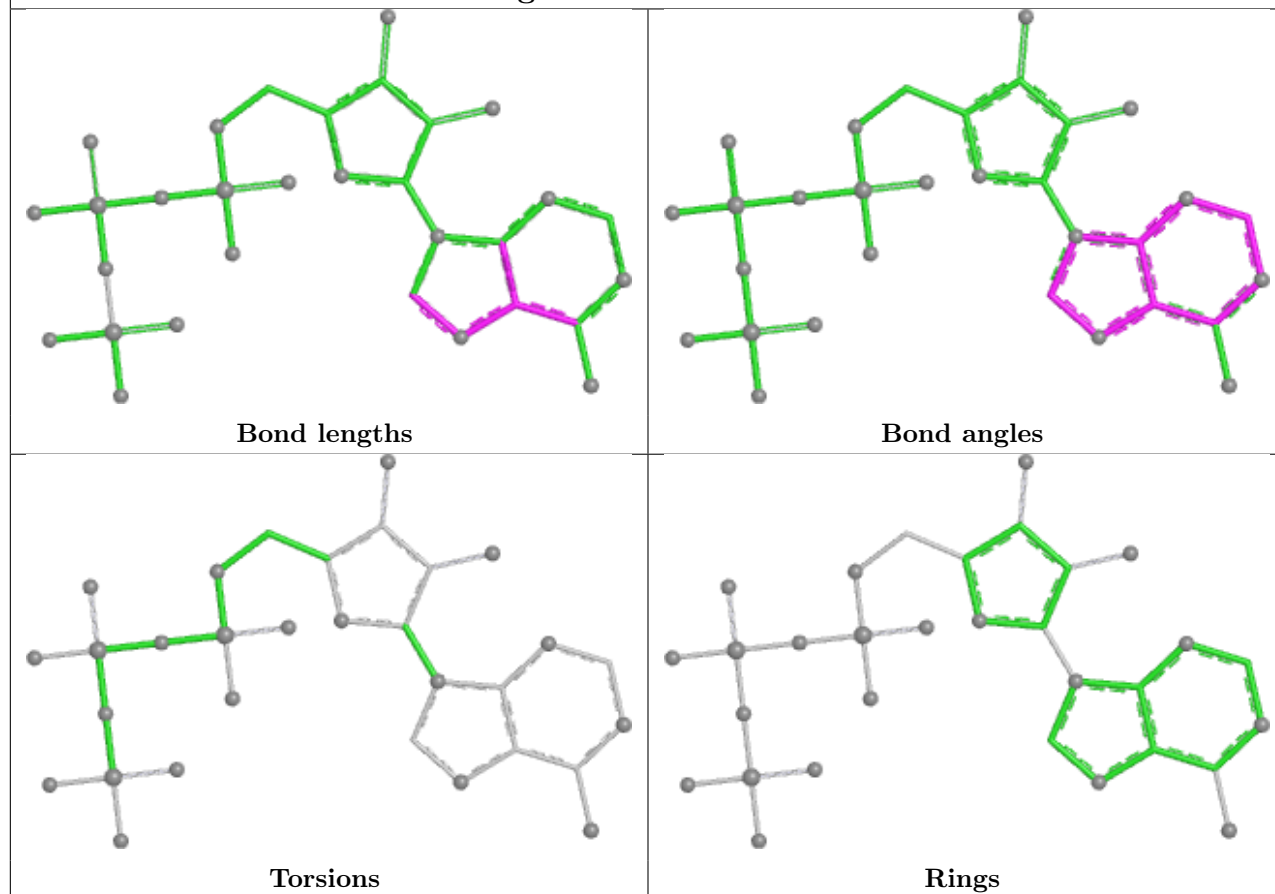


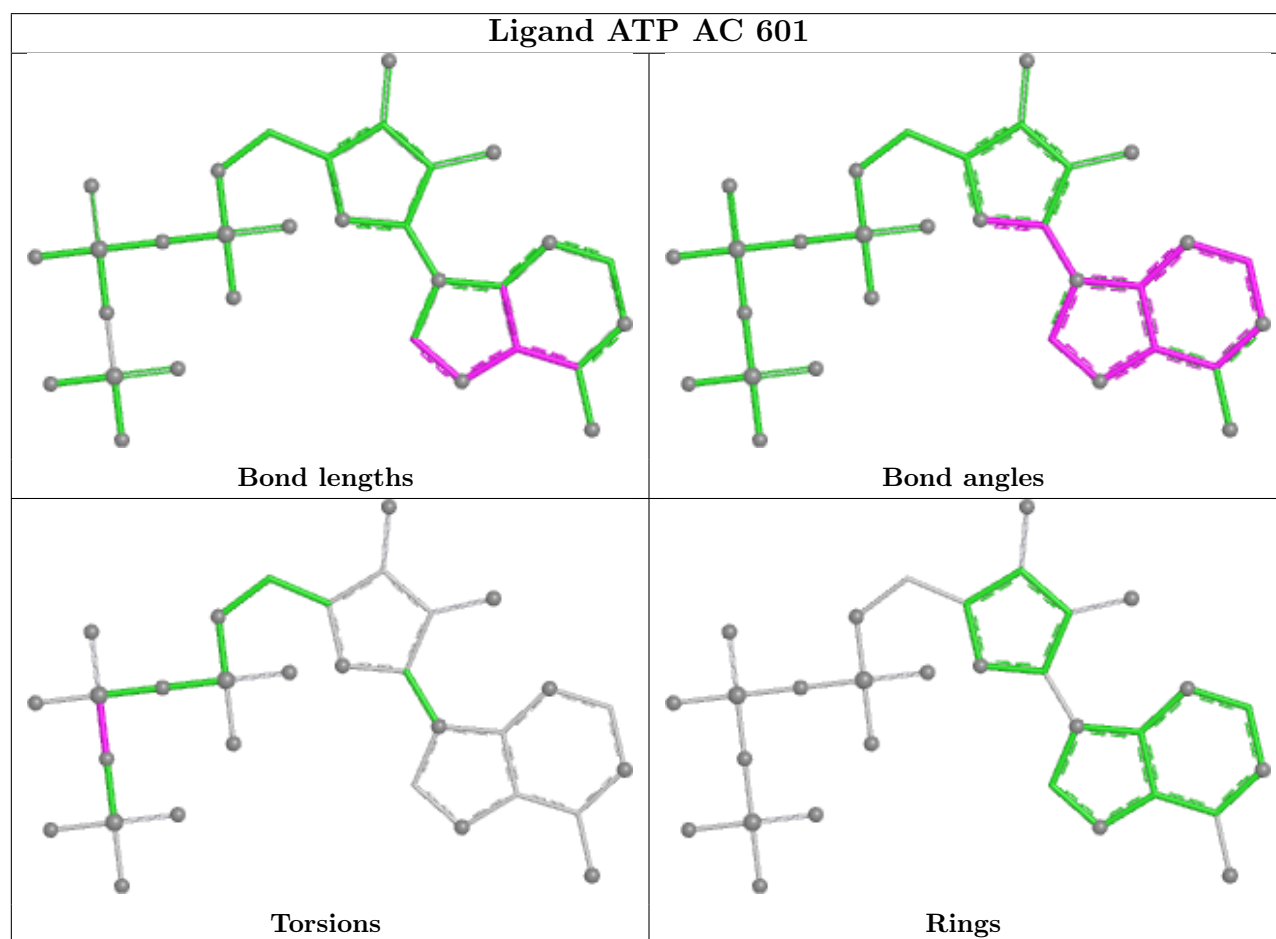
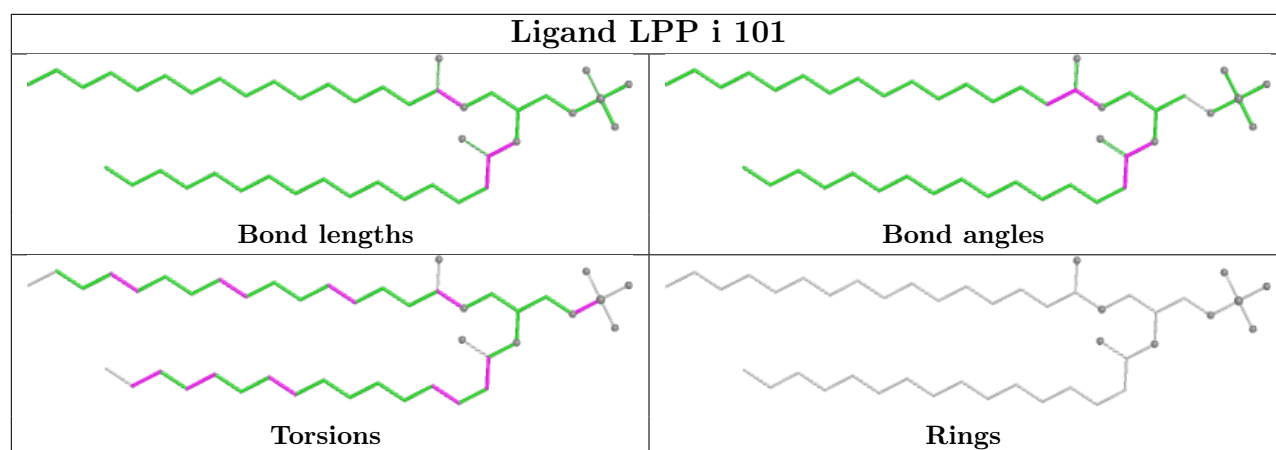


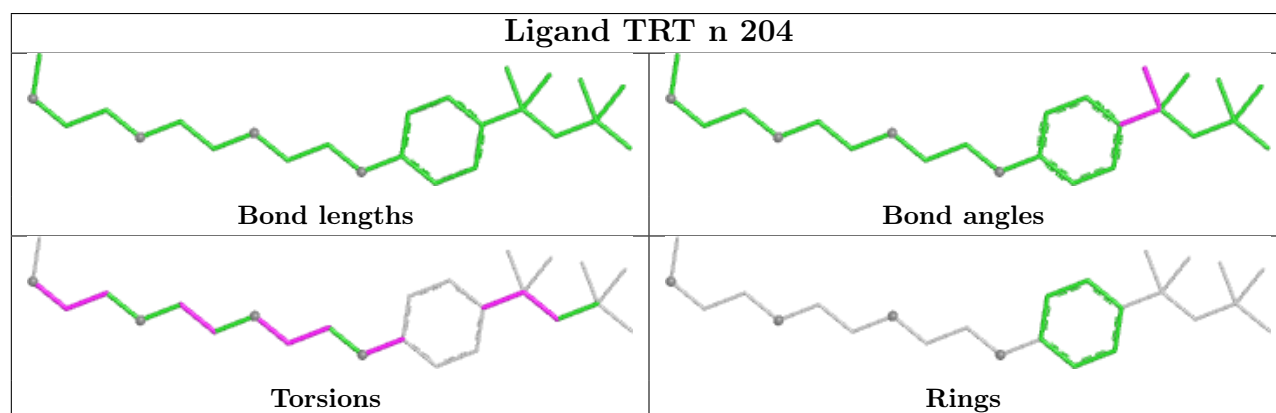
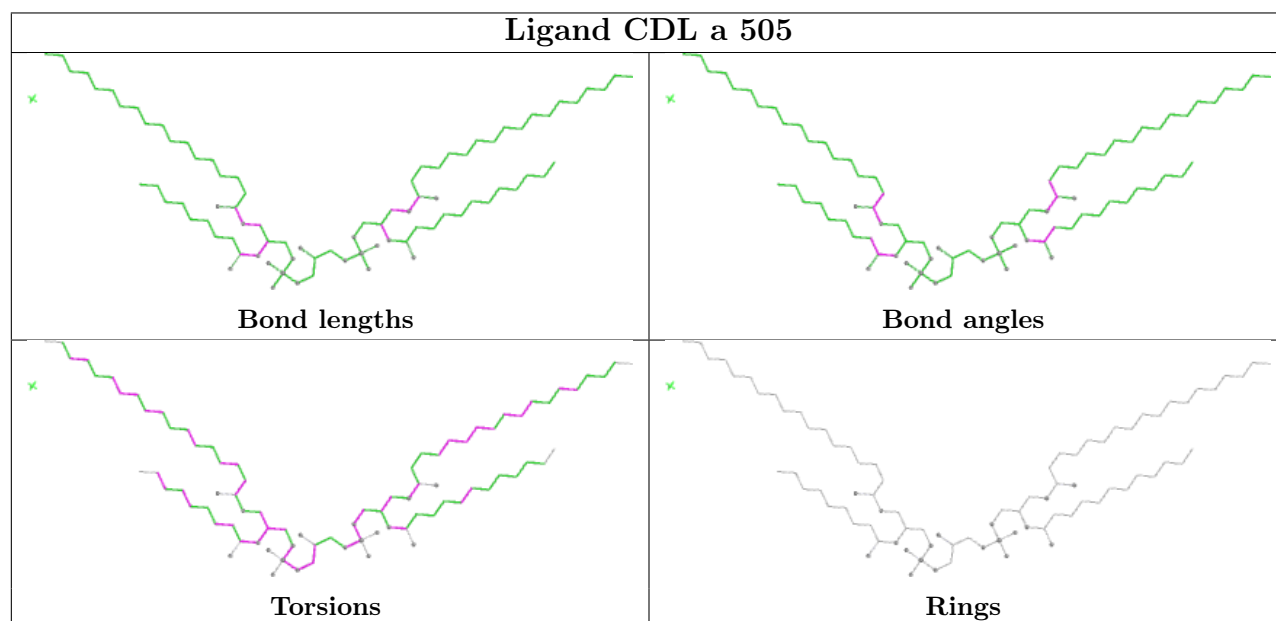
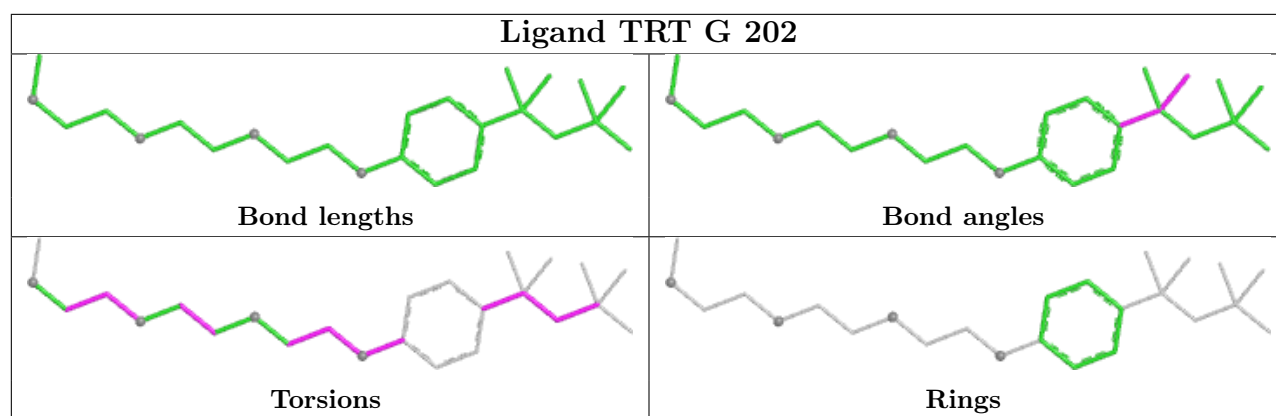
Ligand CDL E 101

