wwPDB EM Validation Summary Report

Apr 2, 2025 – 12:54 am BST

PDB ID	:	6TMK / pdb_00006tmk
EMDB ID	:	EMD-10524
Title	:	Cryo-EM structure of Toxoplasma gondii mitochondrial ATP synthase dimer, composite model
Authors	:	Muhleip, A.; Kock Flygaard, R.; Amunts, A.
Deposited on	:	2019-12-04
Resolution	:	2.90 Å(reported)

This is a wwPDB EM Validation Summary 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:

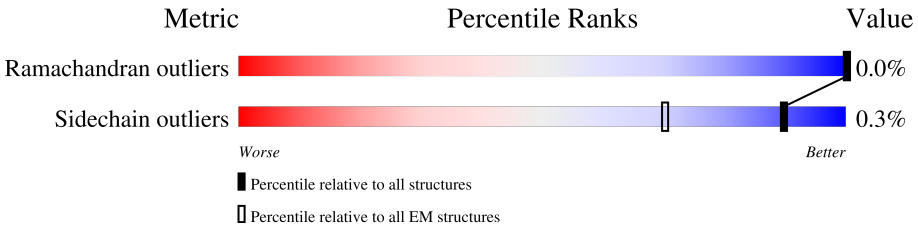
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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	Q	134	98%
1	q	134	99%
2	I	236	38% 62%
2	i	236	38% 62%
3	T	133	69% 31%
3	t	133	69% 31%
4	G	252	44% 56%
4	g	252	44% 56%
5	O	157	95% 5%

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Mol	Chain	Length	Quality of chain
5	o	157	95% 5%
6	K	224	52% 48%
6	k	224	52% 48%
7	J	229	76% 23%
7	j	229	76% 23%
8	S	128	74% 26%
8	s	128	74% 26%
9	U	126	75% 25%
9	u	126	75% 25%
10	H	239	94% 5%
10	h	239	94% 5%
11	E	325	43% 57%
11	e	325	43% 57%
12	X	83	99%
12	x	83	99%
13	B	571	18% 85% 15%
13	b	571	12% 85% 15%
14	R	134	9% 99%
14	r	134	7% 99%
15	P	138	78% 22%
15	p	138	78% 22%
16	V	111	99%
16	v	111	99%
17	L	208	100%
17	l	208	100%

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Mol	Chain	Length	Quality of chain
18	C	398	31% 69%
18	c	398	31% 69%
19	D	310	82% 18%
19	d	310	82% 18%
20	M	205	47% 53%
20	m	205	47% 53%
21	N	166	96%
21	n	166	96%
22	F	267	70% 30%
22	f	267	70% 30%
23	W	106	91% 8%
23	w	106	91% 8%
24	A	536	5% 87% 13%
24	a	536	6% 87% 13%
25	i1	145	28% 72%
25	i2	145	28% 72%
26	A1	565	38% 90% 9%
26	A2	565	51% 90% 9%
26	C1	565	16% 90% 10%
26	C2	565	15% 90% 10%
26	E1	565	33% 90% 10%
26	E2	565	42% 90% 10%
27	B1	560	16% 84% 14%
27	B2	560	21% 85% 14%
27	D1	560	19% 85% 15%

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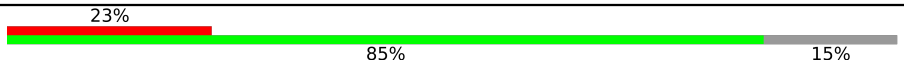
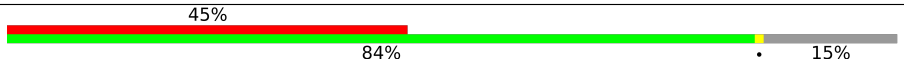
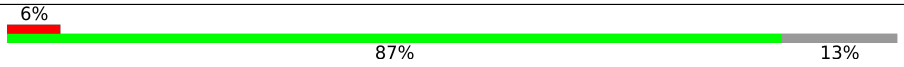
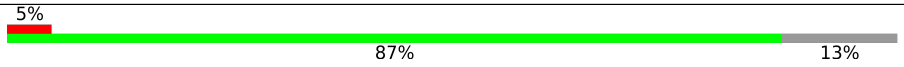
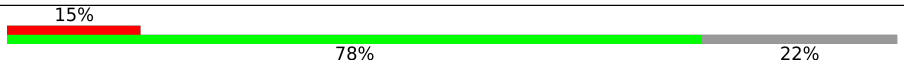
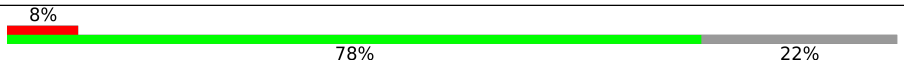
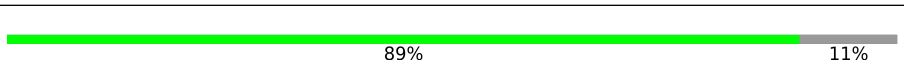
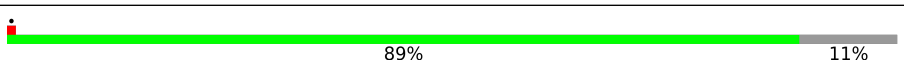
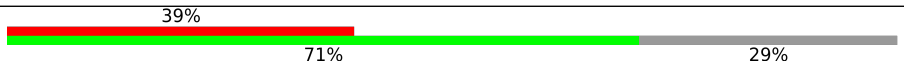
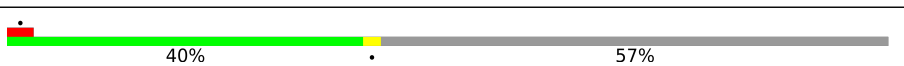
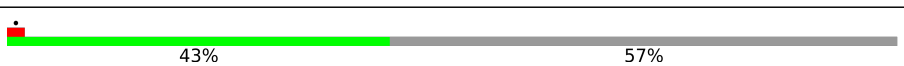
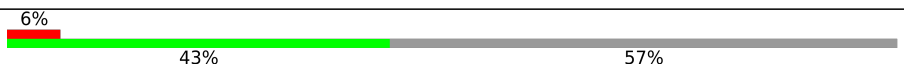
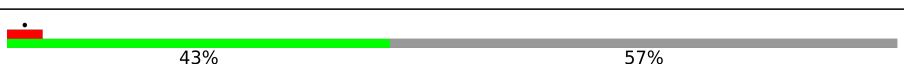
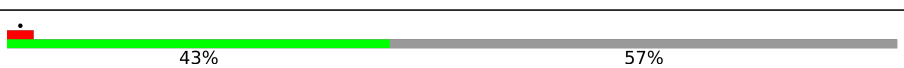
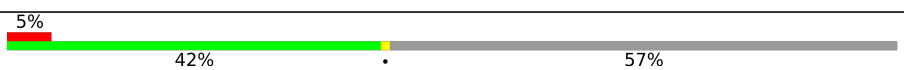
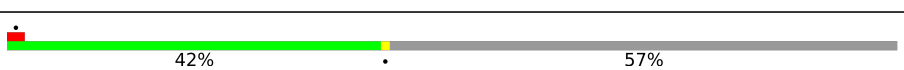
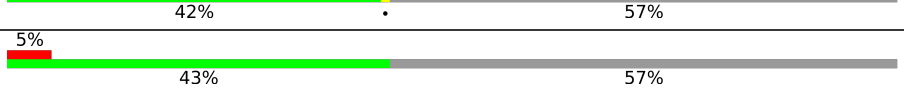
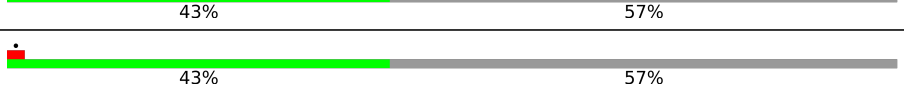
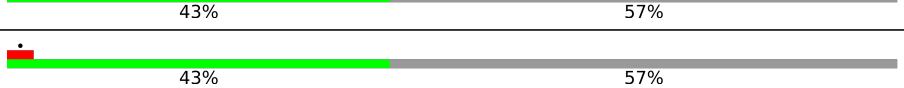
Mol	Chain	Length	Quality of chain
27	D2	560	
27	F1	560	
27	F2	560	
28	g1	314	
28	g2	314	
29	d1	183	
29	d2	183	
30	e1	73	
30	e2	73	
31	G1	252	
31	G2	252	
32	H1	166	
32	H2	166	
32	I1	166	
32	I2	166	
32	J1	166	
32	J2	166	
32	K1	166	
32	K2	166	
32	L1	166	
32	L2	166	
32	M1	166	
32	M2	166	
32	N1	166	
32	N2	166	

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Mol	Chain	Length	Quality of chain
32	O1	166	
32	O2	166	
32	P1	166	
32	P2	166	
32	Q1	166	
32	Q2	166	

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 266834 atoms, of which 134048 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 ATPTG11.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	q	133	Total	C	H	N	O	S	0	0
			2119	674	1044	194	202	5		
1	Q	133	Total	C	H	N	O	S	0	0
			2119	674	1044	194	202	5		