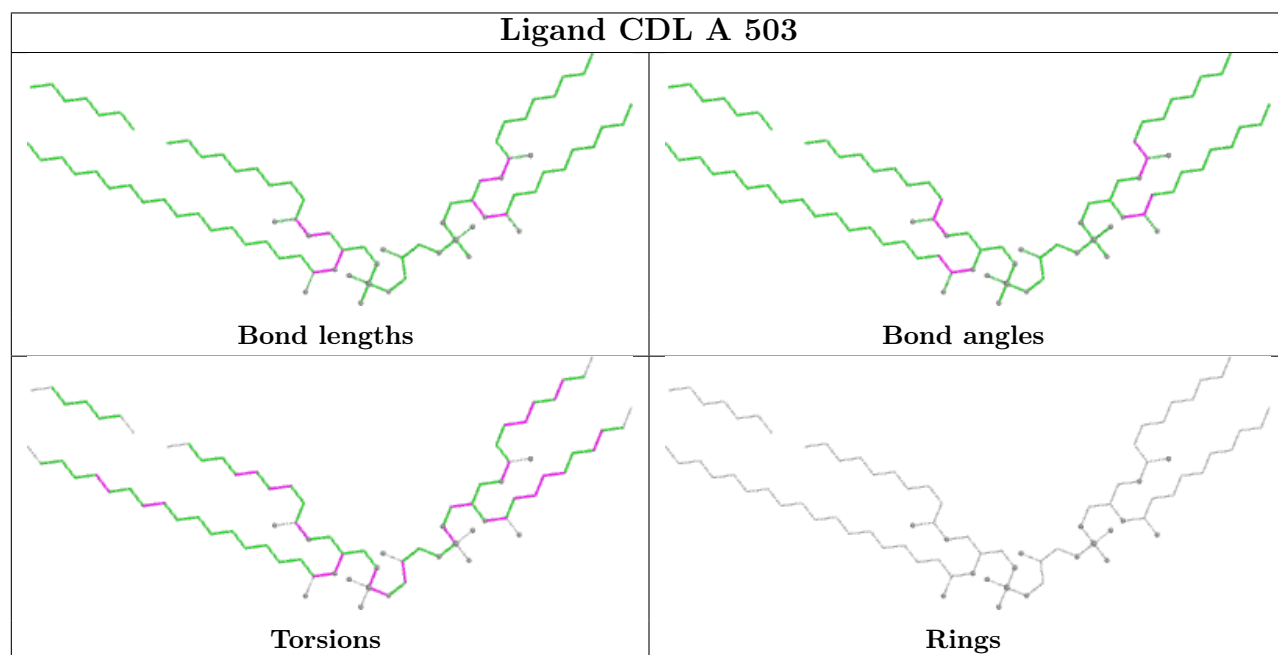
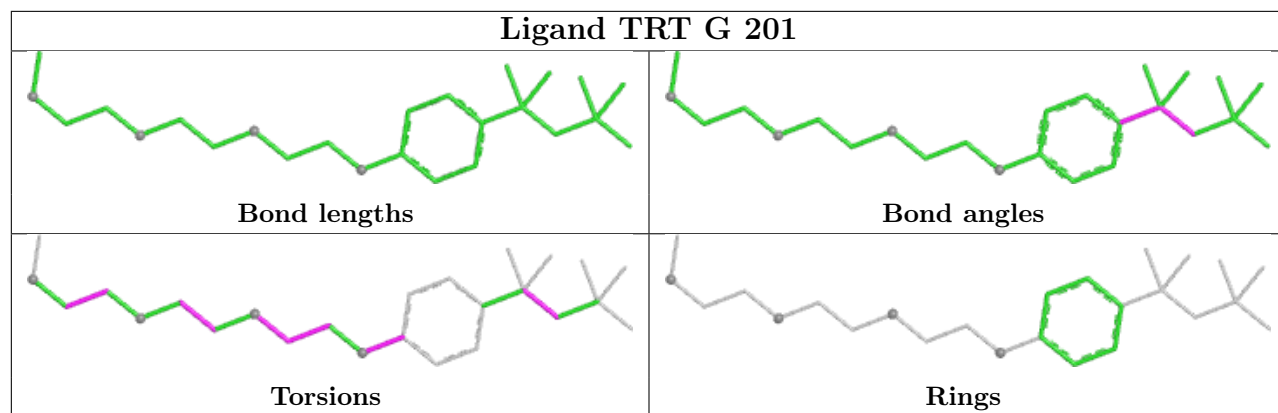


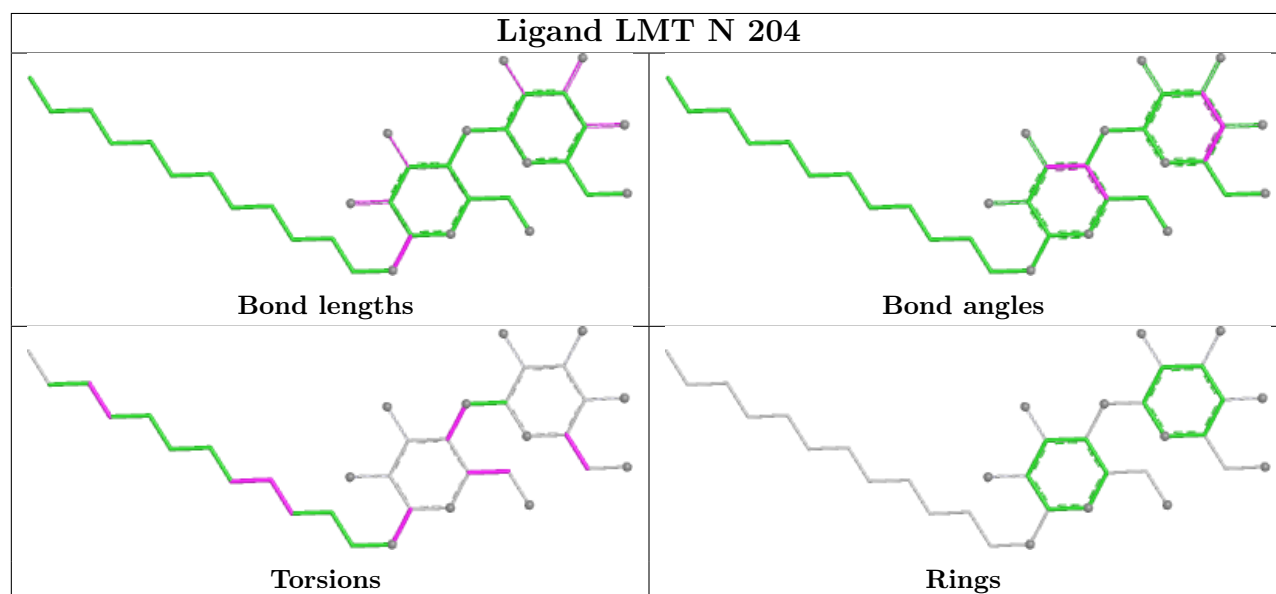
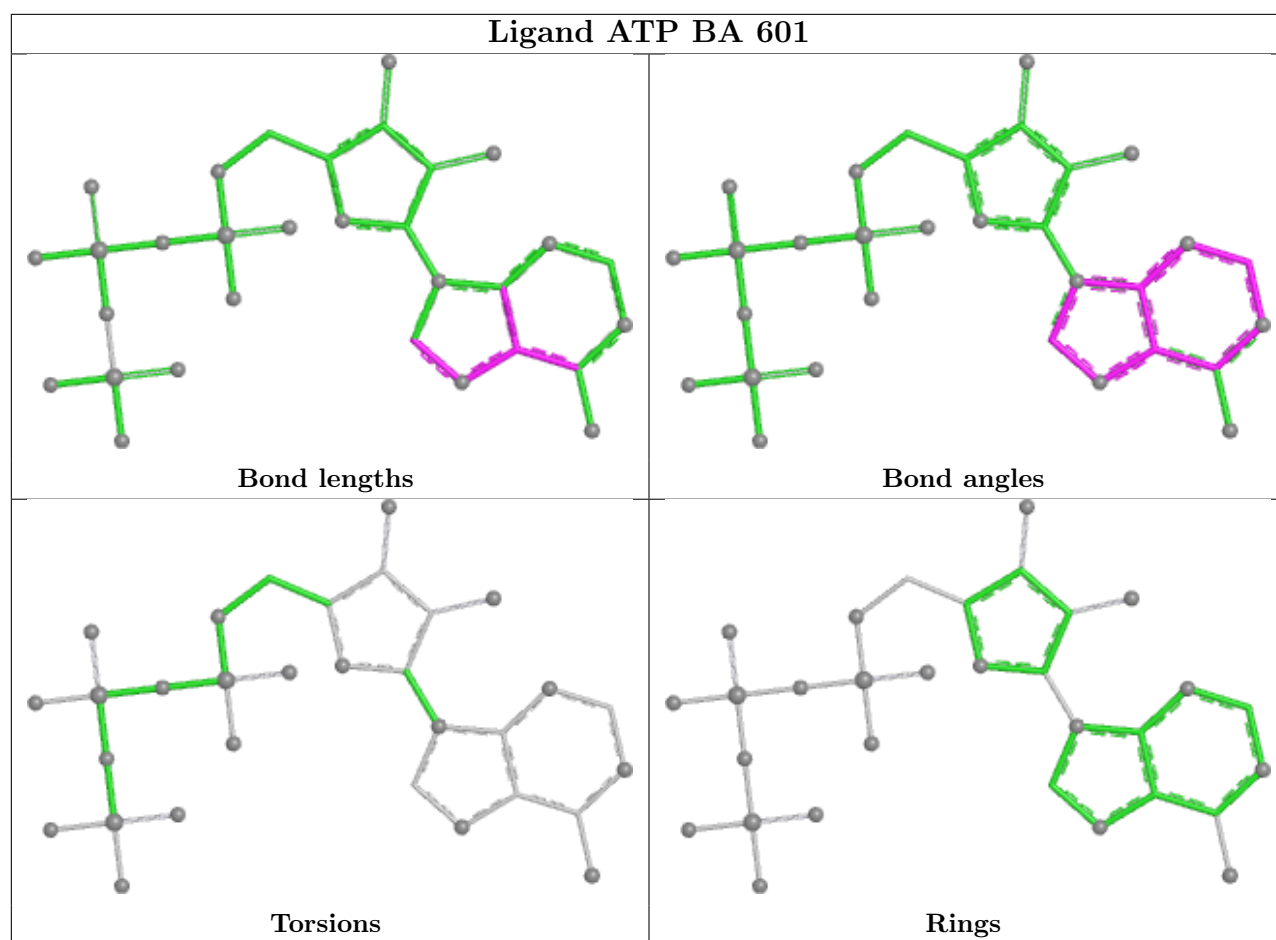
Ligand ATP AA 601

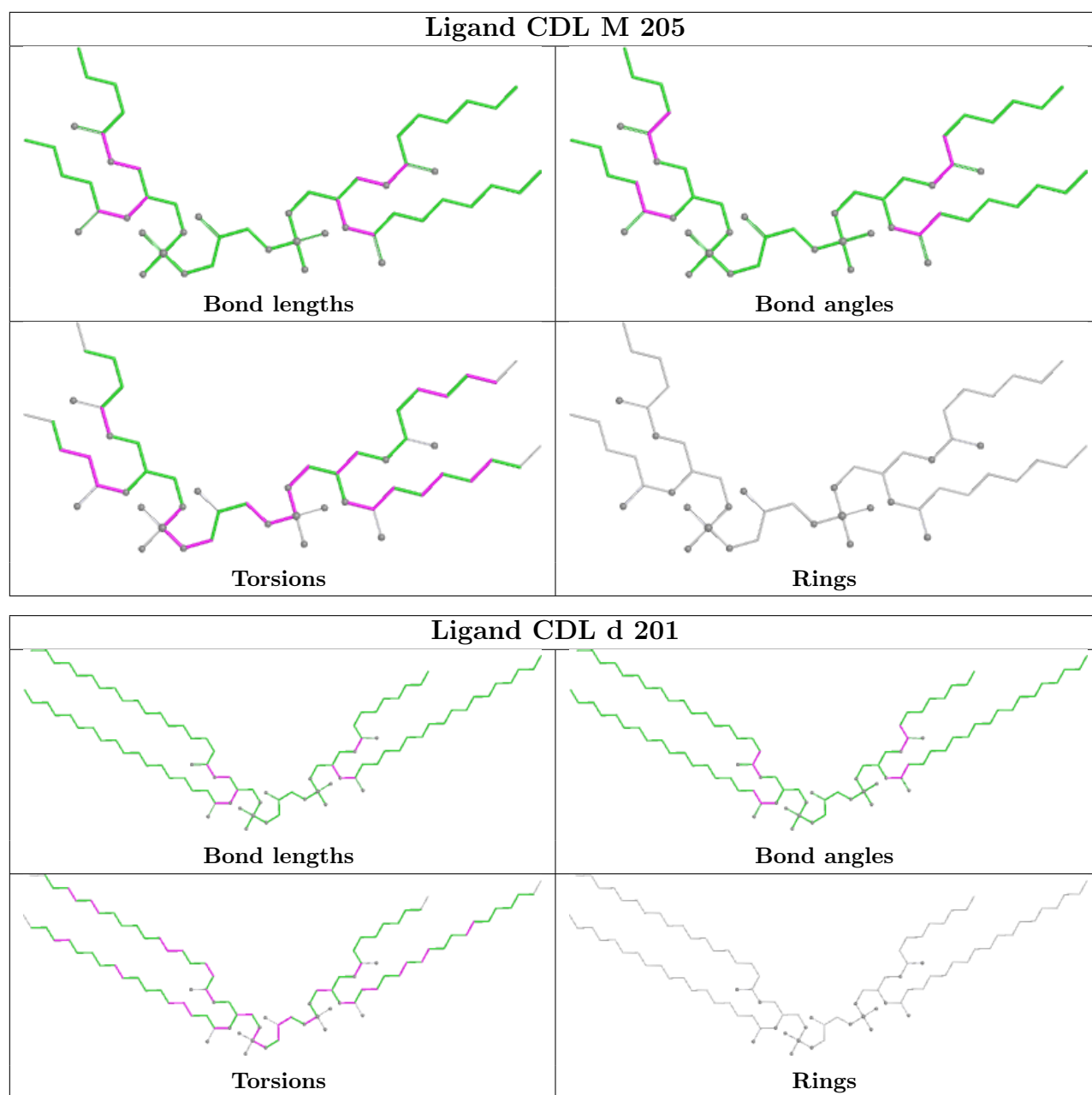


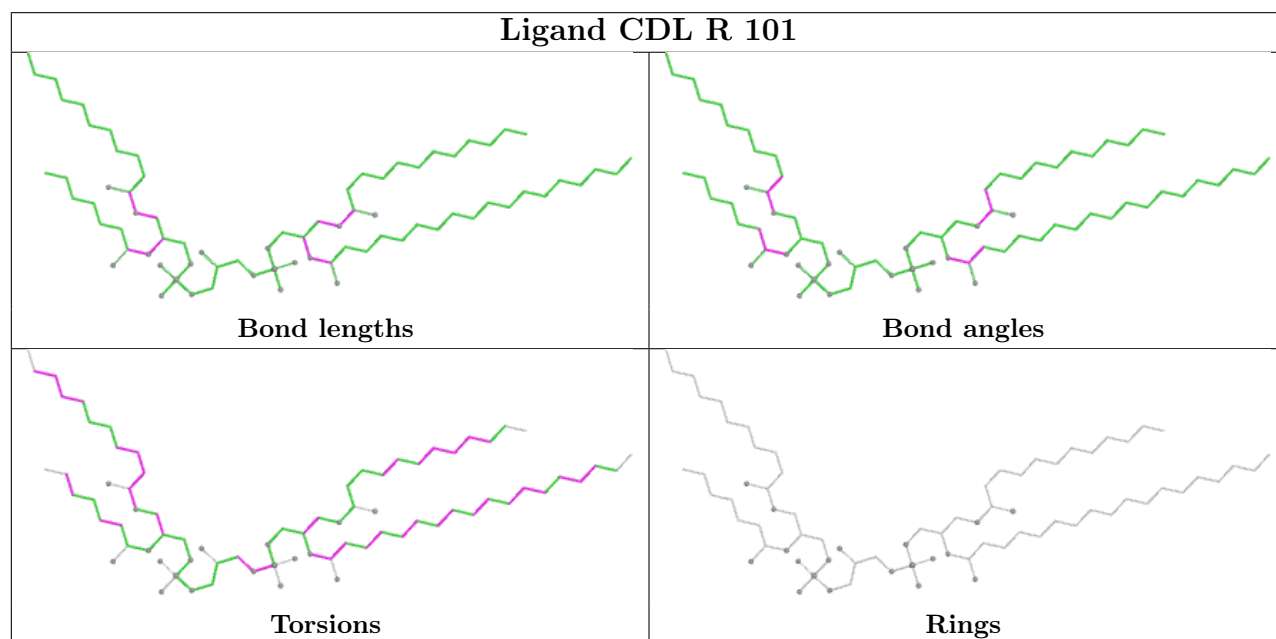
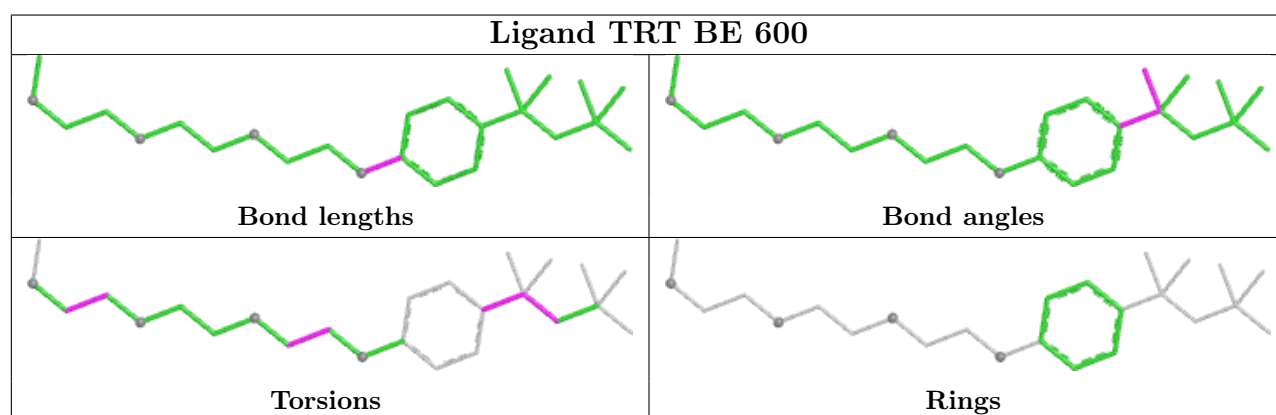
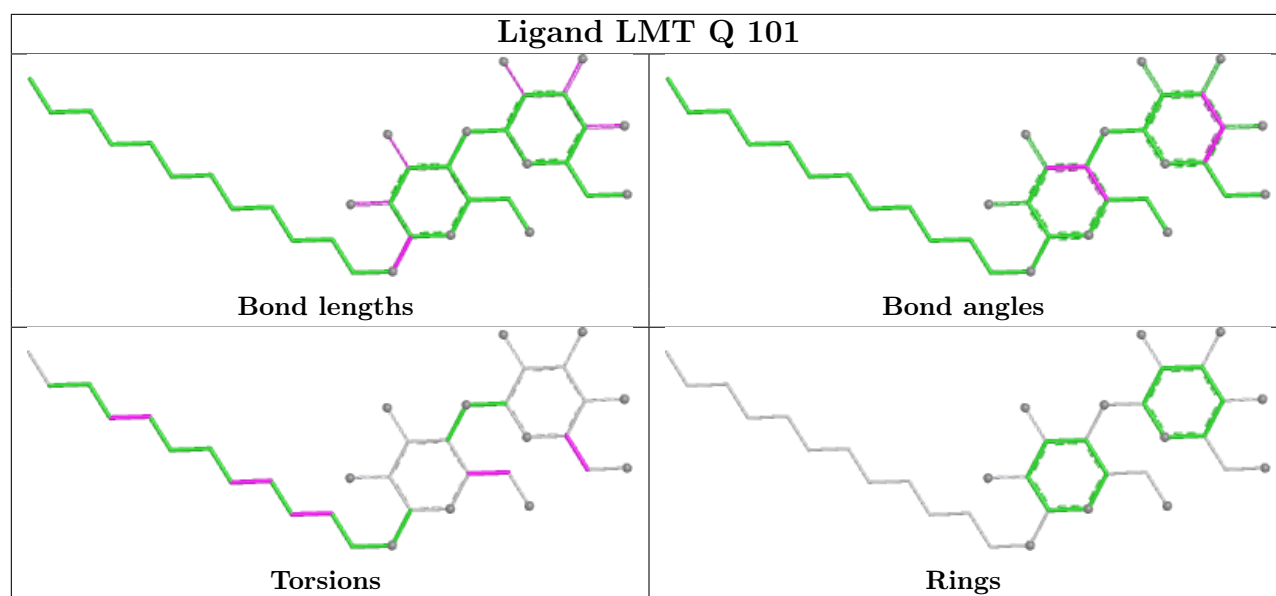




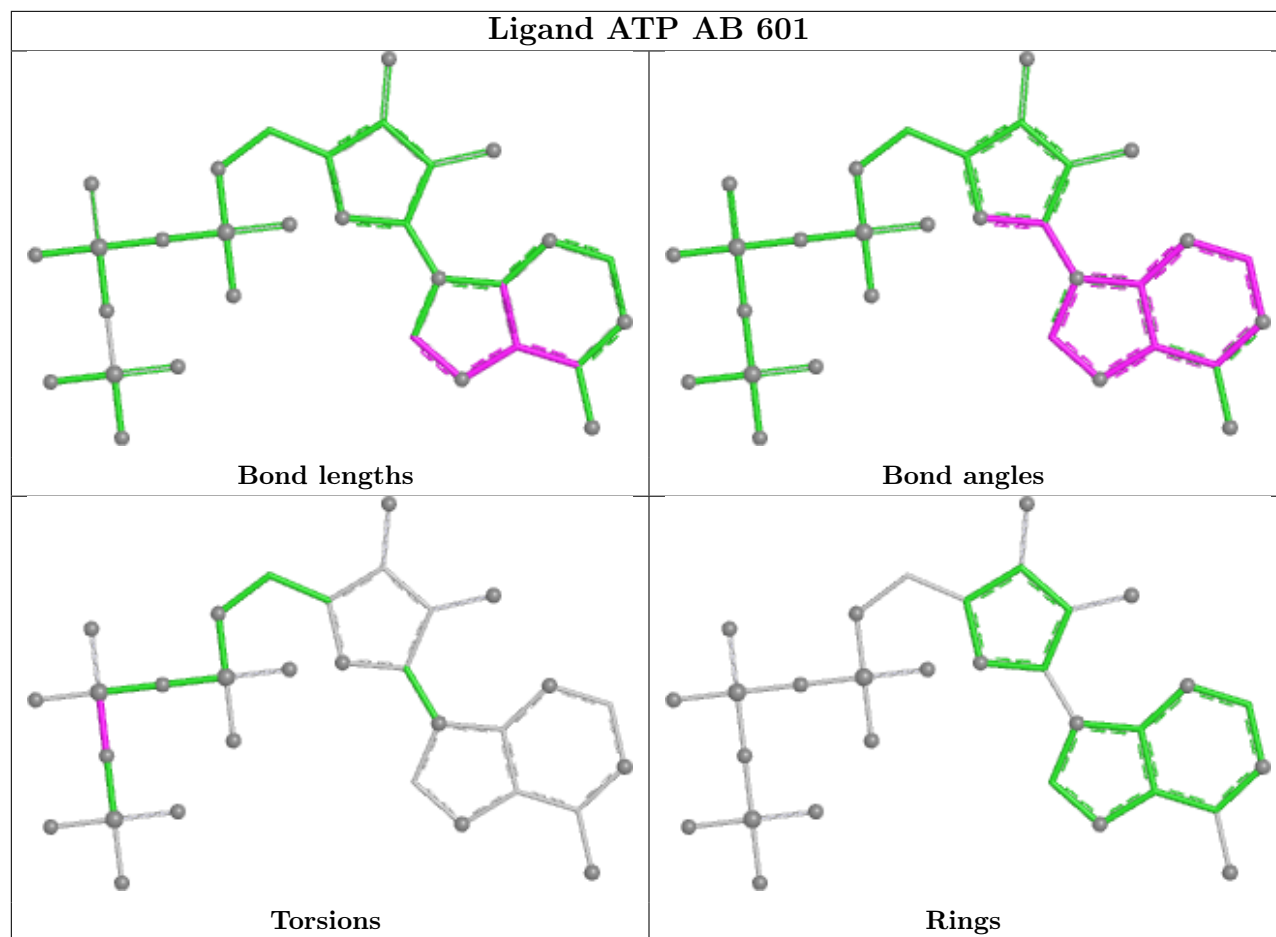




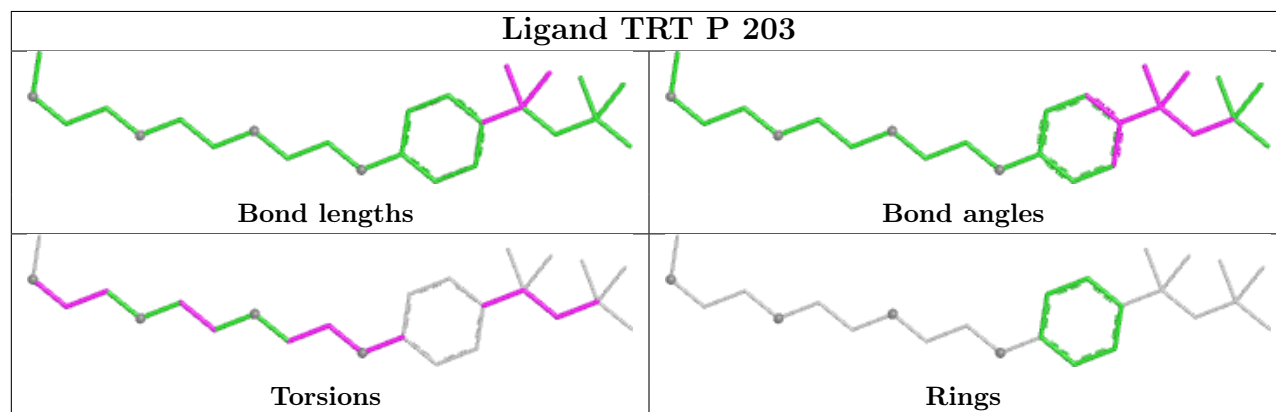


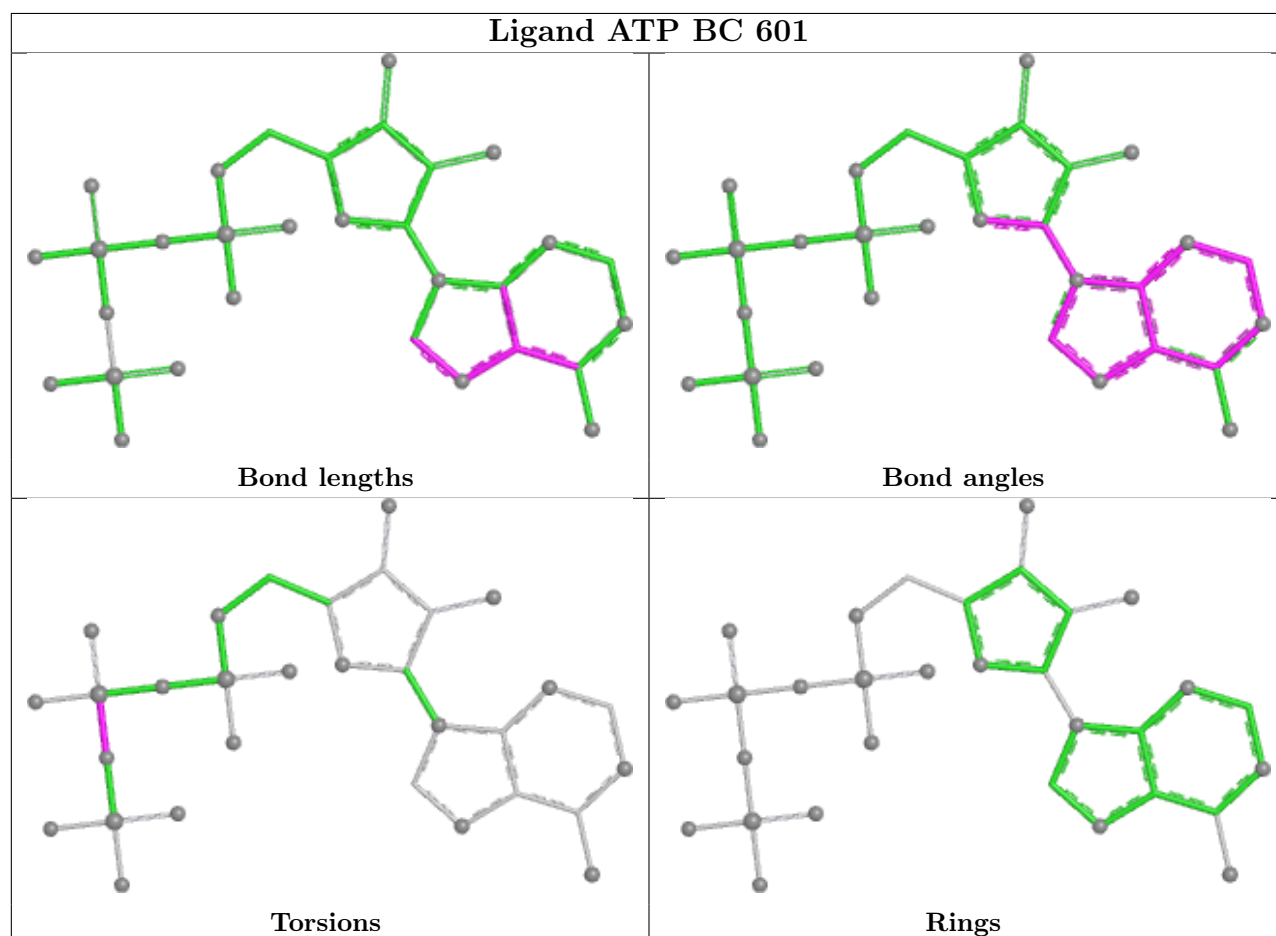
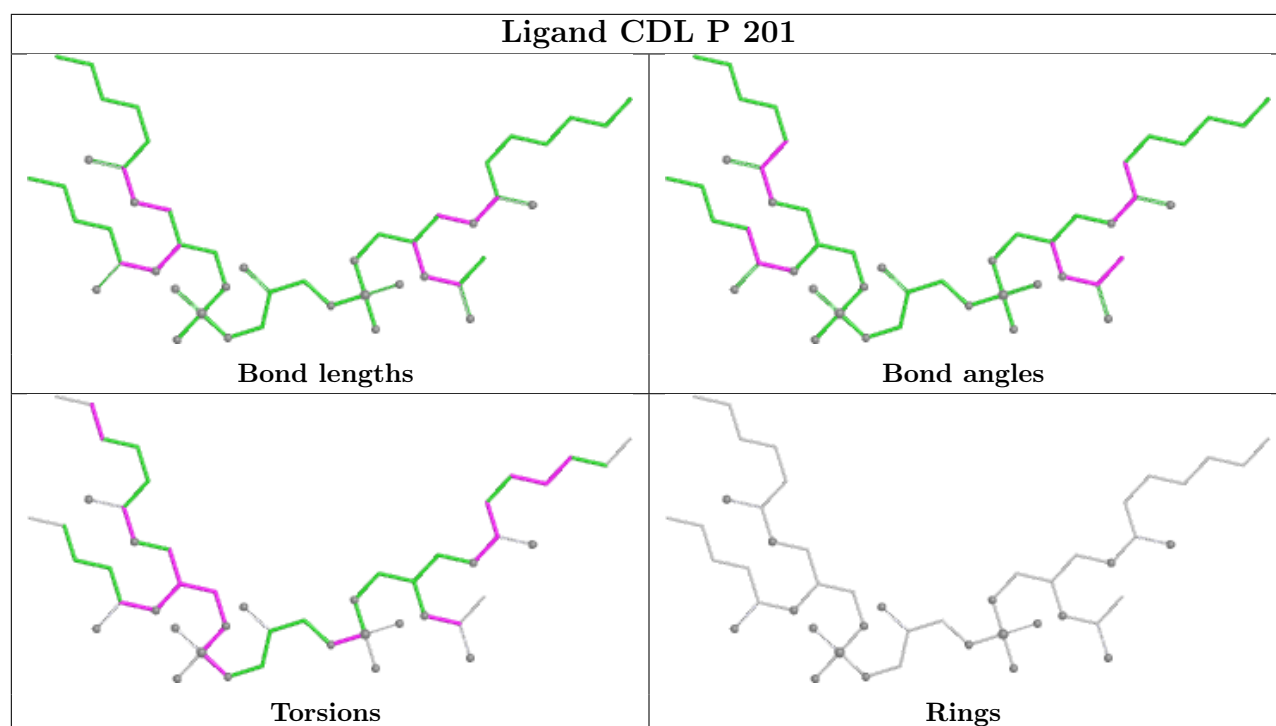