- Molecule 2 is a protein called ATPTG7.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	i	90	Total	C	H	N	O	S	0	0
			1386	433	678	136	129	10		
2	I	90	Total	C	H	N	O	S	0	0
			1386	433	678	136	129	10		

- Molecule 3 is a protein called ATPTG14.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	t	92	Total	C	H	N	O	S	0	0
			1439	463	716	127	129	4		
3	T	92	Total	C	H	N	O	S	0	0
			1439	463	716	127	129	4		

- Molecule 4 is a protein called ATPTG5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	g	112	Total	C	H	N	O	S	0	0
			1732	548	856	152	168	8		
4	G	112	Total	C	H	N	O	S	0	0
			1732	548	856	152	168	8		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	51	VAL	PHE	conflict	UNP S7WD71

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Chain	Residue	Modelled	Actual	Comment	Reference
g	73	CYS	SER	conflict	UNP S7WD71
g	110	LYS	GLU	conflict	UNP S7WD71
g	233	THR	MET	conflict	UNP S7WD71
G	51	VAL	PHE	conflict	UNP S7WD71
G	73	CYS	SER	conflict	UNP S7WD71
G	110	LYS	GLU	conflict	UNP S7WD71
G	233	THR	MET	conflict	UNP S7WD71

- Molecule 5 is a protein called subunit k.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	o	149	Total	C	H	N	O	S	0	0
			2415	786	1195	210	219	5		
5	O	149	Total	C	H	N	O	S	0	0
			2415	786	1195	210	219	5		

- Molecule 6 is a protein called subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	k	117	Total	C	H	N	O	S	0	0
			1904	645	952	145	155	7		
6	K	117	Total	C	H	N	O	S	0	0
			1904	645	952	145	155	7		

- Molecule 7 is a protein called subunit i/j.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	j	176	Total	C	H	N	O	S	0	0
			2981	1003	1469	261	244	4		
7	J	176	Total	C	H	N	O	S	0	0
			2981	1003	1469	261	244	4		

- Molecule 8 is a protein called ATPTG13.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	s	95	Total	C	H	N	O	S	0	0
			1570	526	770	130	142	2		
8	S	95	Total	C	H	N	O	S	0	0
			1570	526	770	130	142	2		

- Molecule 9 is a protein called ATPTG15.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	u	94	Total	C	H	N	O	S	0	0
			1492	482	741	132	133	4		
9	U	94	Total	C	H	N	O	S	0	0
			1492	482	741	132	133	4		

- Molecule 10 is a protein called ATPTG6.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	h	226	Total	C	H	N	O	S	0	0
			3589	1157	1741	334	348	9		
10	H	226	Total	C	H	N	O	S	0	0
			3589	1157	1741	334	348	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	89	ASN	HIS	conflict	UNP A0A125YL08
H	89	ASN	HIS	conflict	UNP A0A125YL08

- Molecule 11 is a protein called ATPTG3.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	e	140	Total	C	H	N	O	S	0	0
			2179	719	1064	187	204	5		
11	E	140	Total	C	H	N	O	S	0	0
			2179	719	1064	187	204	5		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	?	-	LYS	deletion	UNP A0A125YLR0
e	63	PRO	SER	conflict	UNP A0A125YLR0
e	99	LEU	PRO	conflict	UNP A0A125YLR0
e	312	ALA	THR	conflict	UNP A0A125YLR0
E	?	-	LYS	deletion	UNP A0A125YLR0
E	63	PRO	SER	conflict	UNP A0A125YLR0
E	99	LEU	PRO	conflict	UNP A0A125YLR0
E	312	ALA	THR	conflict	UNP A0A125YLR0

- Molecule 12 is a protein called ATPTG17.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	x	82	Total	C	H	N	O	S	0	0
			1298	420	639	116	120	3		
12	X	82	Total	C	H	N	O	S	0	0
			1298	420	639	116	120	3		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	77	TRP	-	expression tag	UNP S7W180
x	78	MET	-	expression tag	UNP S7W180
x	79	PHE	-	expression tag	UNP S7W180
x	80	GLY	-	expression tag	UNP S7W180
x	81	ASN	-	expression tag	UNP S7W180
x	82	SER	-	expression tag	UNP S7W180
x	83	TYR	-	expression tag	UNP S7W180
X	77	TRP	-	expression tag	UNP S7W180
X	78	MET	-	expression tag	UNP S7W180
X	79	PHE	-	expression tag	UNP S7W180
X	80	GLY	-	expression tag	UNP S7W180
X	81	ASN	-	expression tag	UNP S7W180
X	82	SER	-	expression tag	UNP S7W180
X	83	TYR	-	expression tag	UNP S7W180

- Molecule 13 is a protein called subunit b.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	b	484	Total	C	H	N	O	S	0	0
			7841	2525	3909	652	740	15		
13	B	484	Total	C	H	N	O	S	0	0
			7841	2525	3909	652	740	15		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	48	LEU	SER	conflict	UNP S7V2T0
b	472	THR	ALA	conflict	UNP S7V2T0
B	48	LEU	SER	conflict	UNP S7V2T0
B	472	THR	ALA	conflict	UNP S7V2T0

- Molecule 14 is a protein called ATPTG12.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	r	133	Total	C	H	N	O	S	0	0
			2144	681	1073	182	202	6		
14	R	133	Total	C	H	N	O	S	0	0
			2144	681	1073	182	202	6		

- Molecule 15 is a protein called ATPTG10.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	p	108	Total	C	H	N	O	S	0	0
			1711	553	847	148	157	6		
15	P	108	Total	C	H	N	O	S	0	0
			1711	553	847	148	157	6		

- Molecule 16 is a protein called subunit f.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	v	110	Total	C	H	N	O	S	0	0
			1801	590	888	170	148	5		
16	V	110	Total	C	H	N	O	S	0	0
			1801	590	888	170	148	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	54	ALA	VAL	conflict	UNP S7UQT7
V	54	ALA	VAL	conflict	UNP S7UQT7

- Molecule 17 is a protein called ATPTG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	l	207	Total	C	H	N	O	S	0	0
			3273	1013	1647	298	305	10		
17	L	207	Total	C	H	N	O	S	0	0
			3273	1013	1647	298	305	10		

- Molecule 18 is a protein called ATPTG1.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	c	122	Total	C	H	N	O	S	0	0
			2029	656	999	189	184	1		
18	C	122	Total	C	H	N	O	S	0	0
			2029	656	999	189	184	1		

- Molecule 19 is a protein called ATPTG2.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	d	255	Total	C	H	N	O	S	0	0
			4056	1326	1975	366	381	8		
19	D	255	Total	C	H	N	O	S	0	0
			4056	1326	1975	366	381	8		

- Molecule 20 is a protein called subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	m	96	Total	C	H	N	O	S	0	0
			1509	501	744	126	131	7		
20	M	96	Total	C	H	N	O	S	0	0
			1509	501	744	126	131	7		

- Molecule 21 is a protein called ATPTG9.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	n	160	Total	C	H	N	O	S	0	0
			2449	774	1202	227	235	11		
21	N	160	Total	C	H	N	O	S	0	0
			2449	774	1202	227	235	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	140	SER	ALA	conflict	UNP A0A125YUZ2
N	140	SER	ALA	conflict	UNP A0A125YUZ2

- Molecule 22 is a protein called ATPTG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	f	188	Total	C	H	N	O	S	0	0
			2867	919	1425	245	274	4		
22	F	188	Total	C	H	N	O	S	0	0
			2867	919	1425	245	274	4		

- Molecule 23 is a protein called ATPTG16.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	w	97	Total	C	H	N	O	S	0	0
			1520	497	760	128	131	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	97	Total	C	H	N	O	S	0	0
			1520	497	760	128	131	4		

- Molecule 24 is a protein called subunit d.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	a	467	Total	C	H	N	O	S	0	0
			7396	2405	3616	656	698	21		
24	A	467	Total	C	H	N	O	S	0	0
			7396	2405	3616	656	698	21		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	351	THR	ALA	conflict	UNP S7V493
A	351	THR	ALA	conflict	UNP S7V493

- Molecule 25 is a protein called Inhibitor of F1.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	i2	40	Total	C	H	N	O	S	0	0
			660	213	324	56	66	1		
25	i1	40	Total	C	H	N	O	S	0	0
			660	213	324	56	66	1		

- Molecule 26 is a protein called ATP synthase subunit alpha,subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	A2	512	Total	C	H	N	O	S	0	0
			7925	2464	4003	688	751	19		
26	E2	507	Total	C	H	N	O	S	0	0
			7848	2441	3962	682	744	19		
26	C2	507	Total	C	H	N	O	S	0	0
			7849	2442	3967	682	739	19		
26	A1	512	Total	C	H	N	O	S	0	0
			7925	2464	4003	688	751	19		
26	E1	507	Total	C	H	N	O	S	0	0
			7848	2441	3962	682	744	19		
26	C1	507	Total	C	H	N	O	S	0	0
			7849	2442	3967	682	739	19		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
27	B2	479	Total	C	H	N	O	S	0	0
			7314	2293	3676	628	703	14		
27	F2	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		
27	D2	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		
27	B1	479	Total	C	H	N	O	S	0	0
			7314	2293	3676	628	703	14		
27	F1	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		
27	D1	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		

- Molecule 28 is a protein called ATP synthase subunit gamma.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	g2	272	Total	C	H	N	O	S	0	0
			4289	1330	2173	376	394	16		
28	g1	272	Total	C	H	N	O	S	0	0
			4289	1330	2173	376	394	16		

- Molecule 29 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	d2	143	Total	C	H	N	O	S	0	0
			2145	667	1076	181	216	5		
29	d1	143	Total	C	H	N	O	S	0	0
			2145	667	1076	181	216	5		

- Molecule 30 is a protein called ATP synthase subunit epsilon.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	e2	65	Total	C	H	N	O	S	0	0
			1077	337	539	99	98	4		
30	e1	65	Total	C	H	N	O	S	0	0
			1077	337	539	99	98	4		

- Molecule 31 is a protein called Oligomycin sensitivity conferring protein (OSCP).