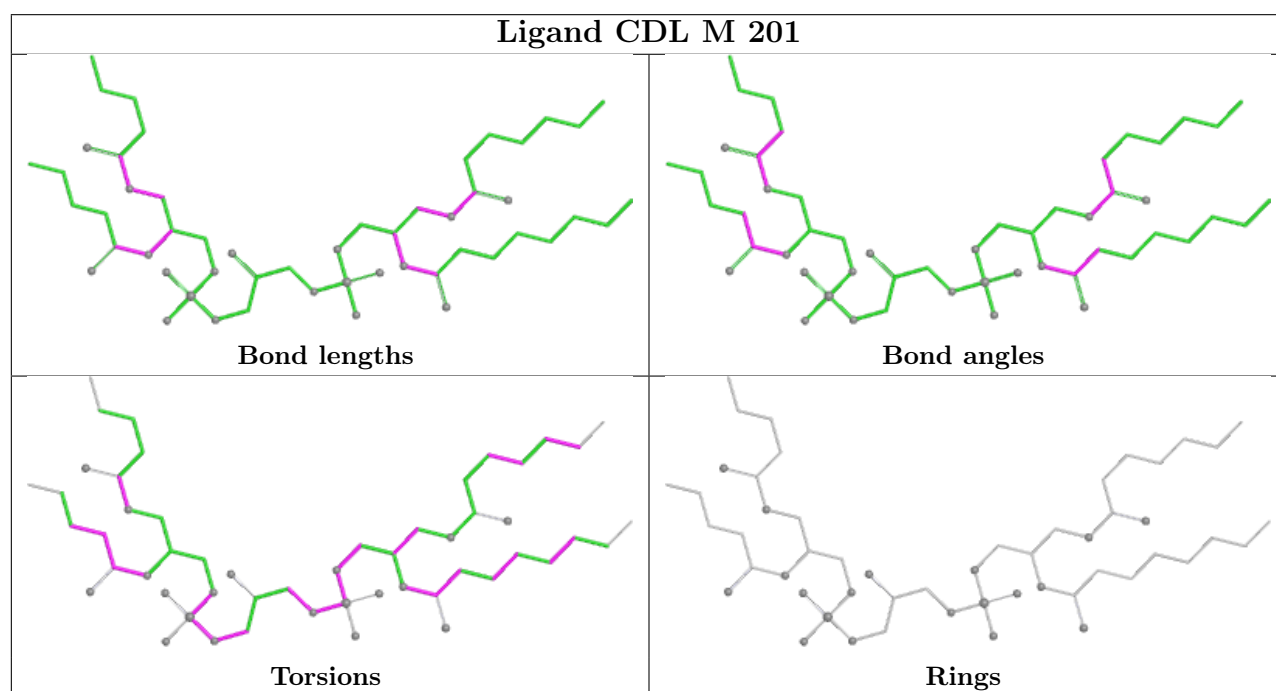
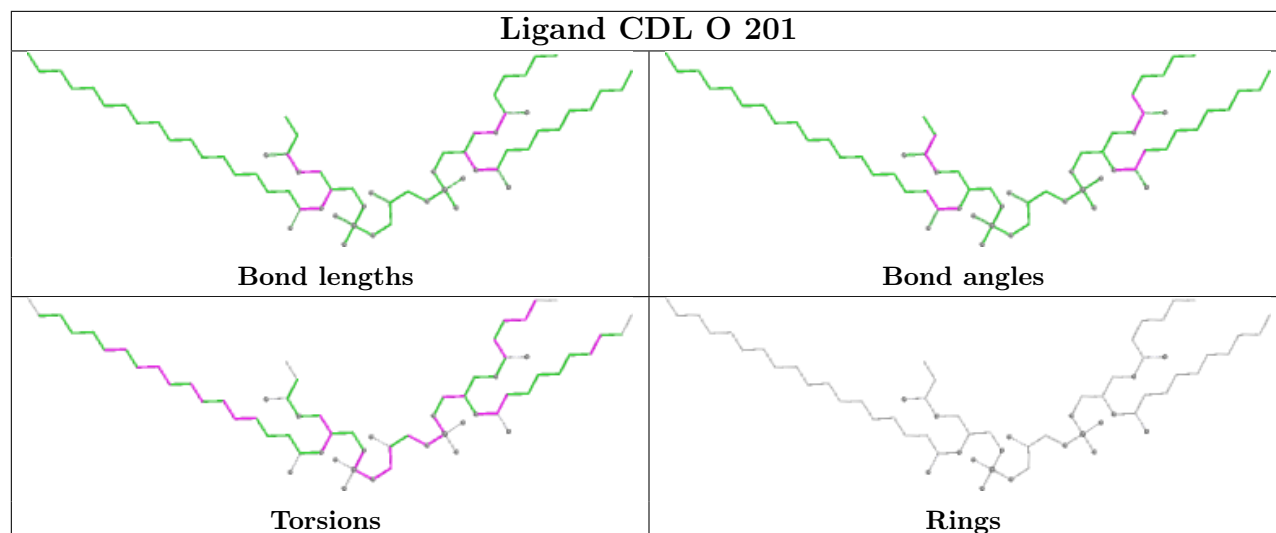
Ligand ATP AB 601

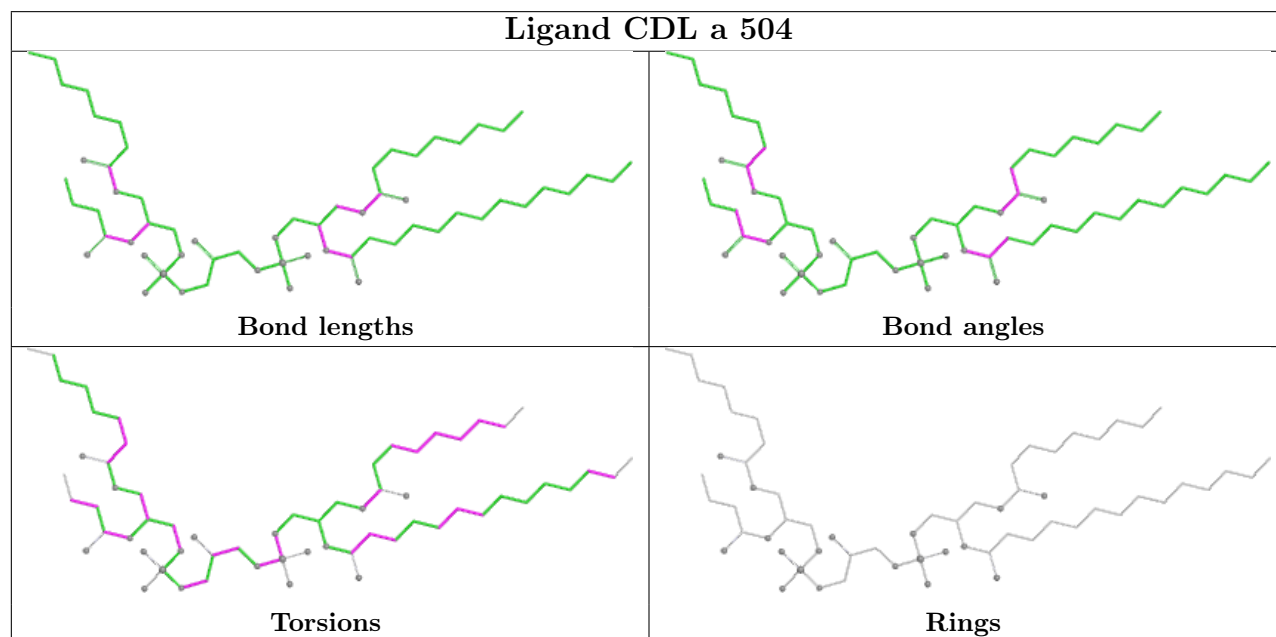
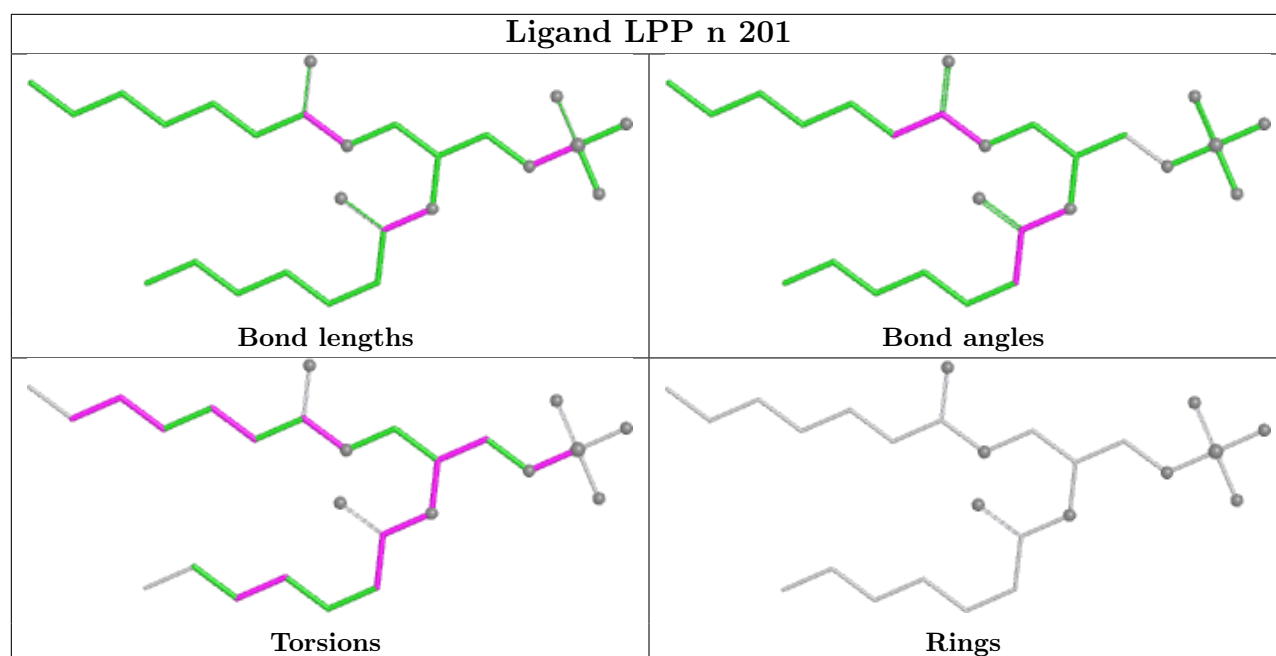


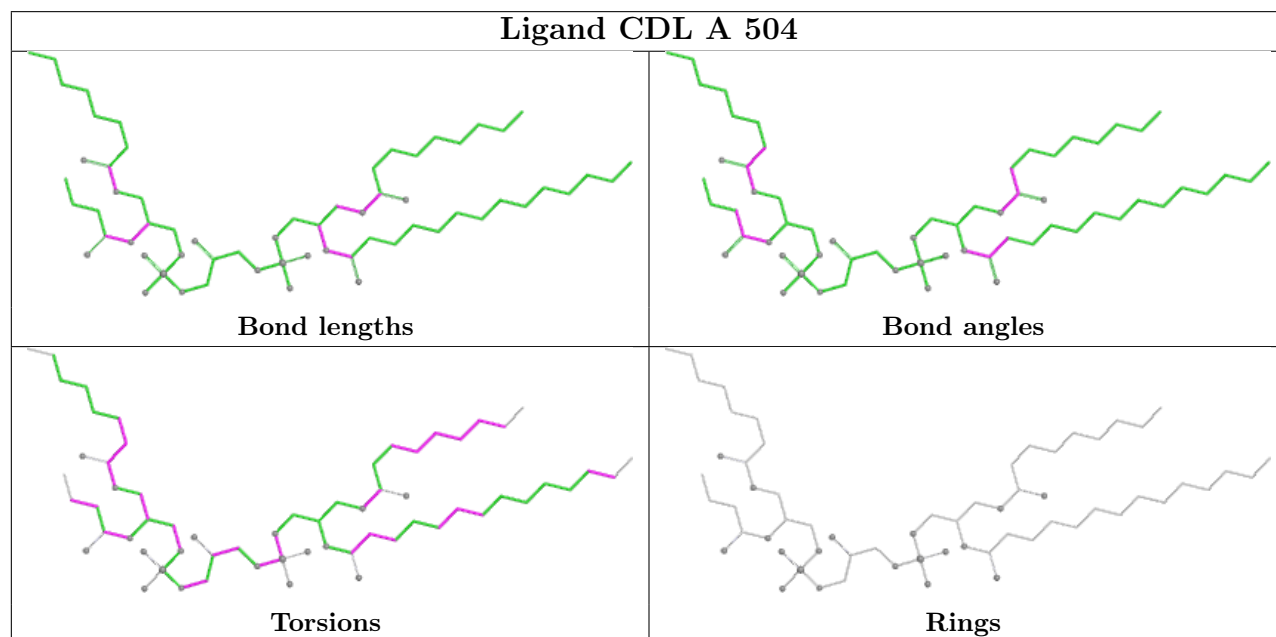
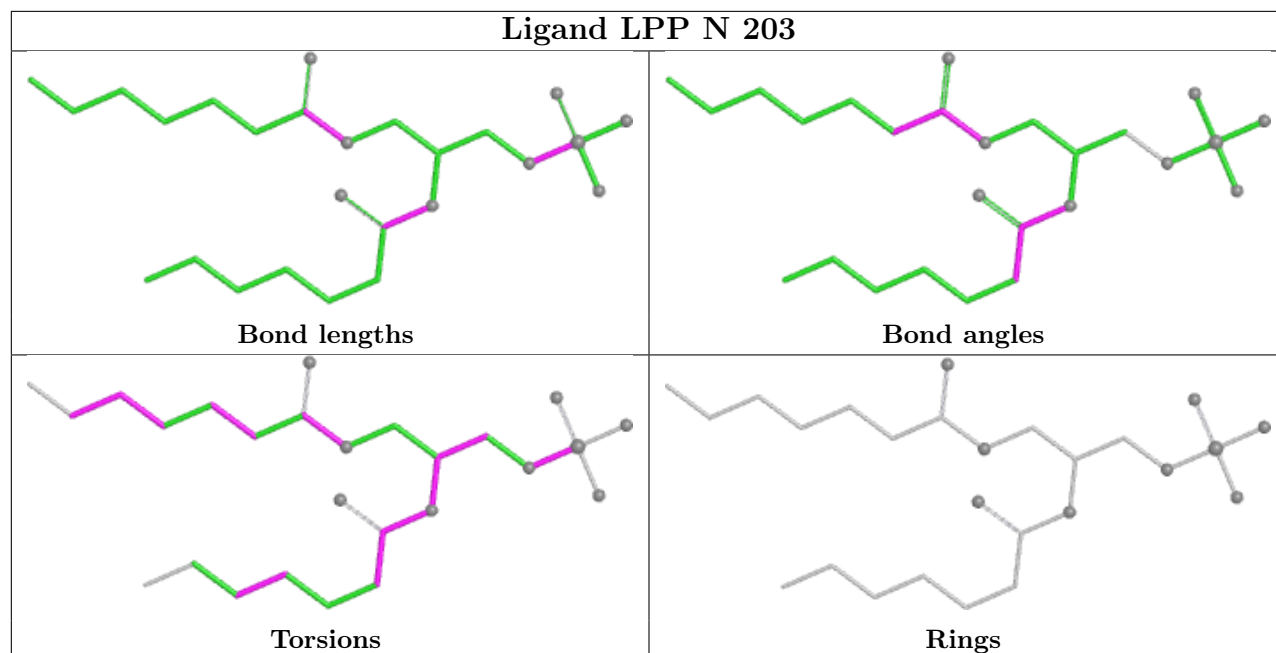
Ligand TRT P 203

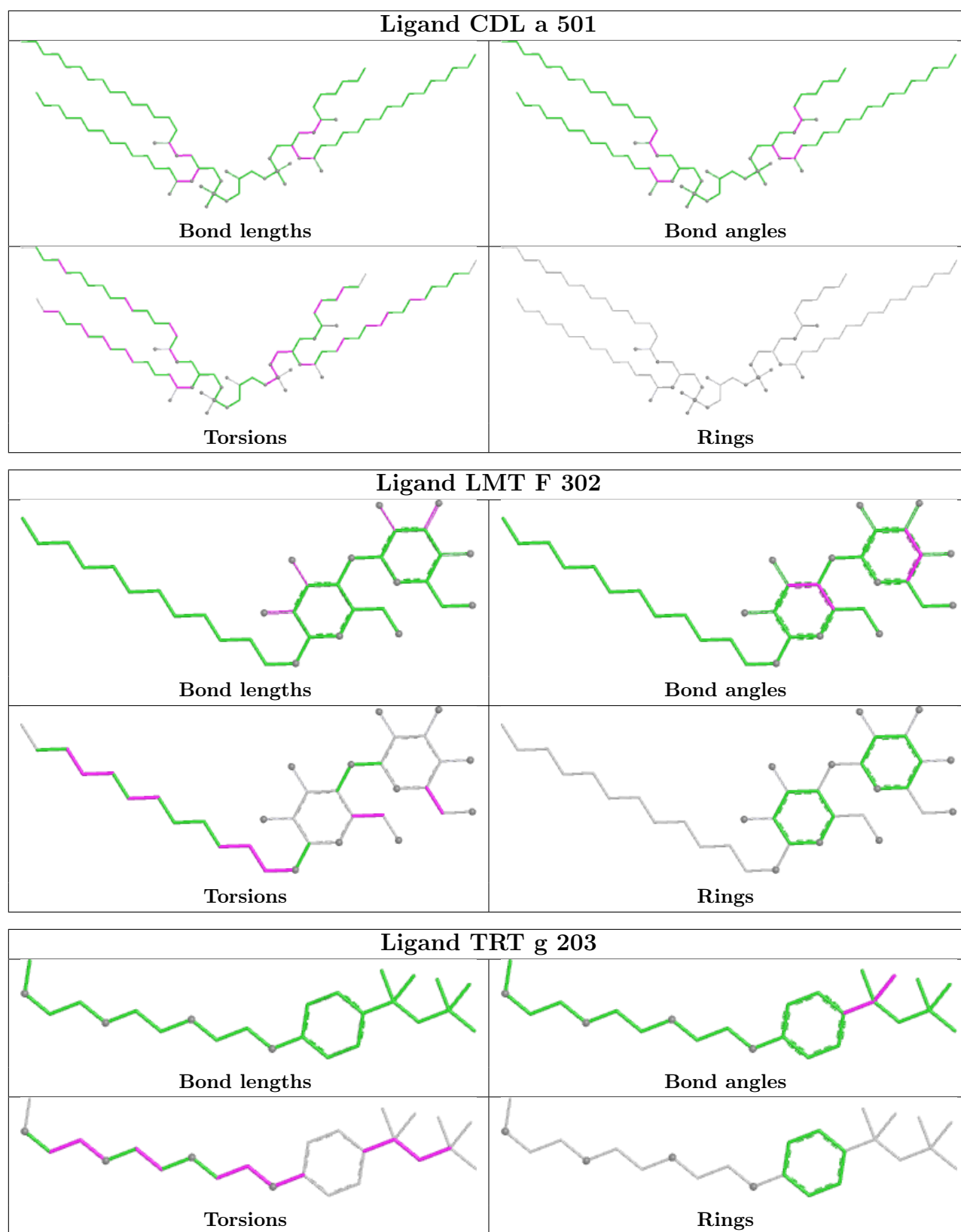


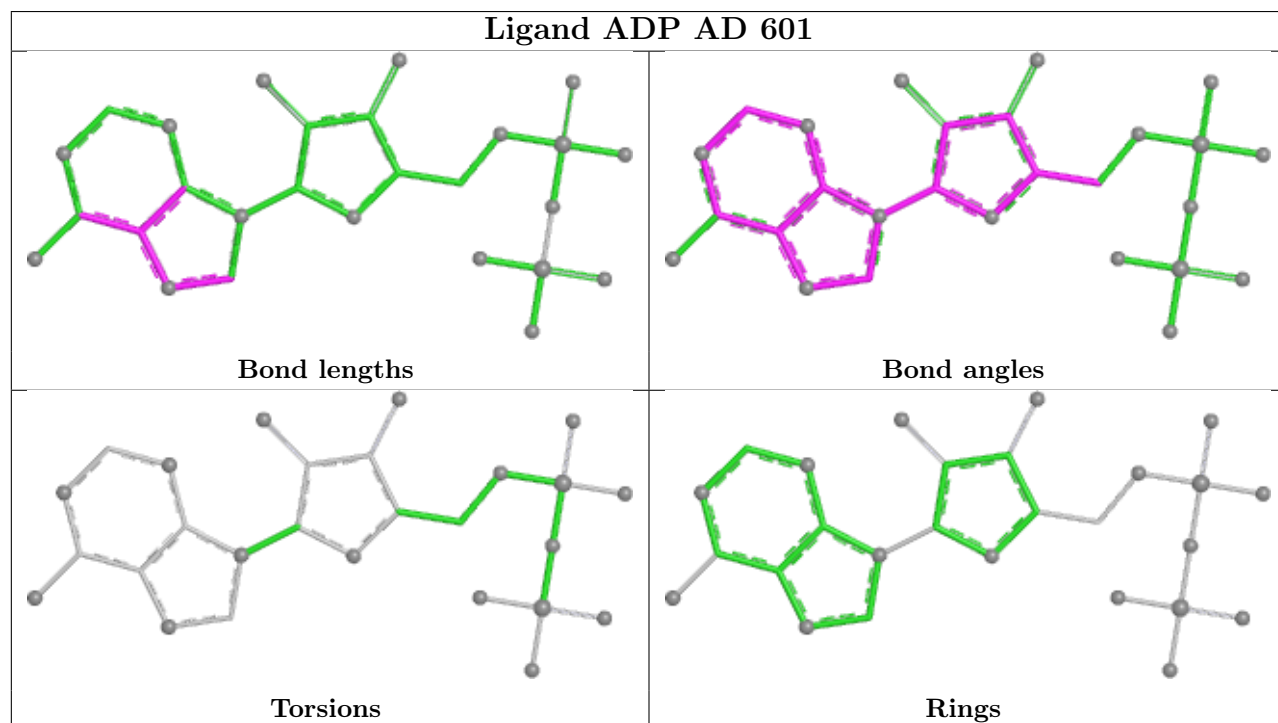
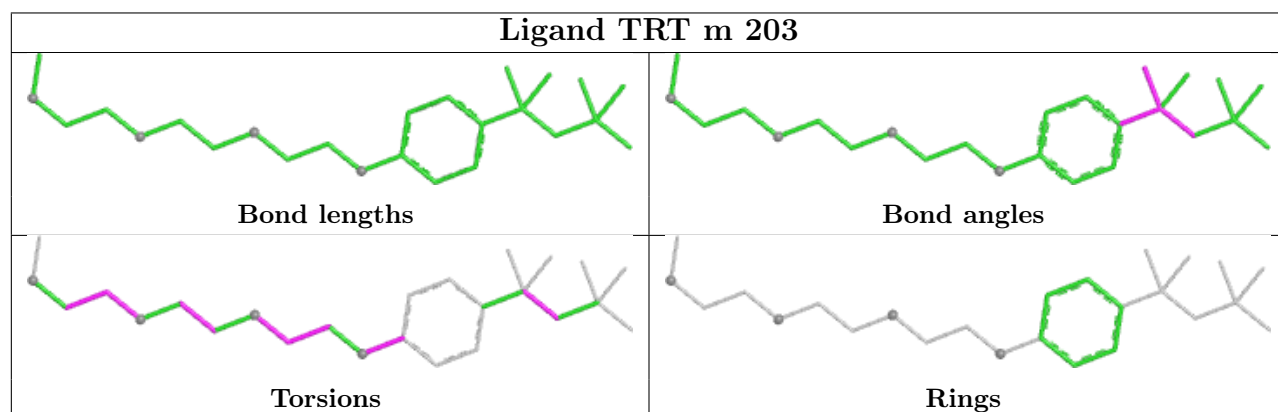
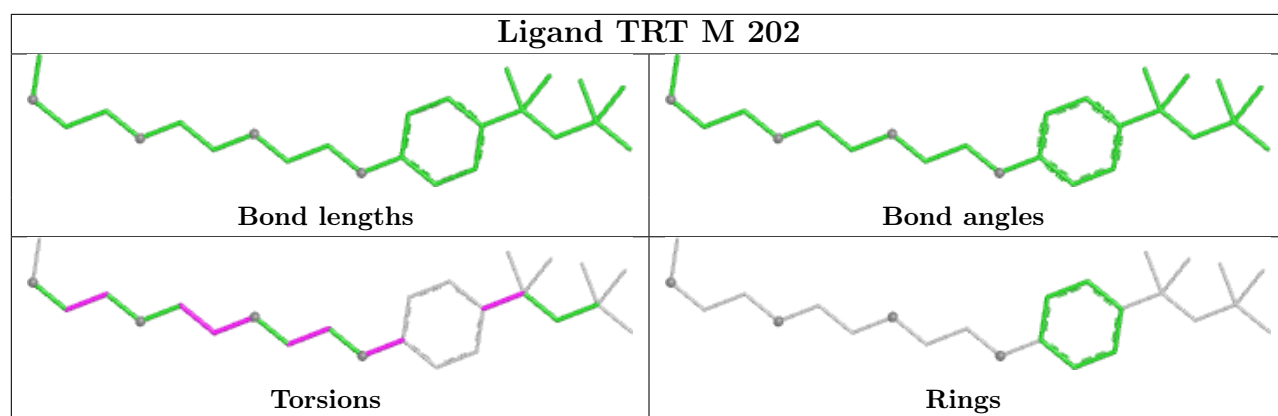


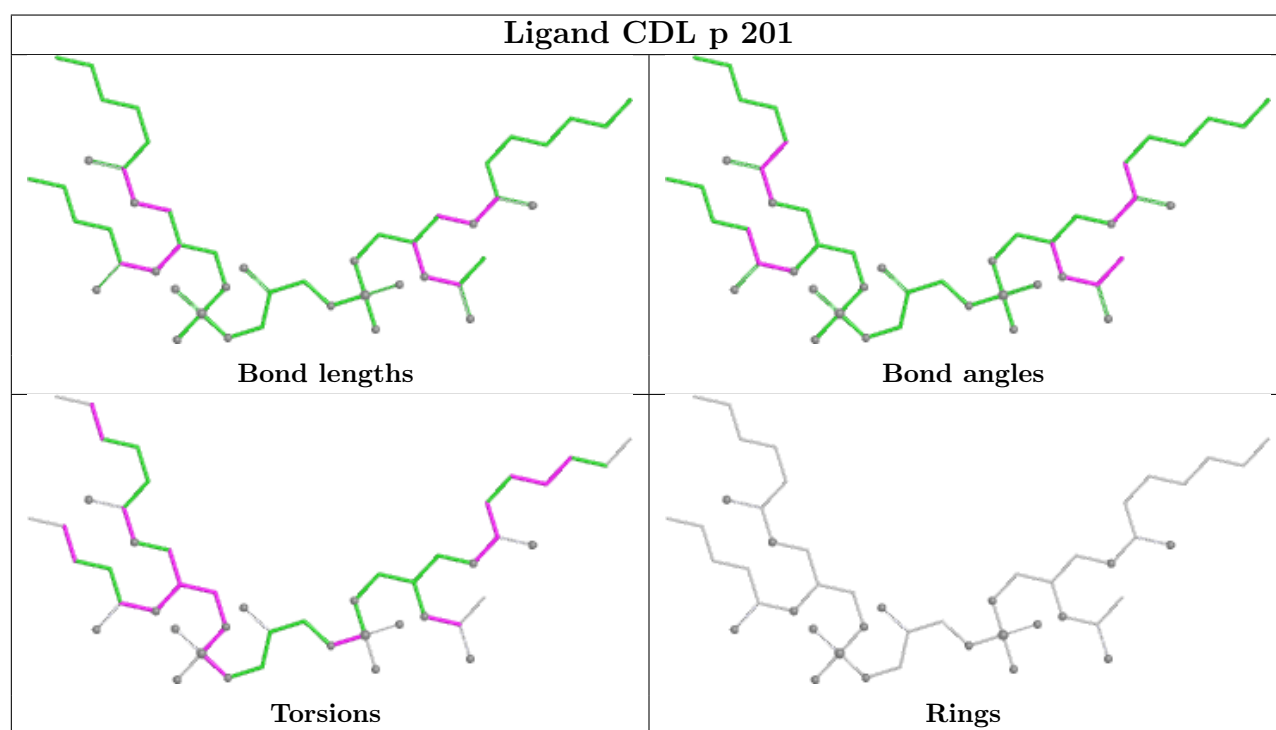
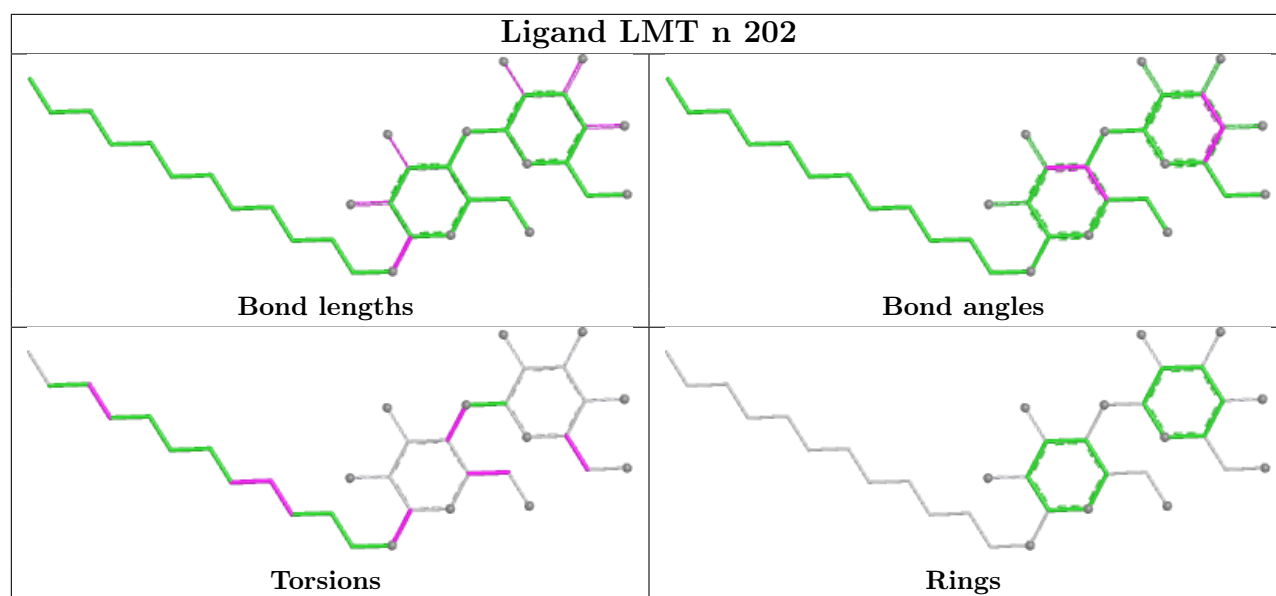