Mol	Chain	Residues	Atoms						AltConf	Trace
31	G2	180	Total	C	H	N	O	S	0	0
			2901	895	1486	255	261	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
31	G1	180	Total	C	H	N	O	S	0	0
			2901	895	1486	255	261	4		

- Molecule 32 is a protein called subunit c.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	H2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	I2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	J2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	K2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	L2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	M2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	N2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	O2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	P2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	Q2	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	H1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	I1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	J1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	K1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	L1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	M1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	N1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	O1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		

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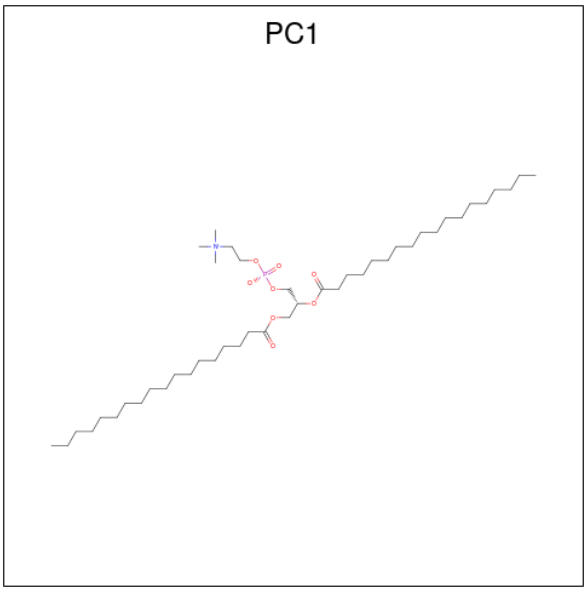
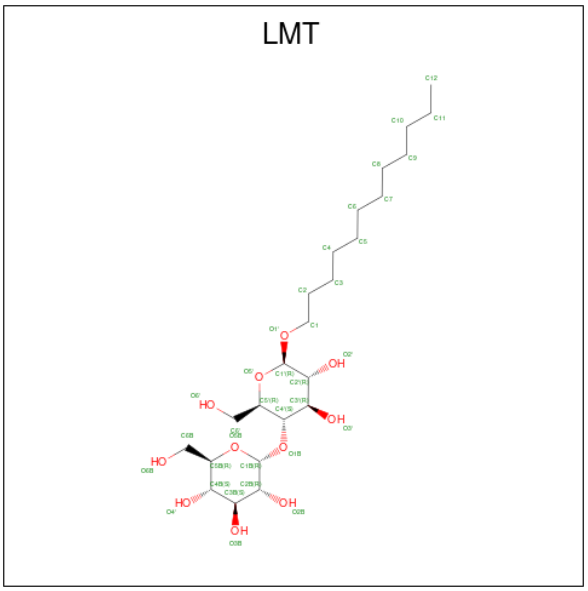
Mol	Chain	Residues	Atoms						AltConf	Trace
32	P1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	Q1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		

- Molecule 33 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



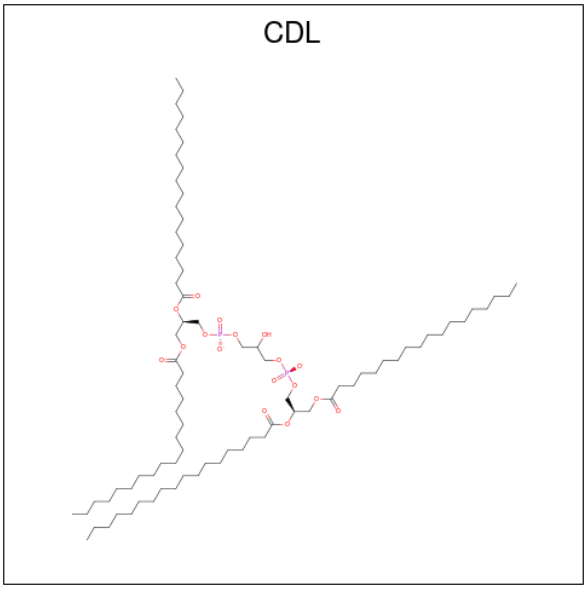
Mol	Chain	Residues	Atoms						AltConf
33	o	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
33	o	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
33	v	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
33	O	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
33	O	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
33	V	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

- Molecule 34 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms				AltConf
34	o	1	Total	C	H	O	0
			81	24	46	11	
34	h	1	Total	C	H	O	0
			81	24	46	11	
34	x	1	Total	C	H	O	0
			81	24	46	11	
34	c	1	Total	C	H	O	0
			81	24	46	11	
34	c	1	Total	C	H	O	0
			81	24	46	11	
34	d	1	Total	C	H	O	0
			81	24	46	11	
34	d	1	Total	C	H	O	0
			81	24	46	11	
34	O	1	Total	C	H	O	0
			81	24	46	11	
34	H	1	Total	C	H	O	0
			81	24	46	11	
34	X	1	Total	C	H	O	0
			81	24	46	11	
34	C	1	Total	C	H	O	0
			81	24	46	11	
34	C	1	Total	C	H	O	0
			81	24	46	11	
34	D	1	Total	C	H	O	0
			81	24	46	11	
34	D	1	Total	C	H	O	0
			81	24	46	11	

- Molecule 35 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
35	o	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	u	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	h	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	e	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	b	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	b	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	v	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	c	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	d	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	O	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	U	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	H	1	Total	C	H	O	P	0
			256	81	156	17	2	

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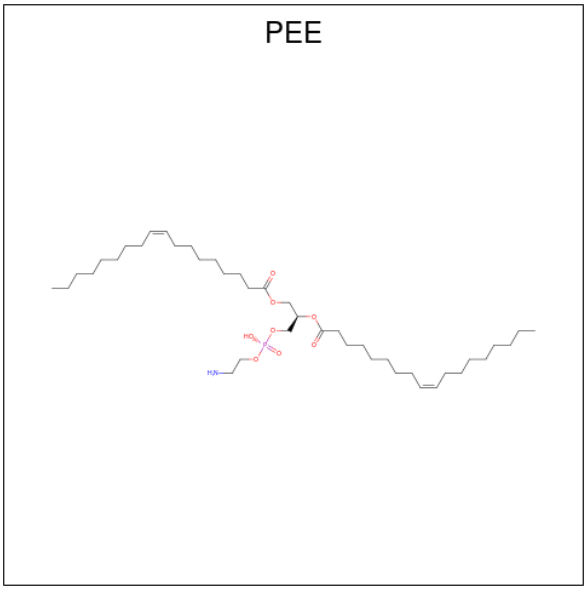
Mol	Chain	Residues	Atoms					AltConf
35	E	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	B	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	B	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	V	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	C	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	D	1	Total	C	H	O	P	0
			256	81	156	17	2	

- Molecule 36 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
36	j	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
36	j	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
36	c	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
36	J	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
36	J	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

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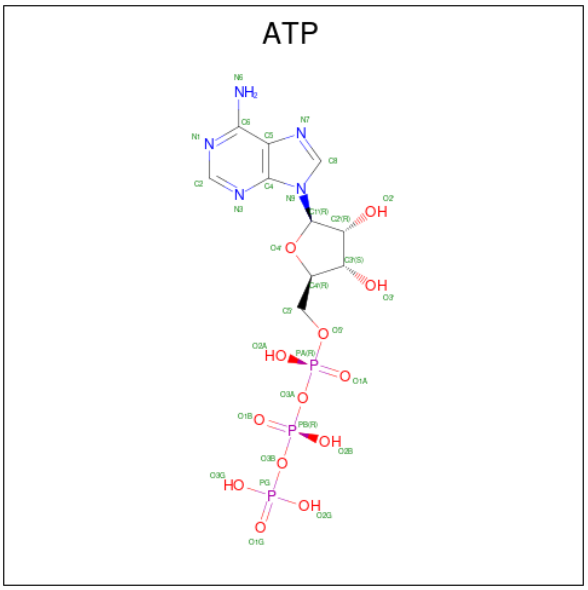
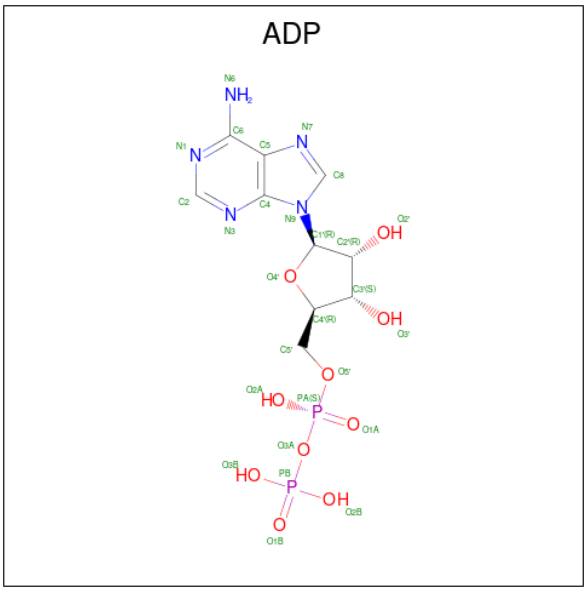
Mol	Chain	Residues	Atoms						AltConf
36	C	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