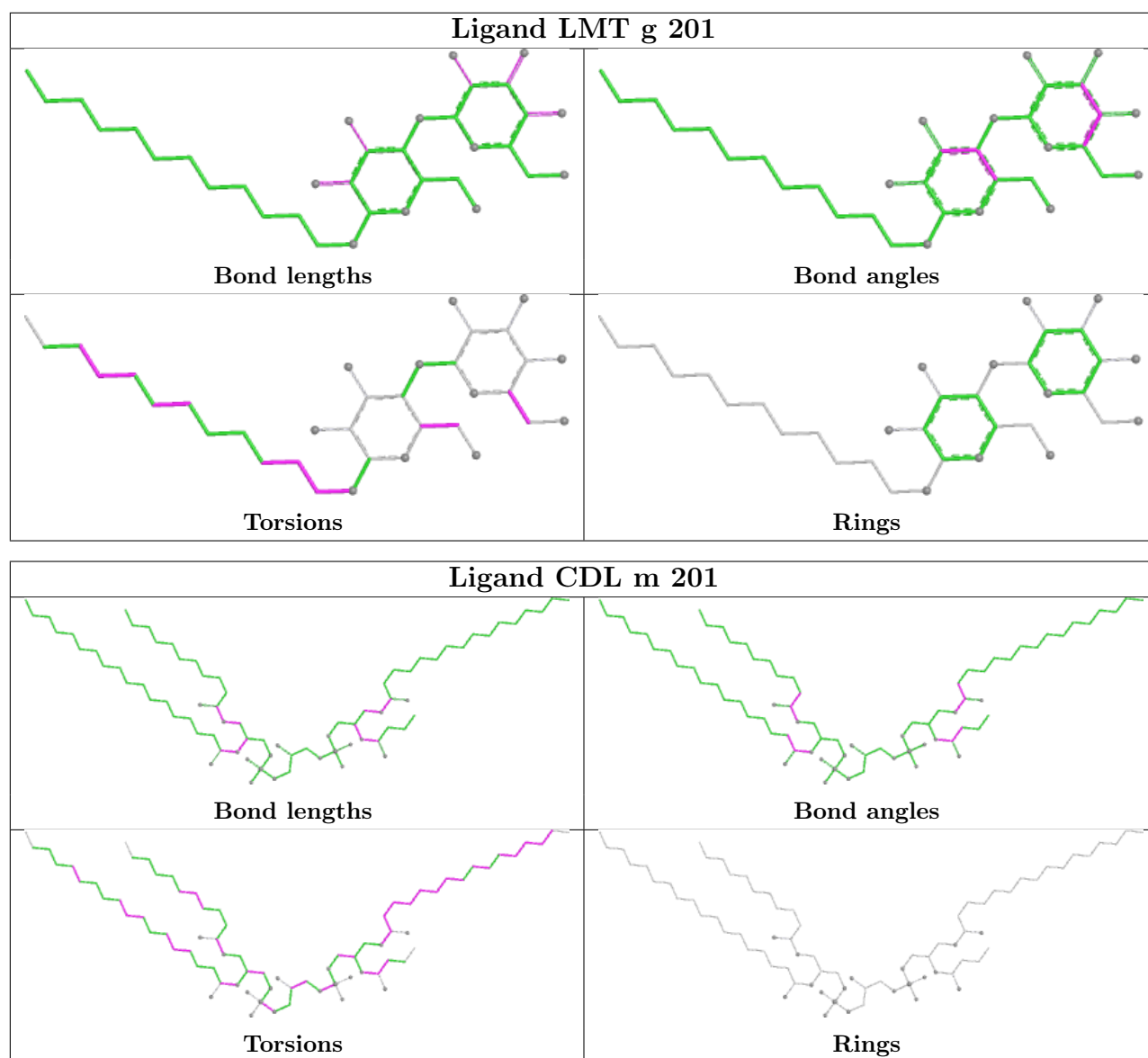


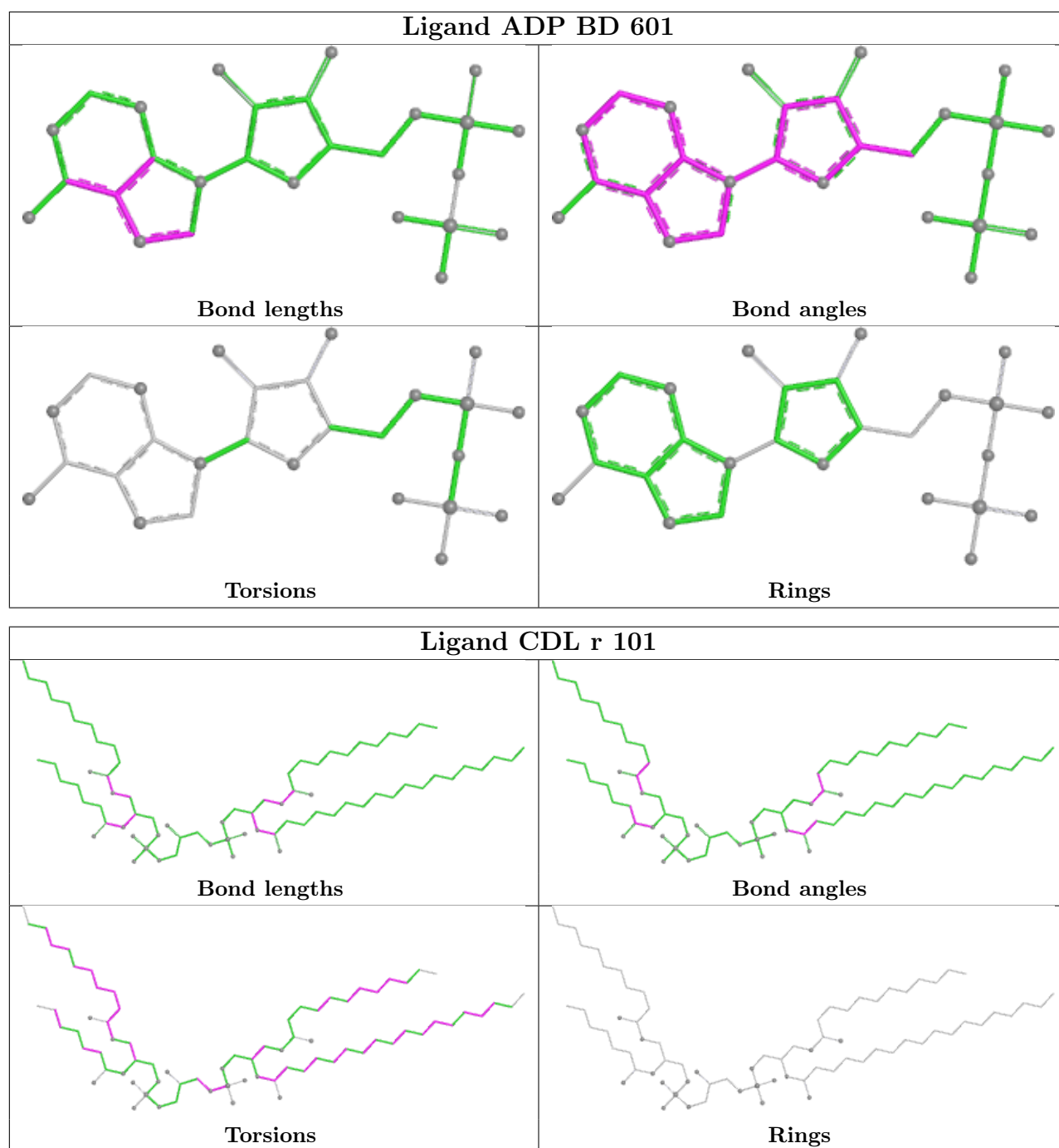












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

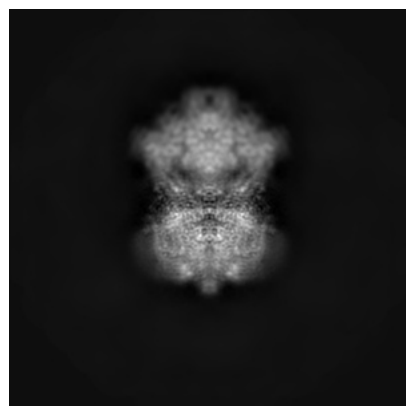
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10467. These allow visual inspection of the internal detail of the map and identification of artifacts.

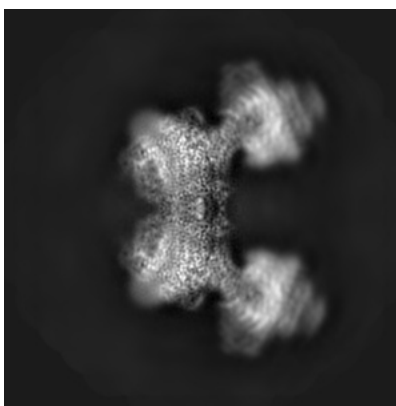
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

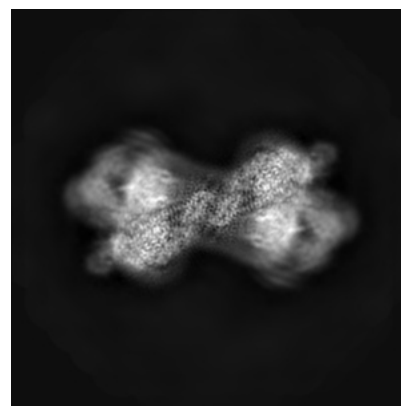
6.1.1 Primary map



X

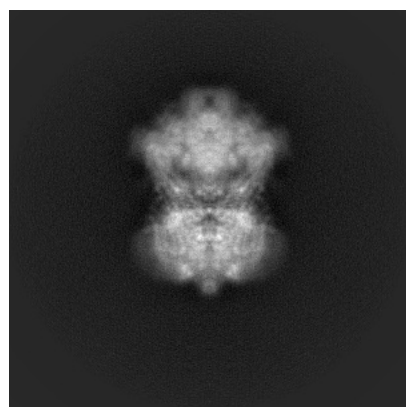


Y

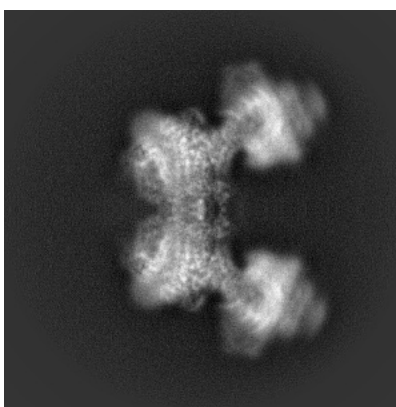


Z

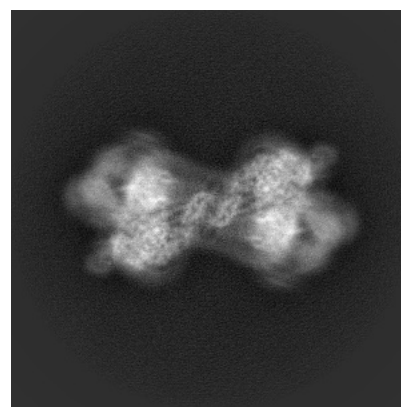
6.1.2 Raw map



X



Y

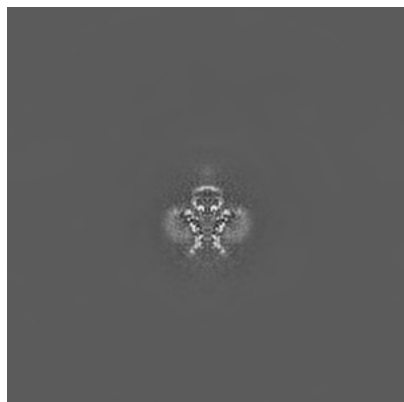


Z

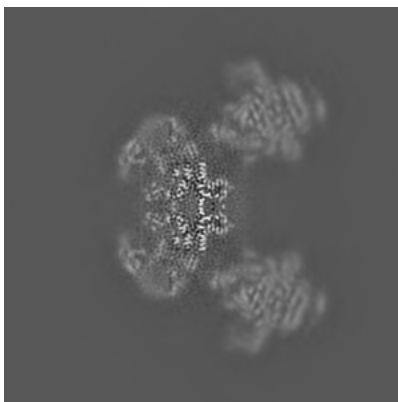
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 220

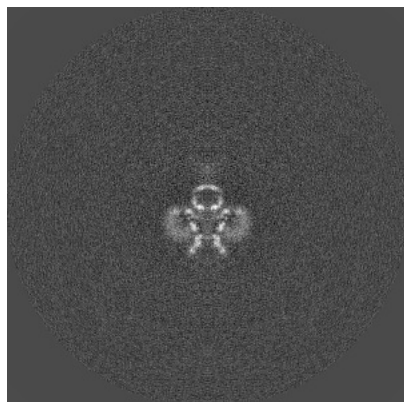


Y Index: 220

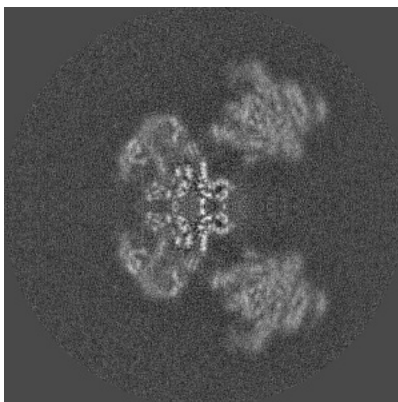


Z Index: 220

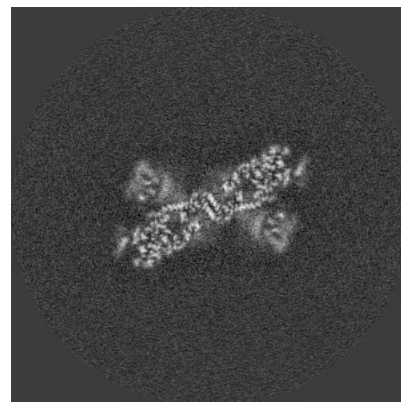
6.2.2 Raw map



X Index: 220



Y Index: 220

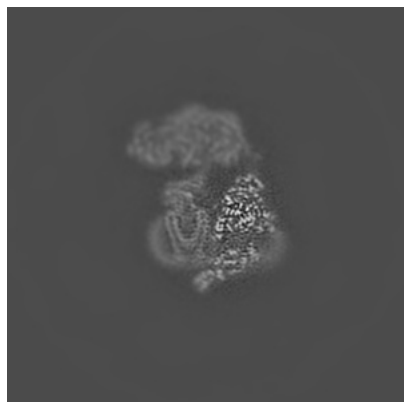


Z Index: 220

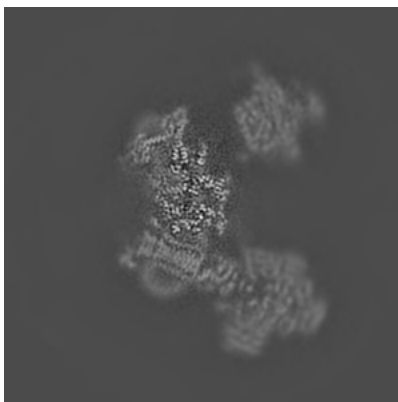
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

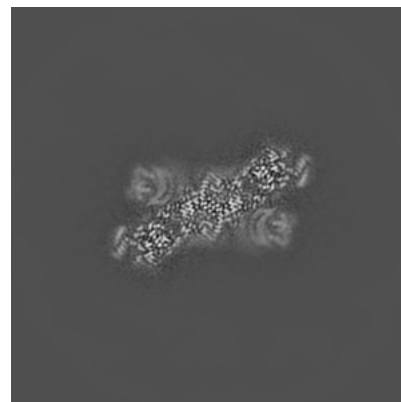
6.3.1 Primary map



X Index: 283

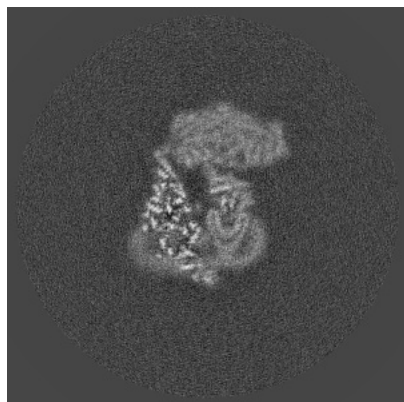


Y Index: 230

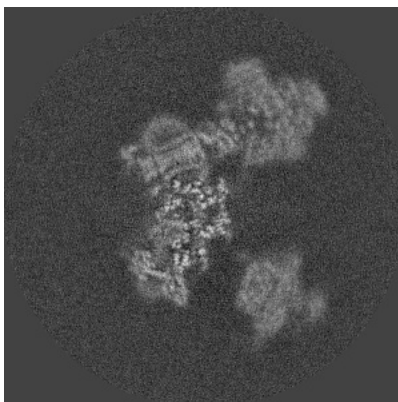


Z Index: 215

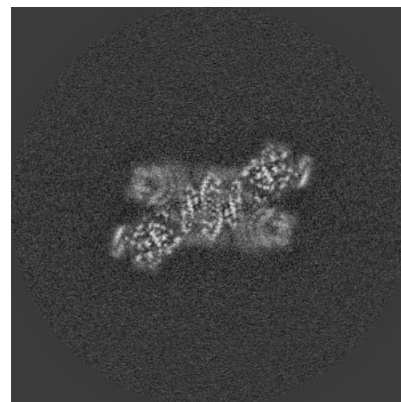
6.3.2 Raw map



X Index: 152



Y Index: 210

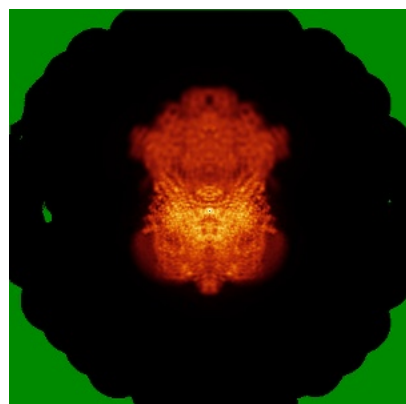


Z Index: 215

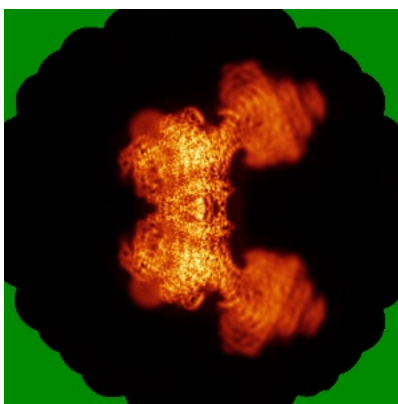
The images above show the largest variance slices of the map in three orthogonal directions.

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

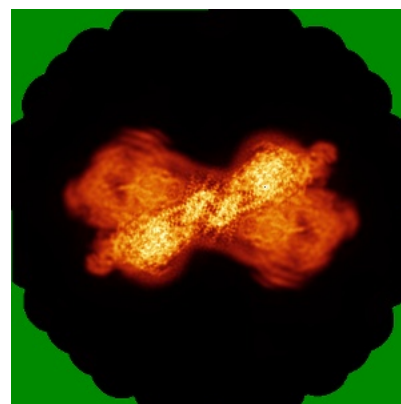
6.4.1 Primary map



X

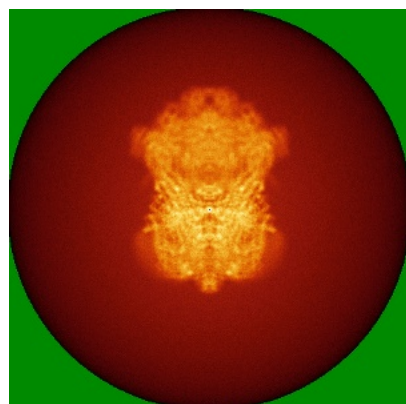


Y

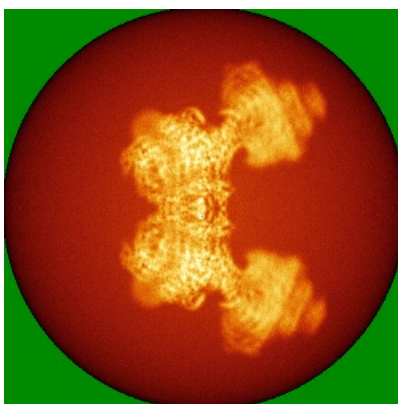


Z

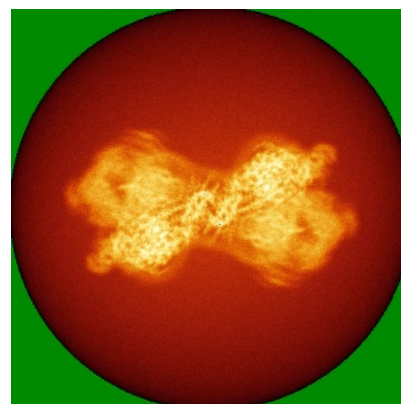
6.4.2 Raw map



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



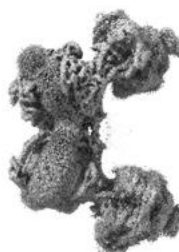
Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

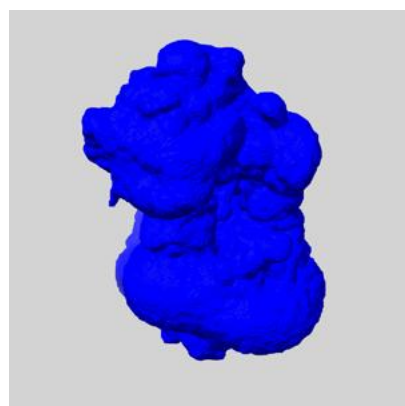
6.6 Mask visualisation [i](#)

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

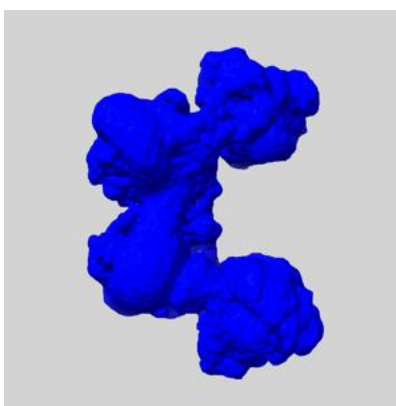
A mask typically either:

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

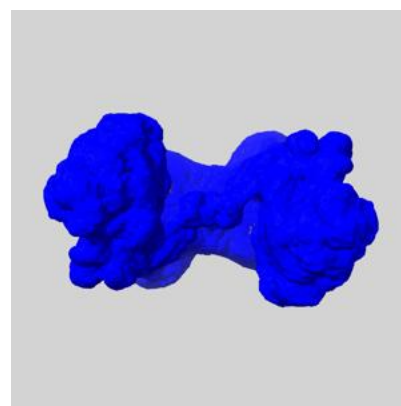
6.6.1 emd_10467_msk_1.map [i](#)



X



Y

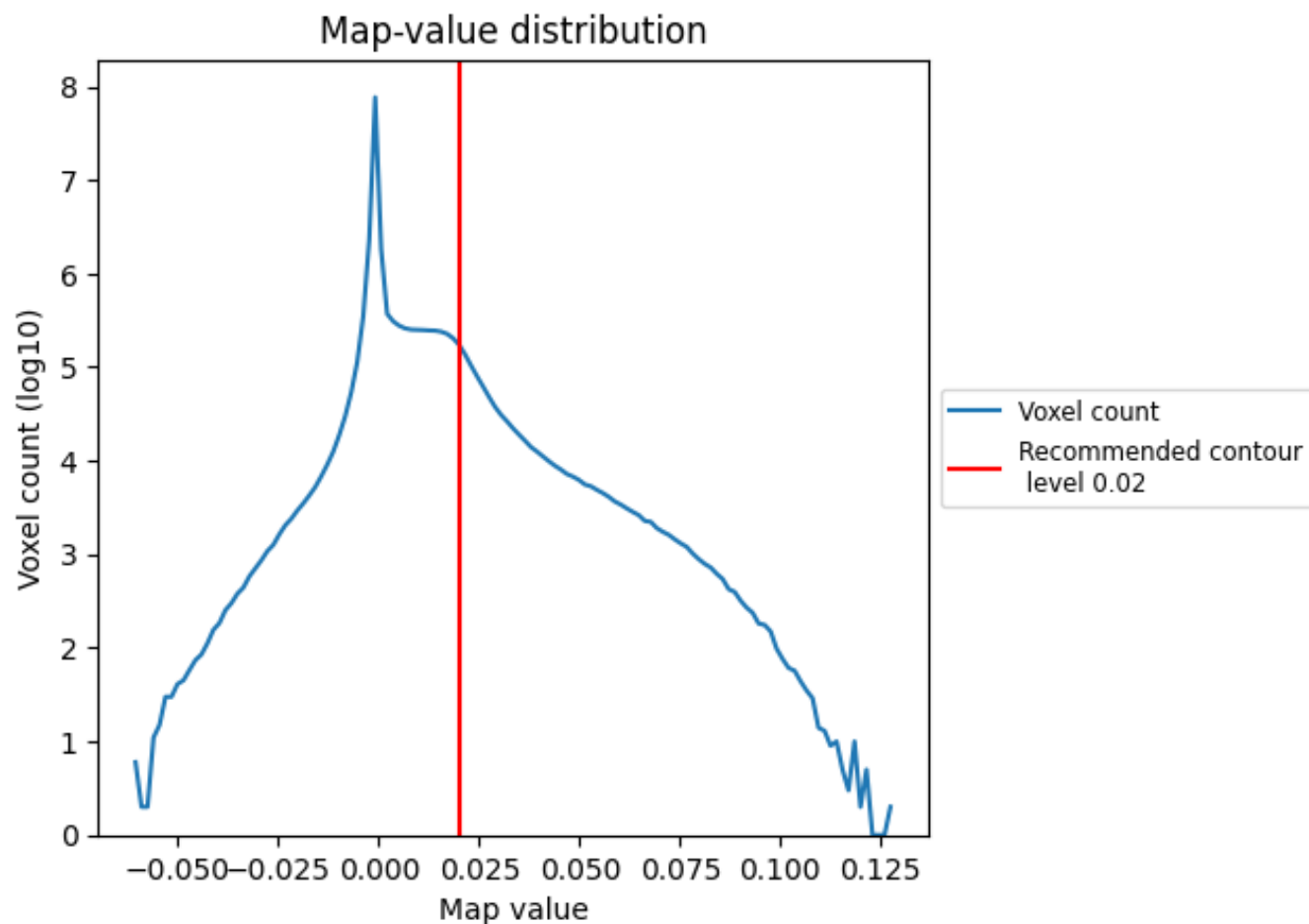


Z

7 Map analysis [i](#)

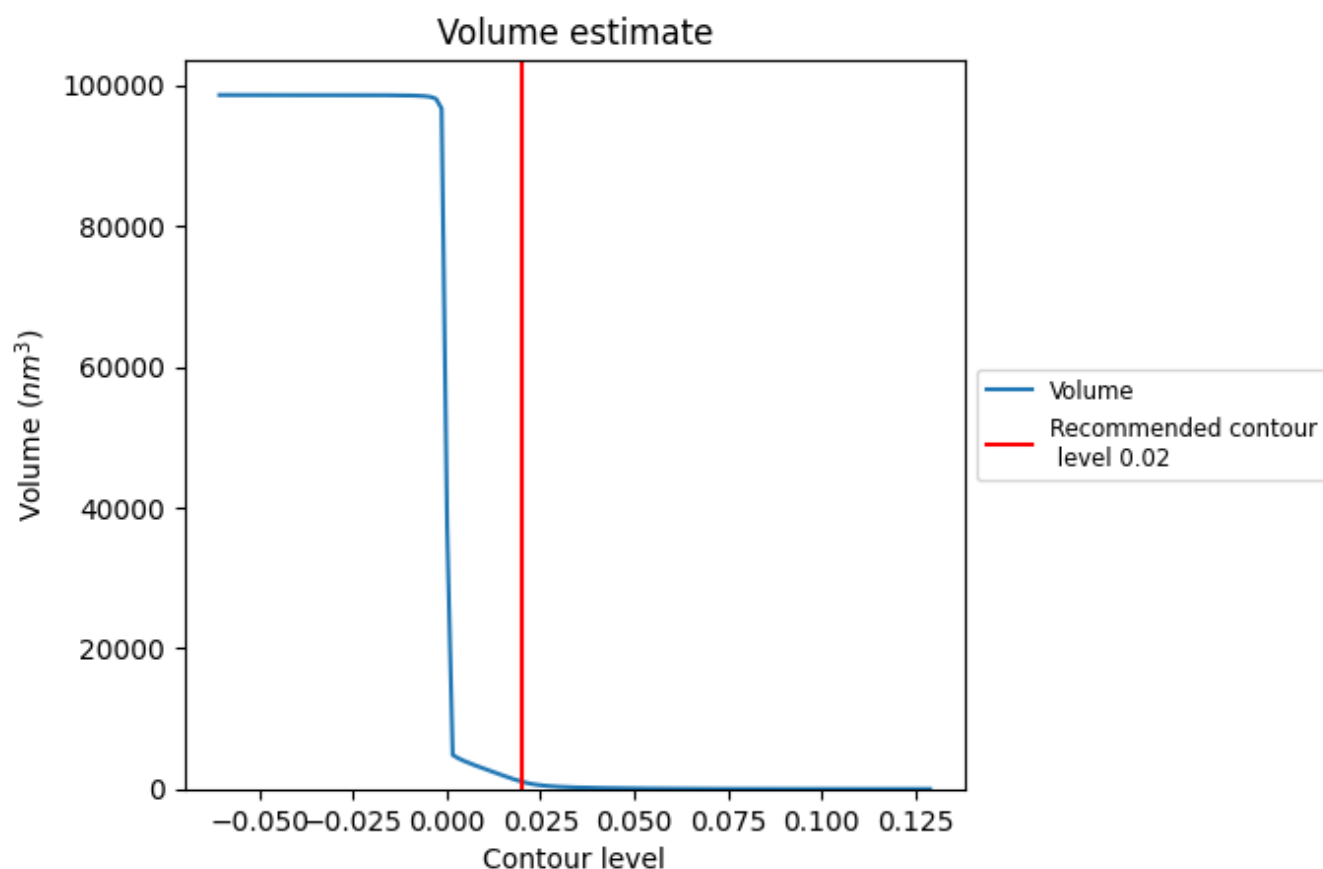
This section contains the results of statistical analysis of the map.

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.

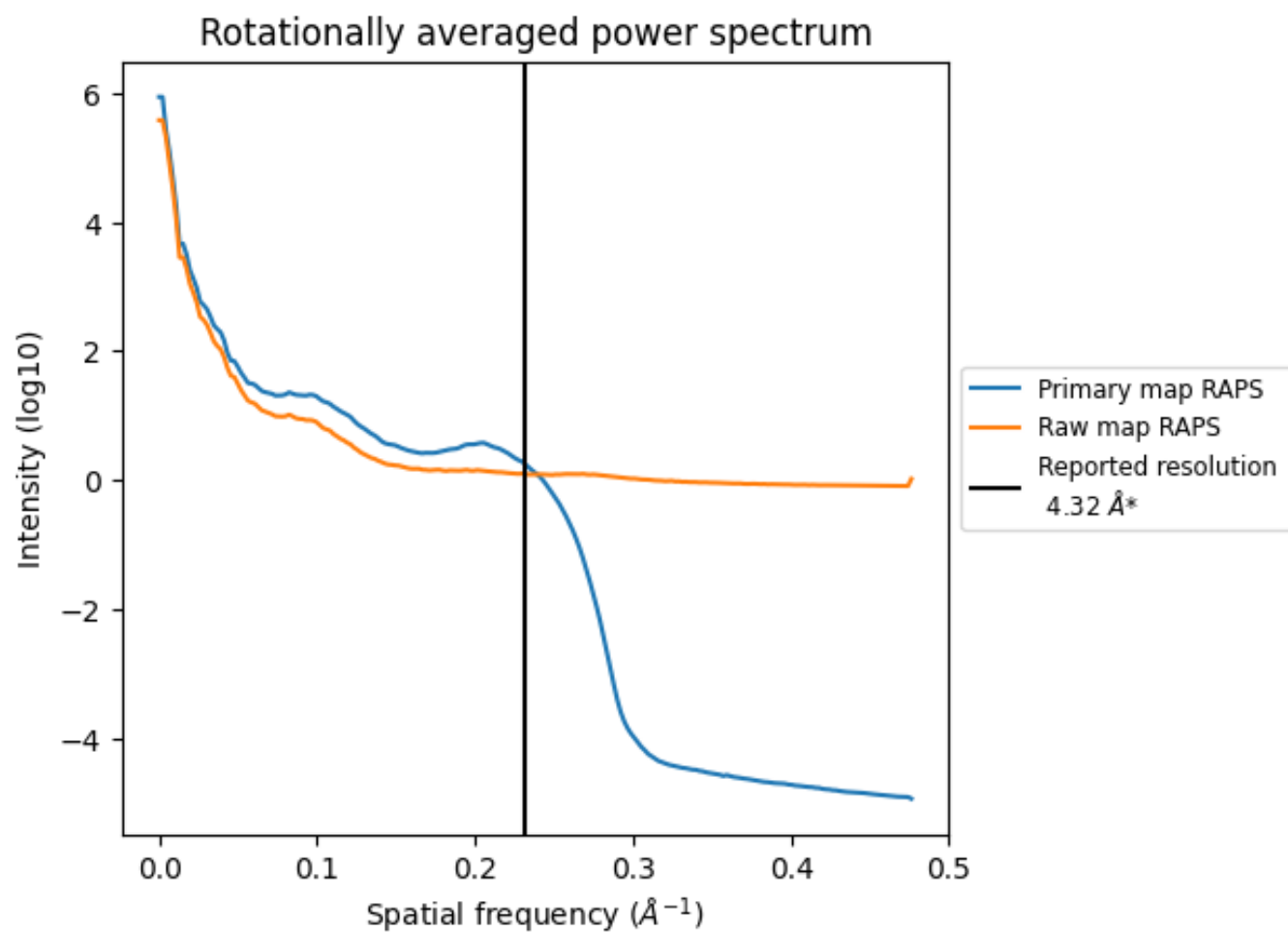
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1048 nm^3 ; this corresponds to an approximate mass of 947 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 ⓘ

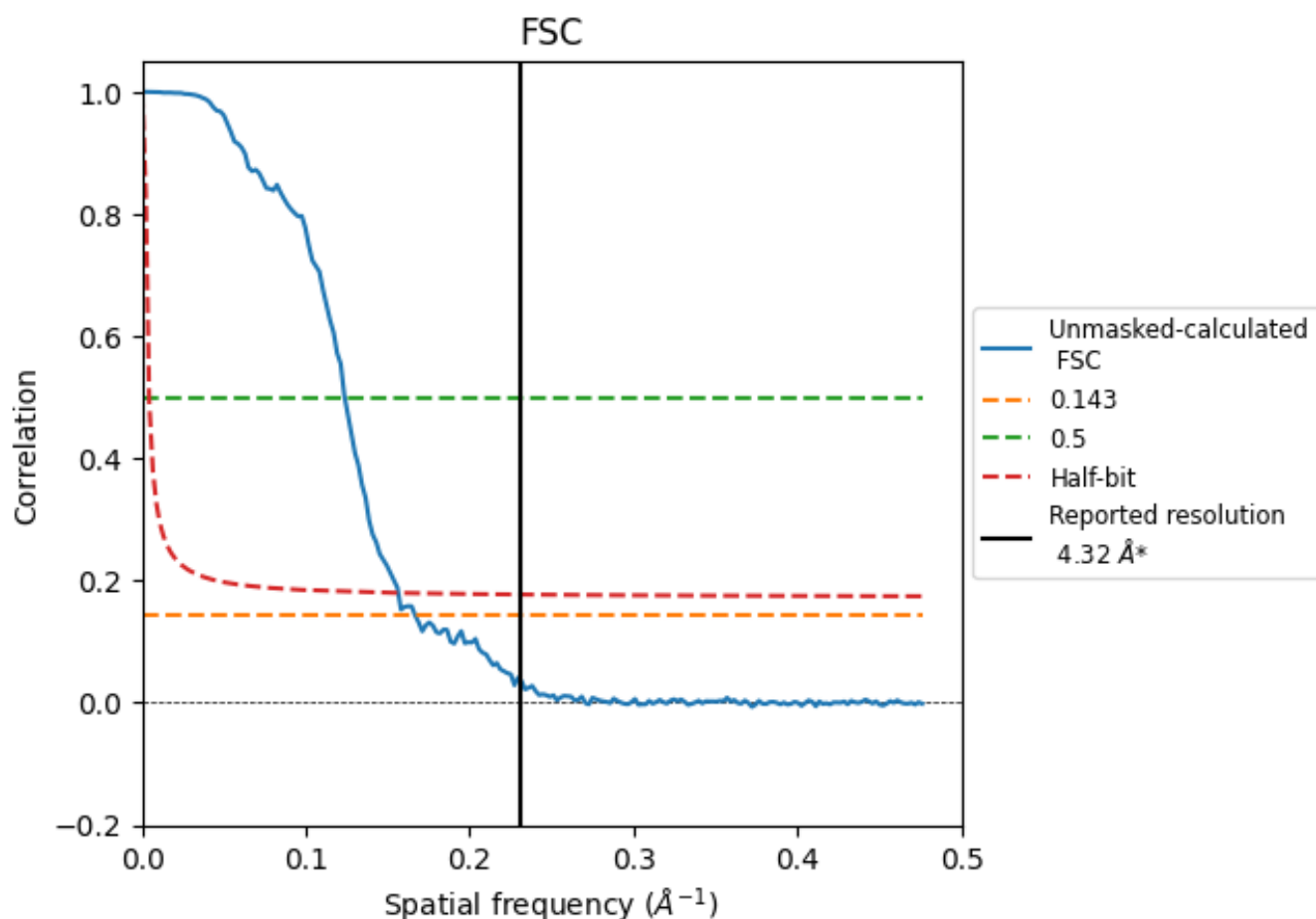


*Reported resolution corresponds to spatial frequency of 0.231 Å⁻¹

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 0.231 Å⁻¹

8.2 Resolution estimates [i](#)

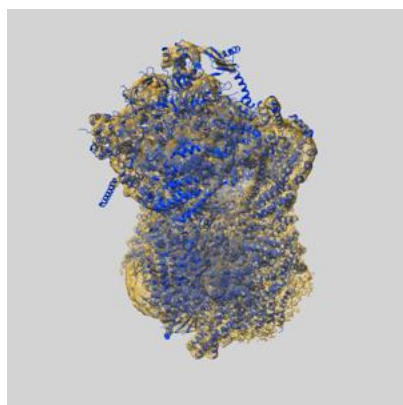
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.32	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.00	8.09	6.39

*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 6.00 differs from the reported value 4.32 by more than 10 %

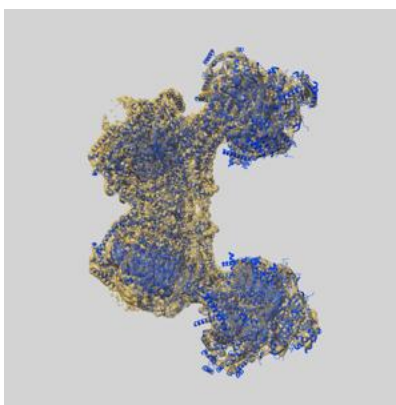
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10467 and PDB model 6TDU. Per-residue inclusion information can be found in section [3](#) on page [22](#).

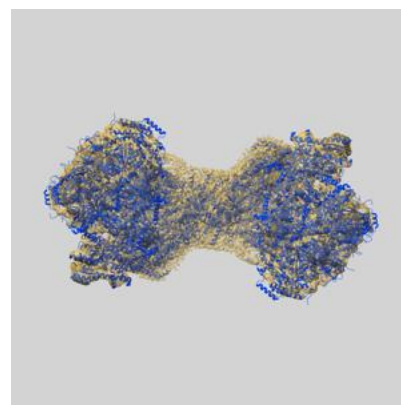
9.1 Map-model overlay [i](#)



X



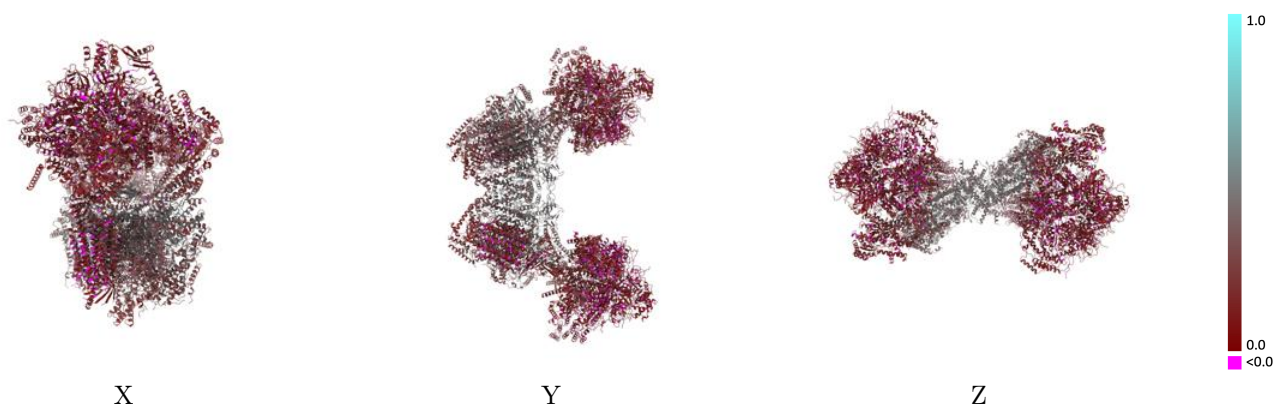
Y



Z

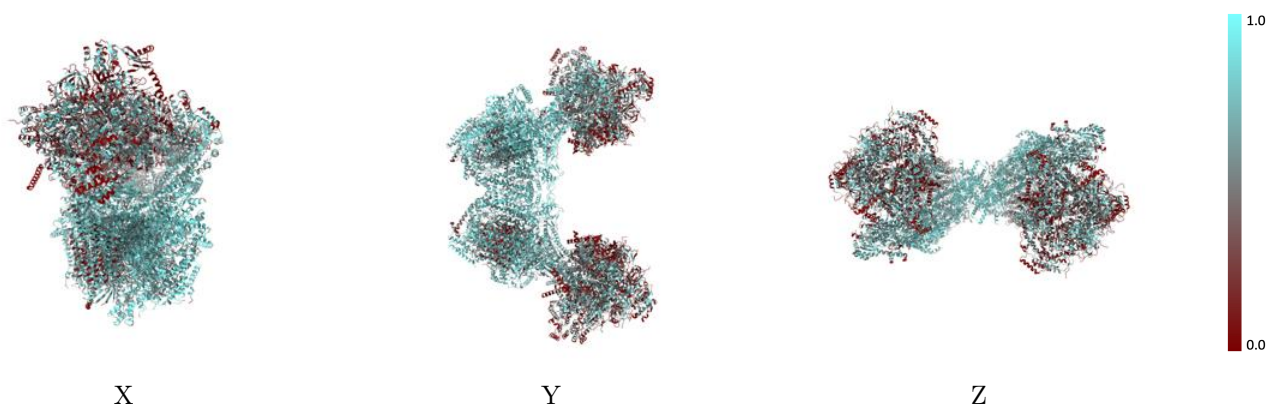
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



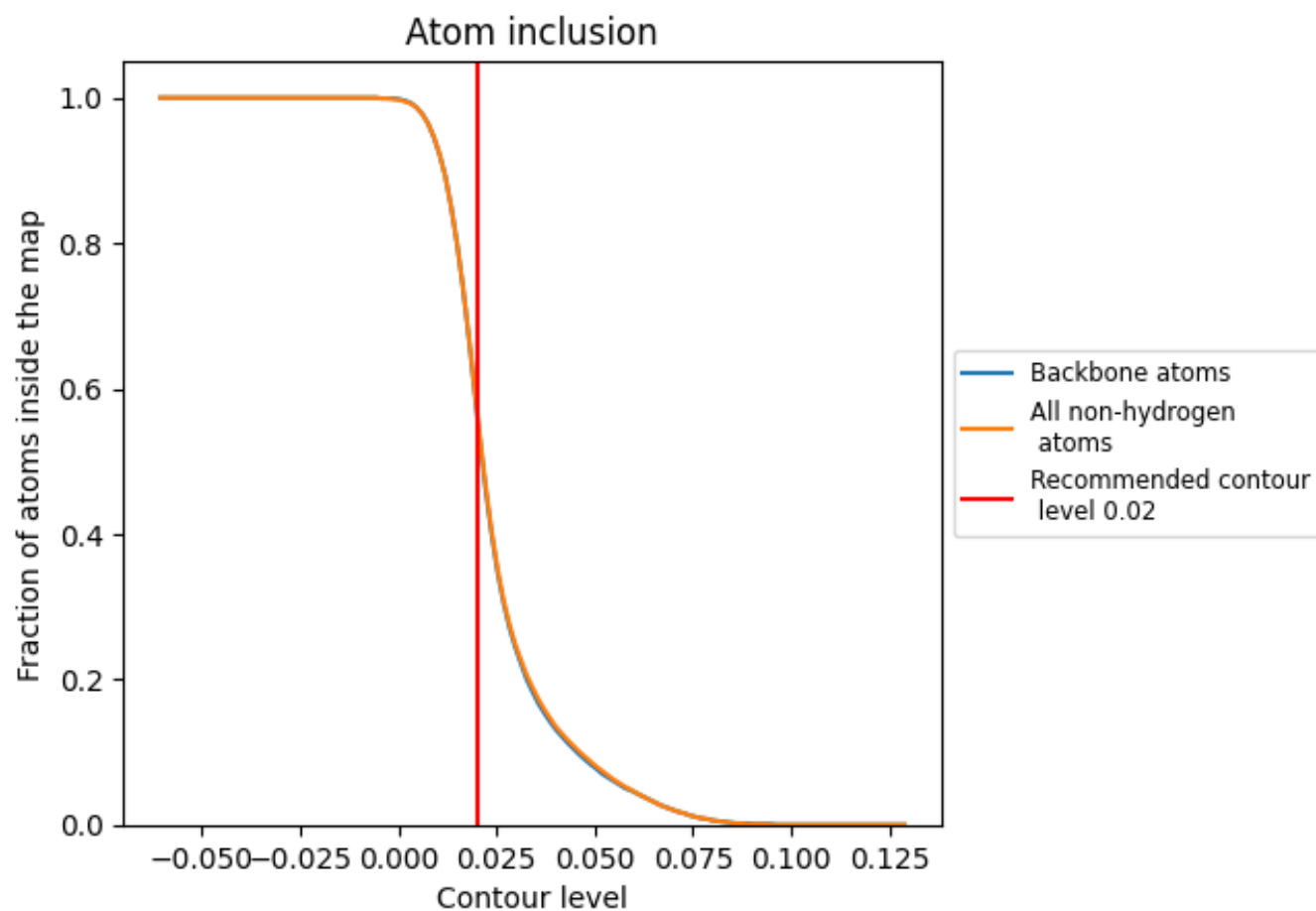
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5710	 0.2360
A	 0.8070	 0.4010
AA	 0.4290	 0.1310
AB	 0.4390	 0.1380
AC	 0.4910	 0.1490
AD	 0.3200	 0.1280
AE	 0.4390	 0.1470
AF	 0.4900	 0.1650
AG	 0.6320	 0.2230
AH	 0.6000	 0.1930
AI	 0.6110	 0.2330
AJ	 0.3050	 0.1400
AK	 0.2100	 0.1420
AL	 0.2610	 0.1490
AM	 0.3490	 0.1510
AN	 0.2930	 0.1840
AO	 0.6000	 0.2070
AP	 0.6660	 0.2470
AQ	 0.6310	 0.2490
AR	 0.5830	 0.2310
AS	 0.5500	 0.1840
AT	 0.5530	 0.1540
AU	 0.6050	 0.1700
AV	 0.6100	 0.1770
AW	 0.5560	 0.1910
AX	 0.5860	 0.1840
B	 0.6300	 0.1910
BA	 0.4390	 0.1340
BB	 0.4490	 0.1450
BC	 0.4870	 0.1440
BD	 0.3180	 0.1300
BE	 0.4460	 0.1570
BF	 0.5000	 0.1640
BG	 0.6420	 0.2250
BH	 0.6010	 0.2070



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
BI	 0.6130	 0.2390
BJ	 0.3040	 0.1460
BK	 0.2210	 0.1400
BL	 0.2720	 0.1510
BM	 0.3460	 0.1560
BN	 0.3050	 0.1850
BO	 0.5950	 0.2010
BP	 0.6640	 0.2400
BQ	 0.6330	 0.2550
BR	 0.6080	 0.2350
BS	 0.5460	 0.1710
BT	 0.5460	 0.1360
BU	 0.5910	 0.1570
BV	 0.6040	 0.1670
BW	 0.5510	 0.1790
BX	 0.5970	 0.1840
C	 0.5400	 0.1490
D	 0.7800	 0.3460
E	 0.7680	 0.3060
F	 0.7920	 0.4060
G	 0.8160	 0.3970
H	 0.7630	 0.3340
I	 0.8030	 0.3950
J	 0.7650	 0.3630
K	 0.7910	 0.3400
L	 0.7920	 0.4220
M	 0.7770	 0.3750
N	 0.7210	 0.3800
O	 0.7070	 0.3290
P	 0.7580	 0.4120
Q	 0.7440	 0.2500
R	 0.7540	 0.3370
S	 0.7750	 0.3860
T	 0.8040	 0.3810
a	 0.8030	 0.4000
b	 0.6330	 0.1890
c	 0.5450	 0.1530
d	 0.7770	 0.3460
e	 0.7700	 0.3040
f	 0.7920	 0.4060
g	 0.8020	 0.3930
h	 0.7630	 0.3350

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Chain	Atom inclusion	Q-score
i	 0.7950	 0.3930
j	 0.7710	 0.3600
k	 0.7890	 0.3360
l	 0.7980	 0.4150
m	 0.7890	 0.3740
n	 0.7060	 0.3810
o	 0.7070	 0.3300
p	 0.7840	 0.4170
q	 0.7420	 0.2500
r	 0.7470	 0.3370
s	 0.7690	 0.3910
t	 0.7940	 0.3770