- Molecule 37 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
37	A2	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
37	E2	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
37	C2	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
37	A1	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
37	E1	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
37	C1	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 38 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



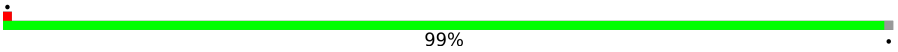
Mol	Chain	Residues	Atoms						AltConf
38	B2	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
38	D2	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	
38	B1	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	
38	D1	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	

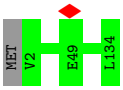
3 Residue-property plots (i)

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

• Molecule 1: ATPTG11

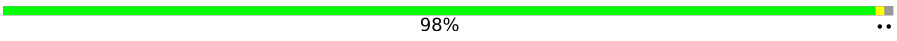
Chain q:

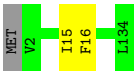




• Molecule 1: ATPTG11

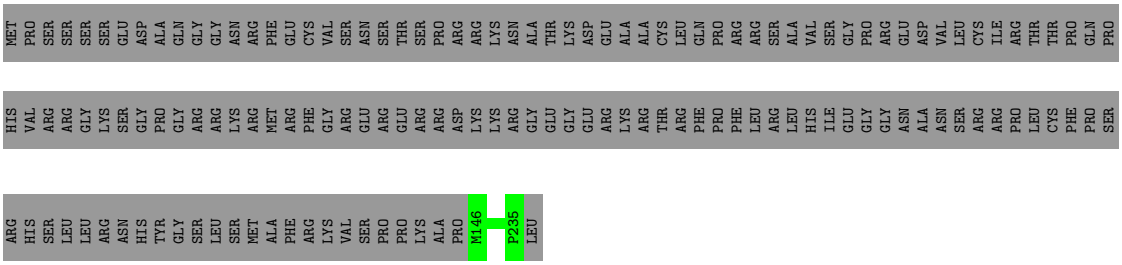
Chain Q:





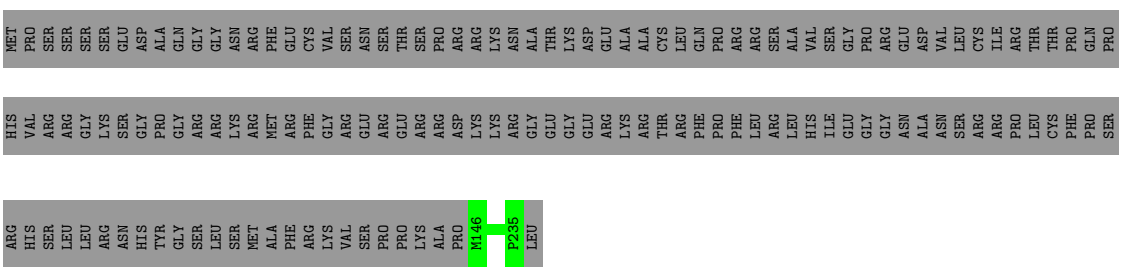
• Molecule 2: ATPTG7

Chain i:



• Molecule 2: ATPTG7

Chain I:



• Molecule 3: ATPTG14

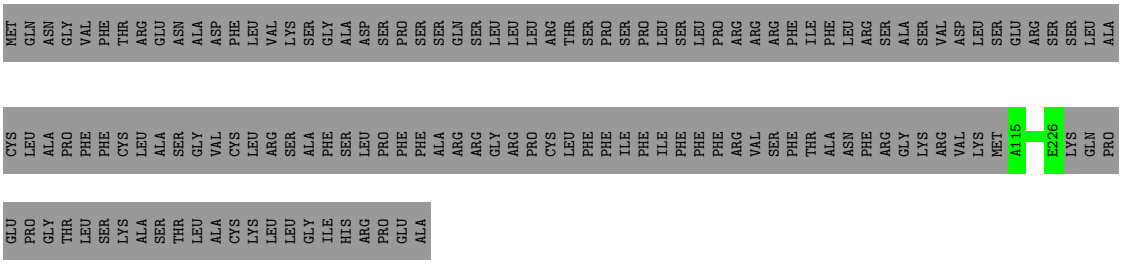
Chain t:

• Molecule 3: ATPTG14

Chain T:

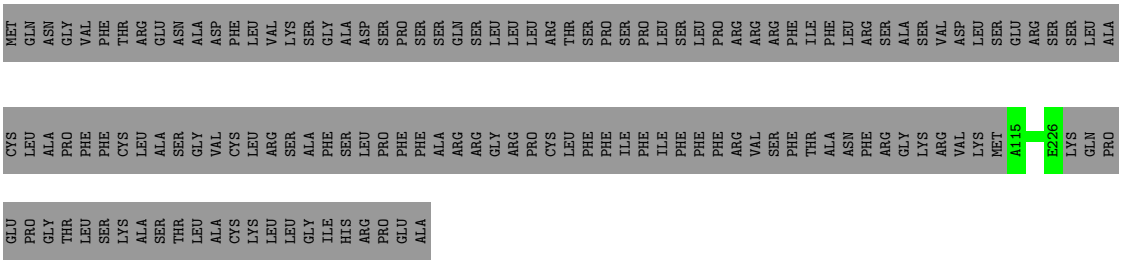
• Molecule 4: ATPTG5

Chain g:



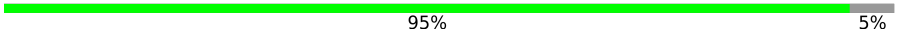
• Molecule 4: ATPTG5

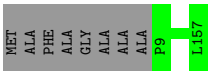
Chain G:



• Molecule 5: subunit k

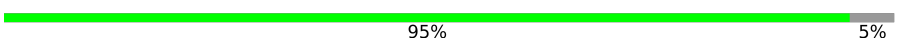
Chain o:

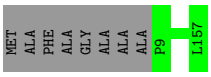




• Molecule 5: subunit k

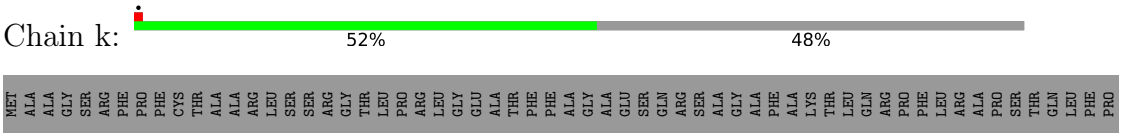
Chain O:





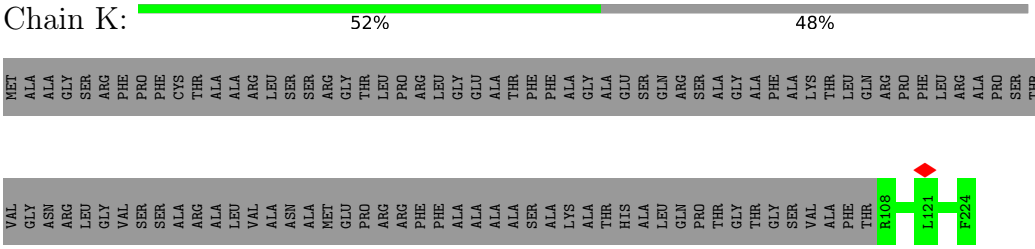
• Molecule 6: subunit a

Chain k:



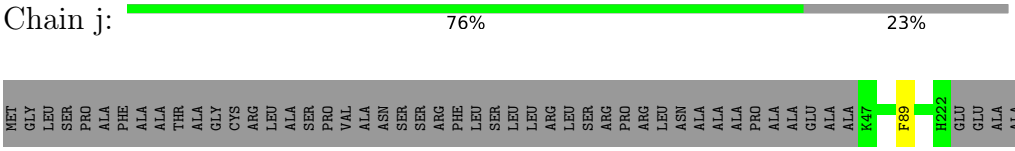
• Molecule 6: subunit a

Chain K:



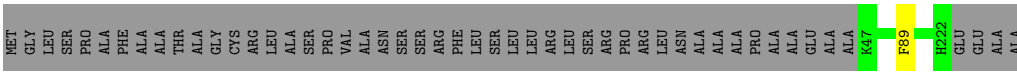
• Molecule 7: subunit i/j

Chain j:



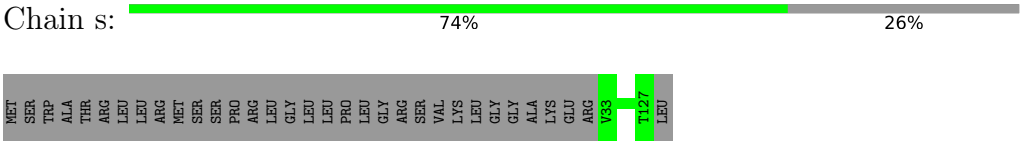
• Molecule 7: subunit i/j

Chain J:



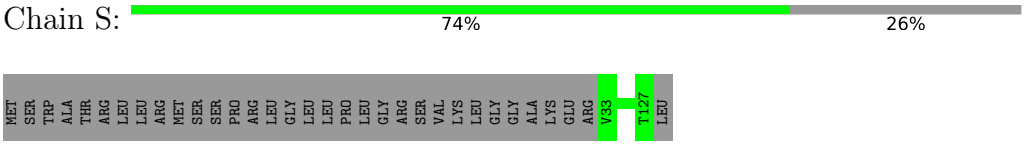
• Molecule 8: ATPTG13

Chain s:



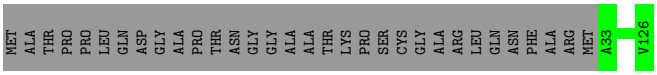
• Molecule 8: ATPTG13

Chain S:



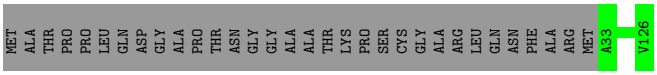
• Molecule 9: ATPTG15

Chain u:



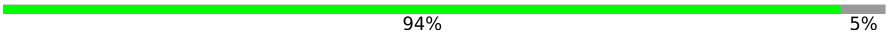
• Molecule 9: ATPTG15

Chain U:



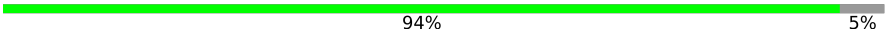
• Molecule 10: ATPTG6

Chain h:



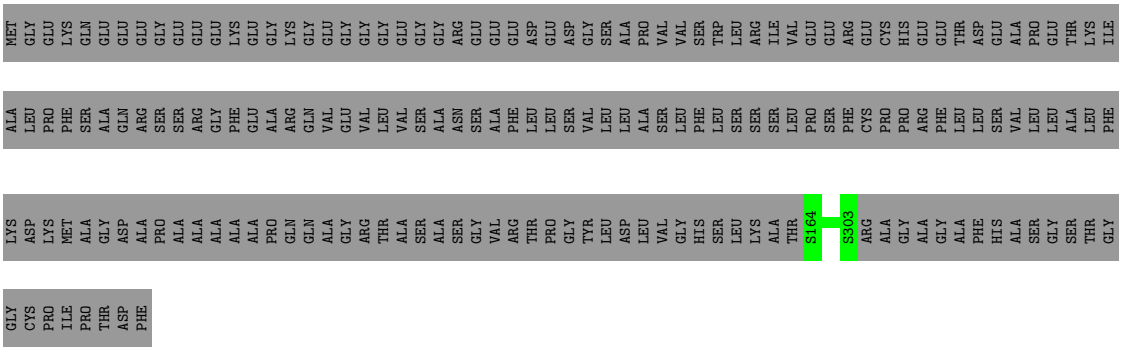
• Molecule 10: ATPTG6

Chain H:



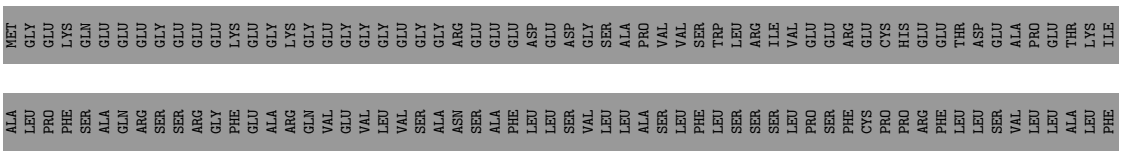
• Molecule 11: ATPTG3

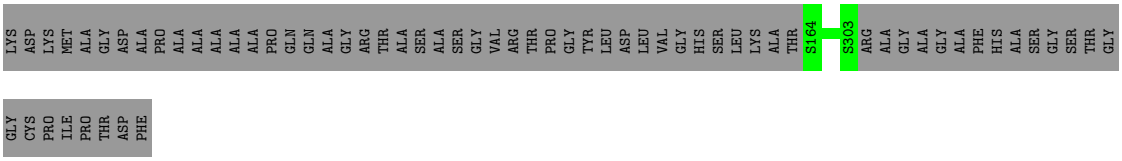
Chain e:



• Molecule 11: ATPTG3

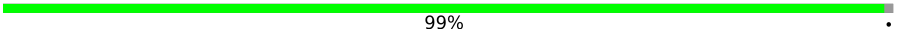
Chain E:





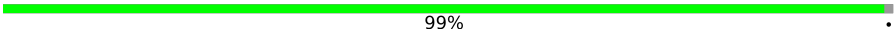
• Molecule 12: ATPTG17

Chain x:



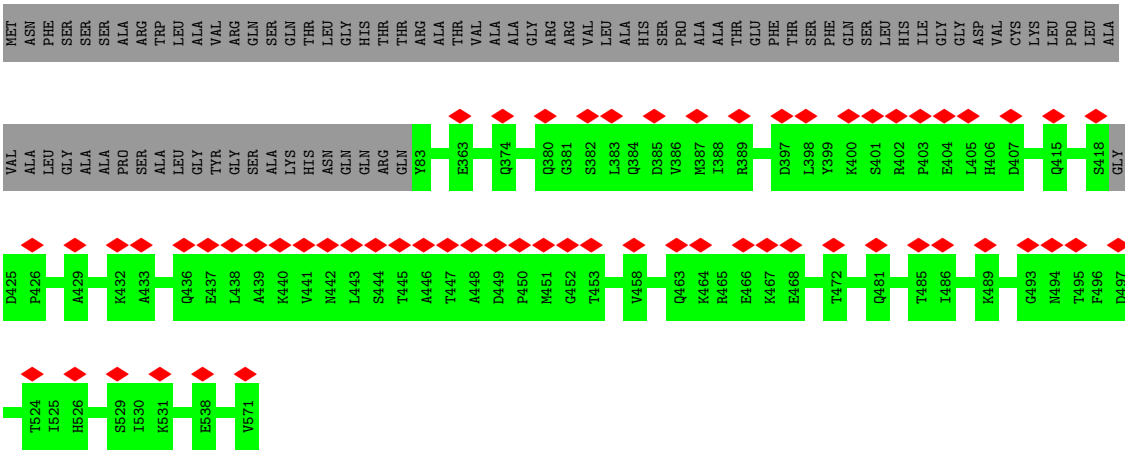
• Molecule 12: ATPTG17

Chain X:



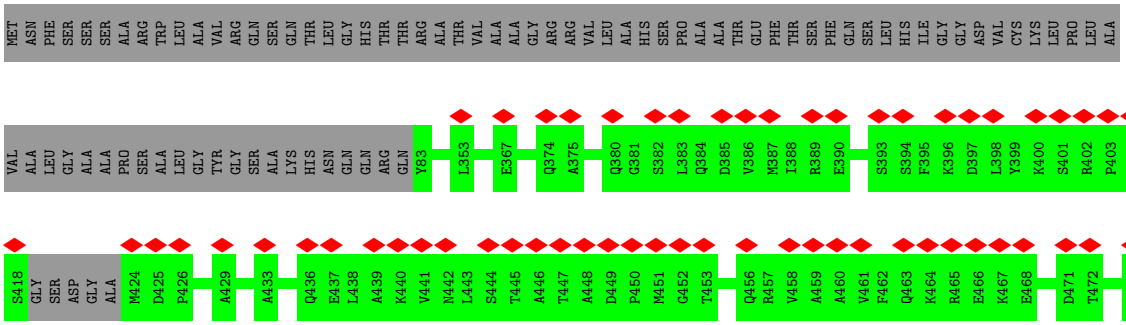
• Molecule 13: subunit b

Chain b:

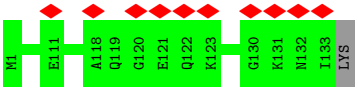


• Molecule 13: subunit b

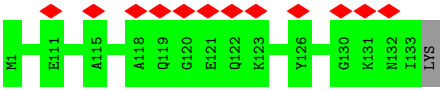
Chain B:



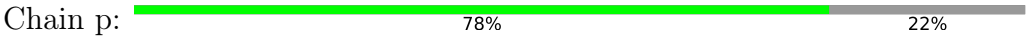
• Molecule 14: ATPTG12

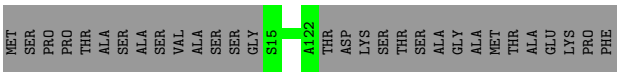


• Molecule 14: ATPTG12

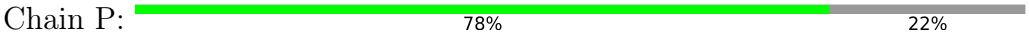


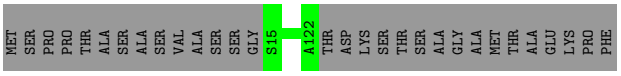
• Molecule 15: ATPTG10





• Molecule 15: ATPTG10





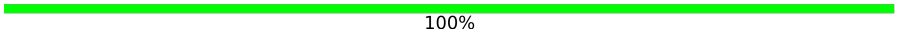
• Molecule 16: subunit f

• Molecule 16: subunit f

• Molecule 17: ATPTG8

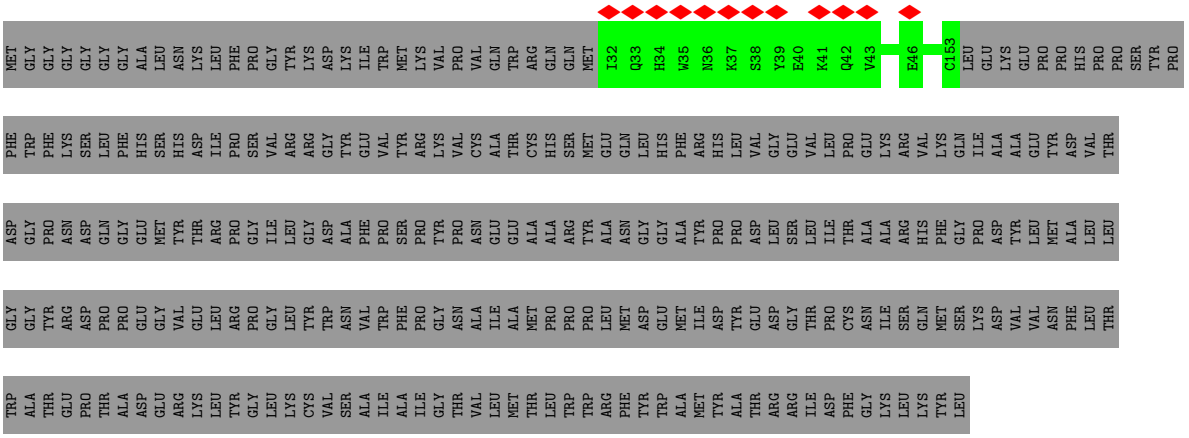
• Molecule 17: ATPTG8

Chain L:



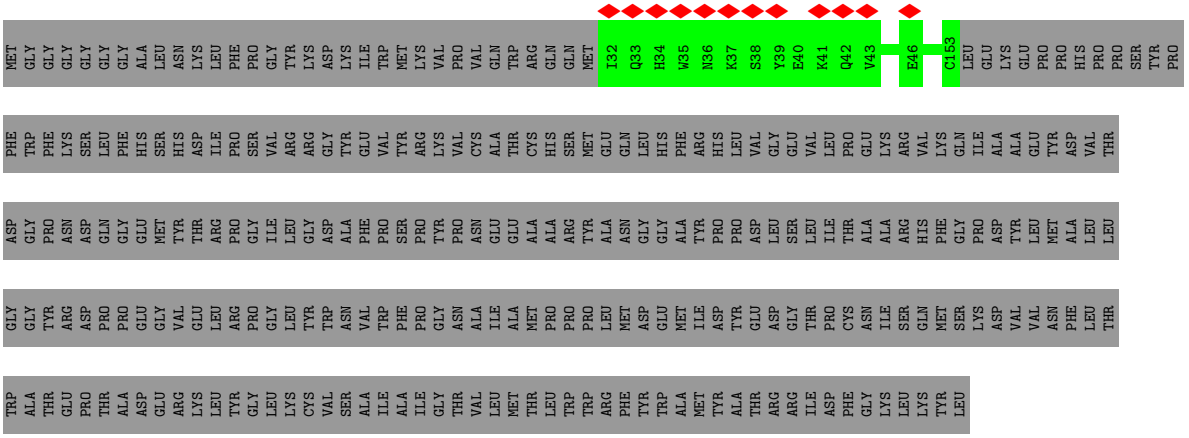
• Molecule 18: ATPTG1

Chain c:



• Molecule 18: ATPTG1

Chain C:



• Molecule 19: ATPTG2

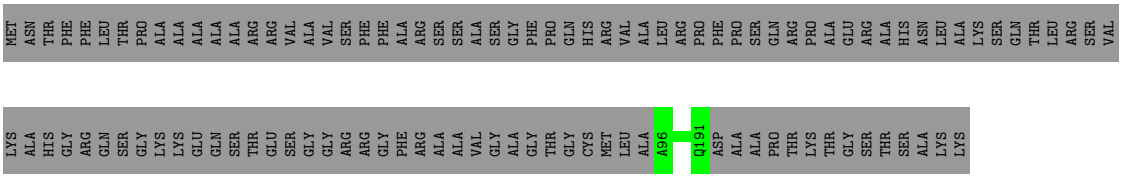
Chain d:

• Molecule 19: ATPTG2

Chain D:

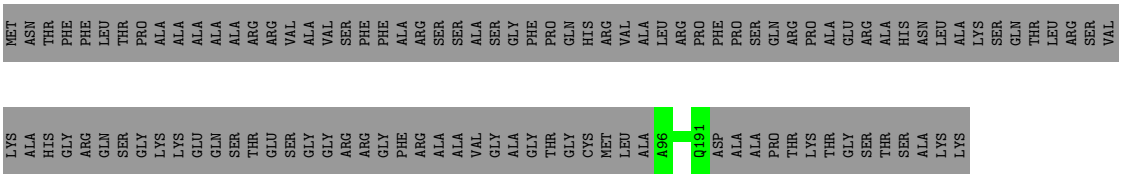
• Molecule 20: subunit 8

Chain m:



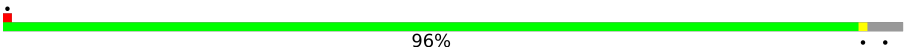
• Molecule 20: subunit 8

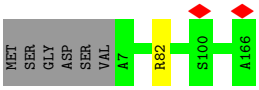
Chain M:



• Molecule 21: ATPTG9

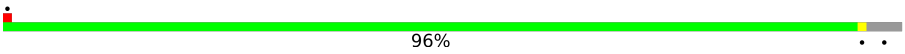
Chain n:

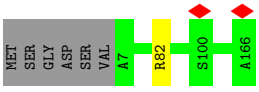




• Molecule 21: ATPTG9

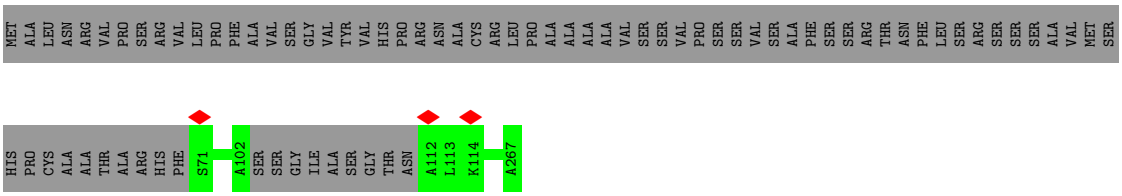
Chain N:





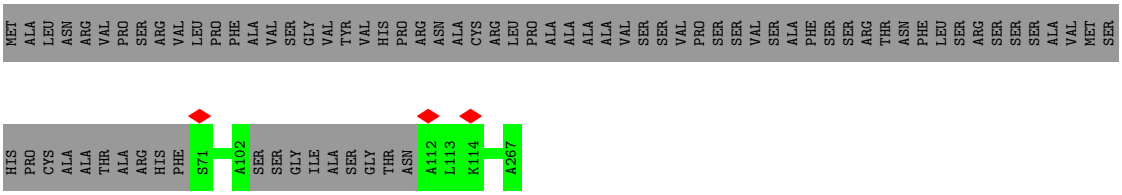
• Molecule 22: ATPTG4

Chain f:



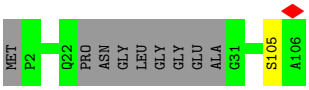
• Molecule 22: ATPTG4

Chain F:



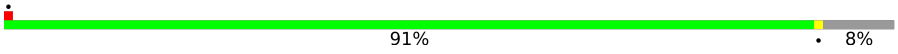
• Molecule 23: ATPTG16

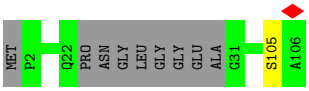
Chain w:



• Molecule 23: ATPTG16

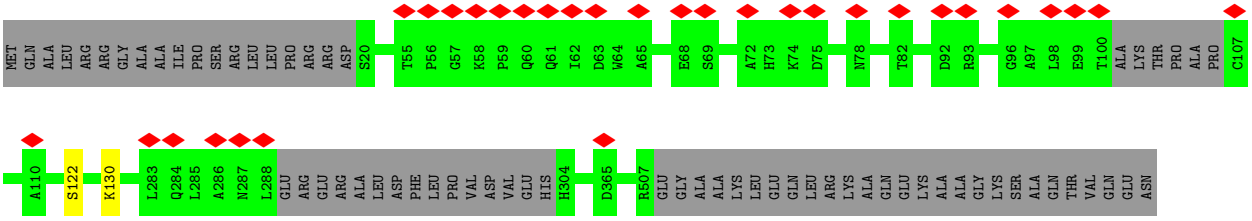
Chain W:





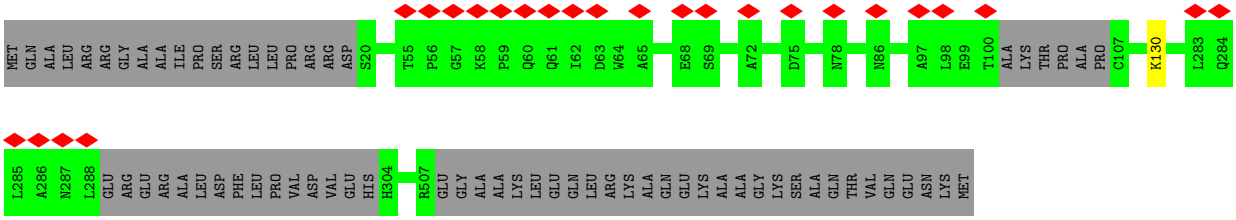
• Molecule 24: subunit d

Chain a:



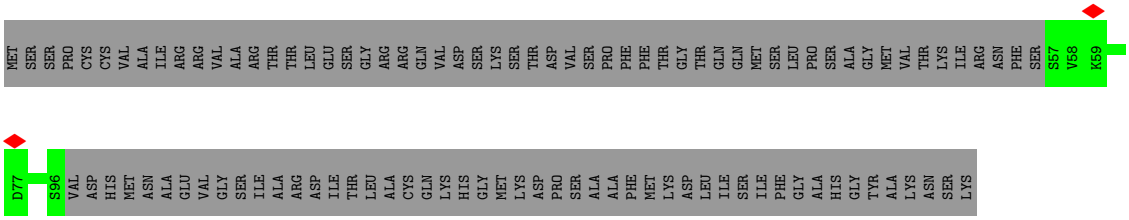
• Molecule 24: subunit d

Chain A:



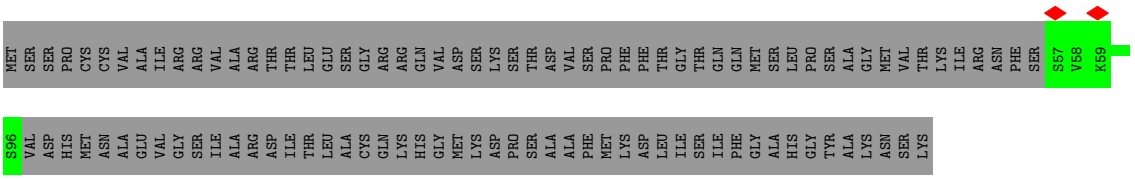
• Molecule 25: Inhibitor of F1

Chain i2:



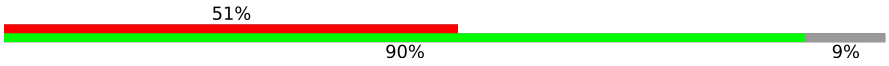
• Molecule 25: Inhibitor of F1

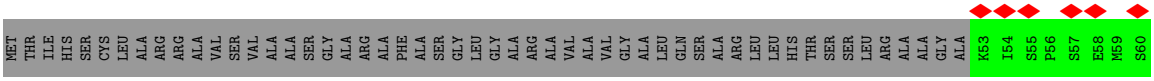
Chain i1:

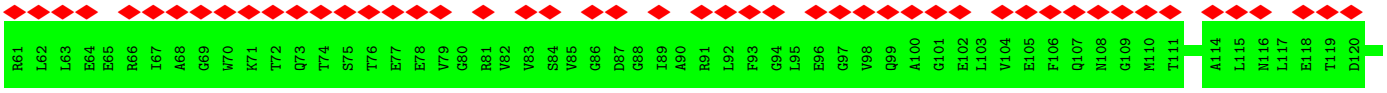


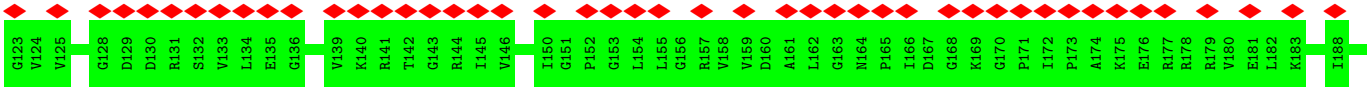
• Molecule 26: ATP synthase subunit alpha,subunit alpha

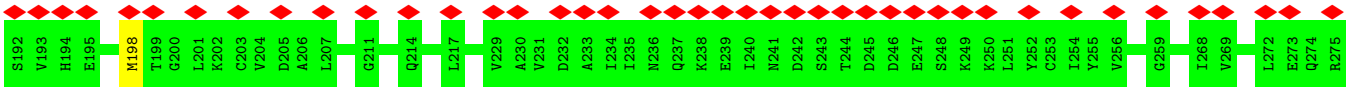
Chain A2:

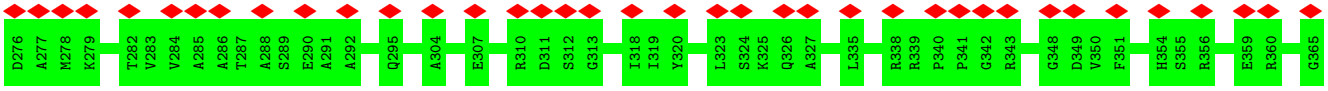


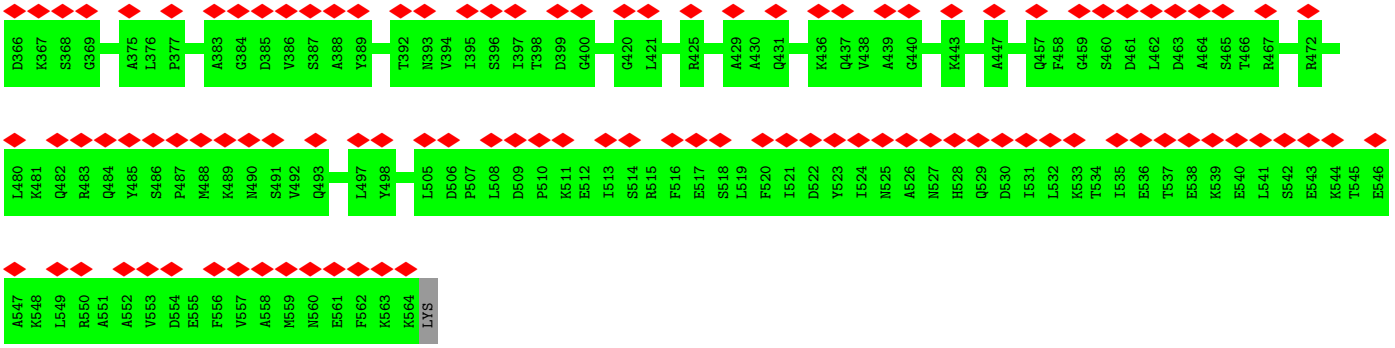






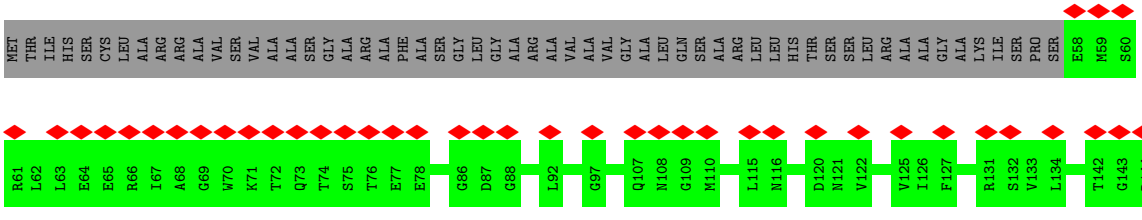






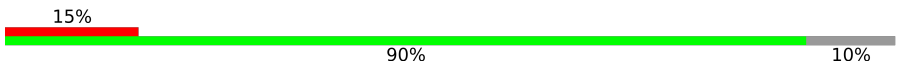
• Molecule 26: ATP synthase subunit alpha,subunit alpha

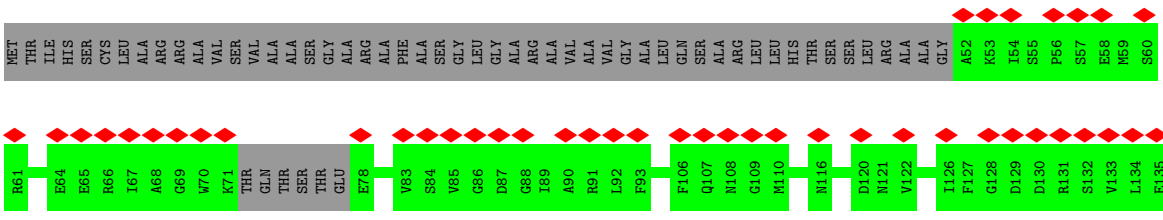
Chain E2:

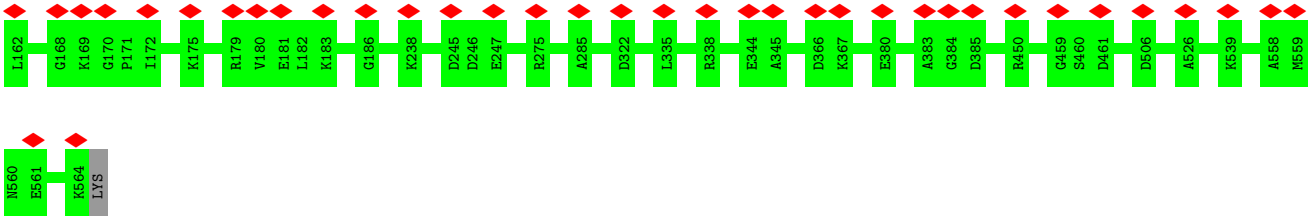


• Molecule 26: ATP synthase subunit alpha,subunit alpha

Chain C2:

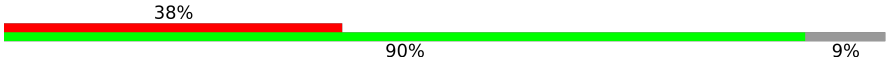


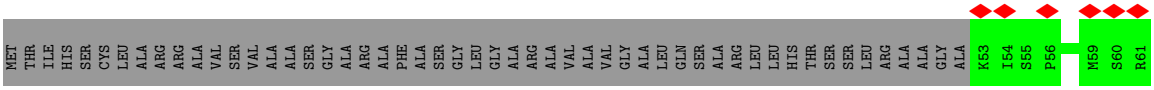


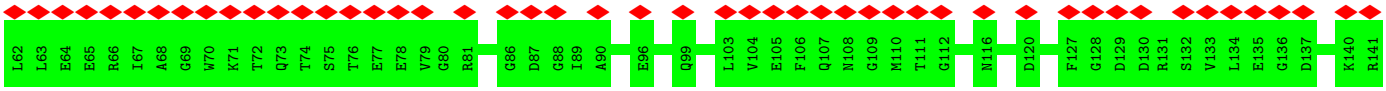


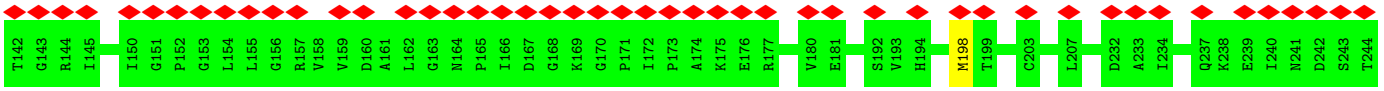
• Molecule 26: ATP synthase subunit alpha,subunit alpha

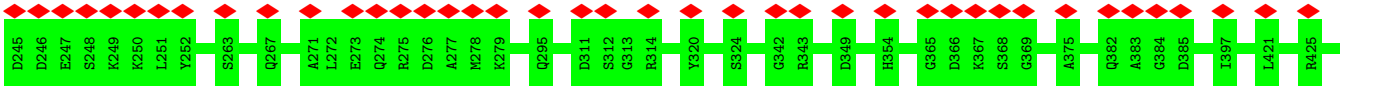
Chain A1:

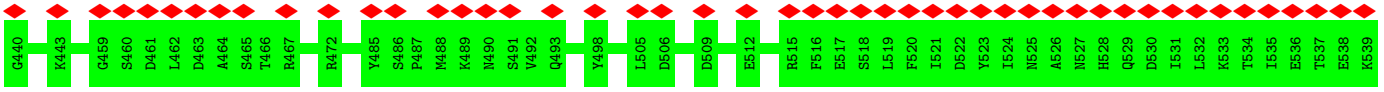


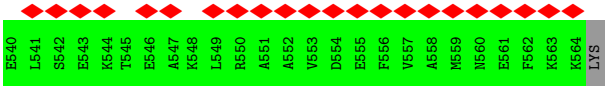






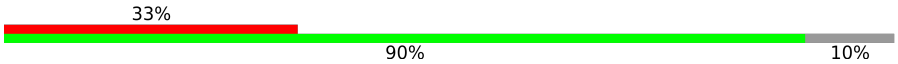


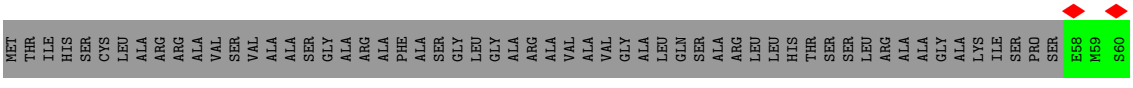


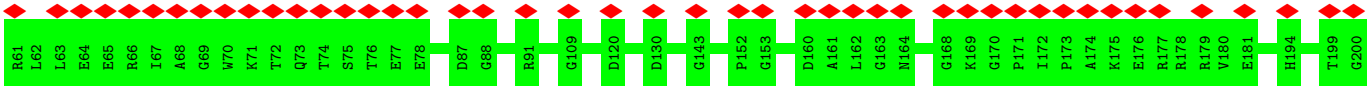


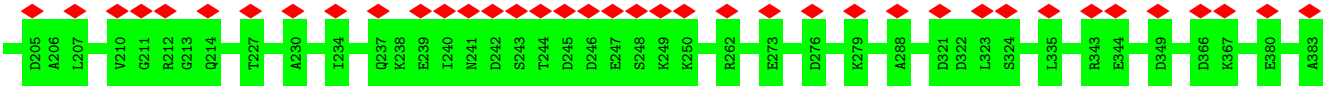
• Molecule 26: ATP synthase subunit alpha,subunit alpha

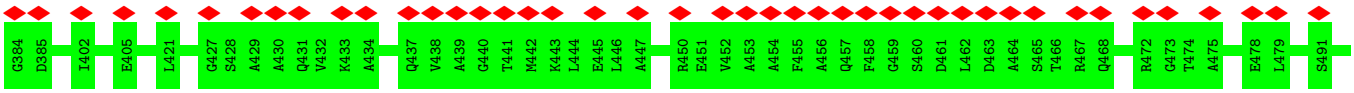
Chain E1:

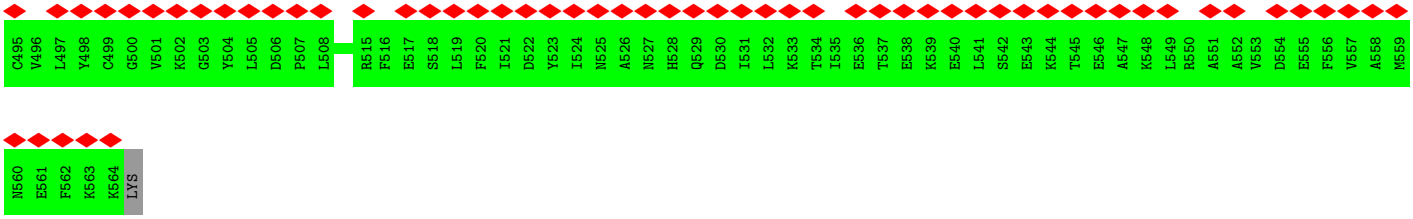






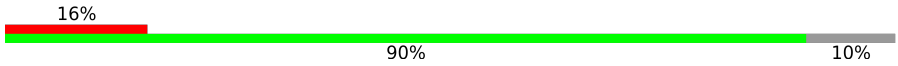


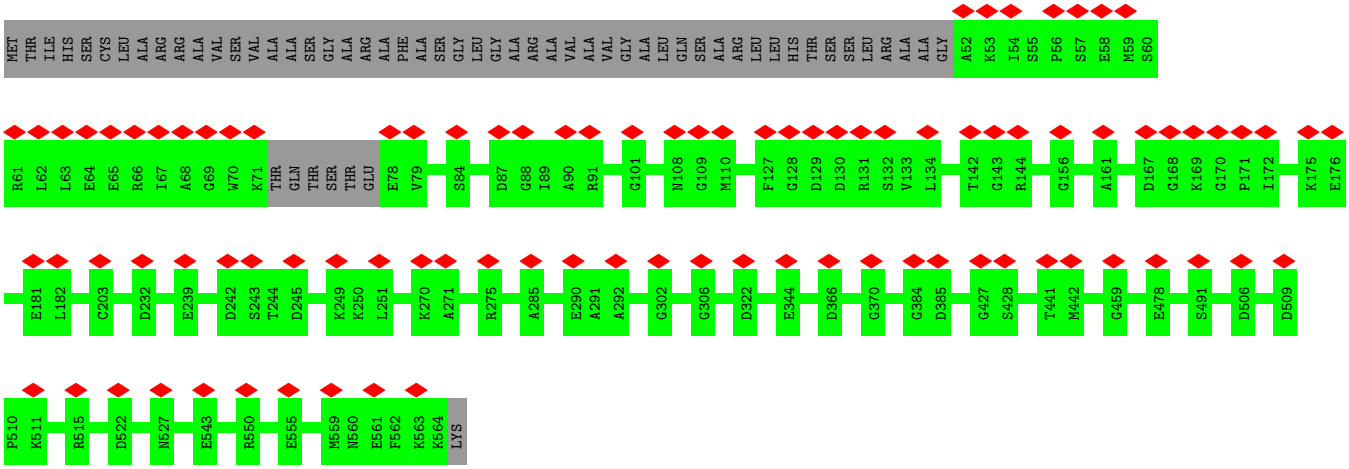




• Molecule 26: ATP synthase subunit alpha,subunit alpha

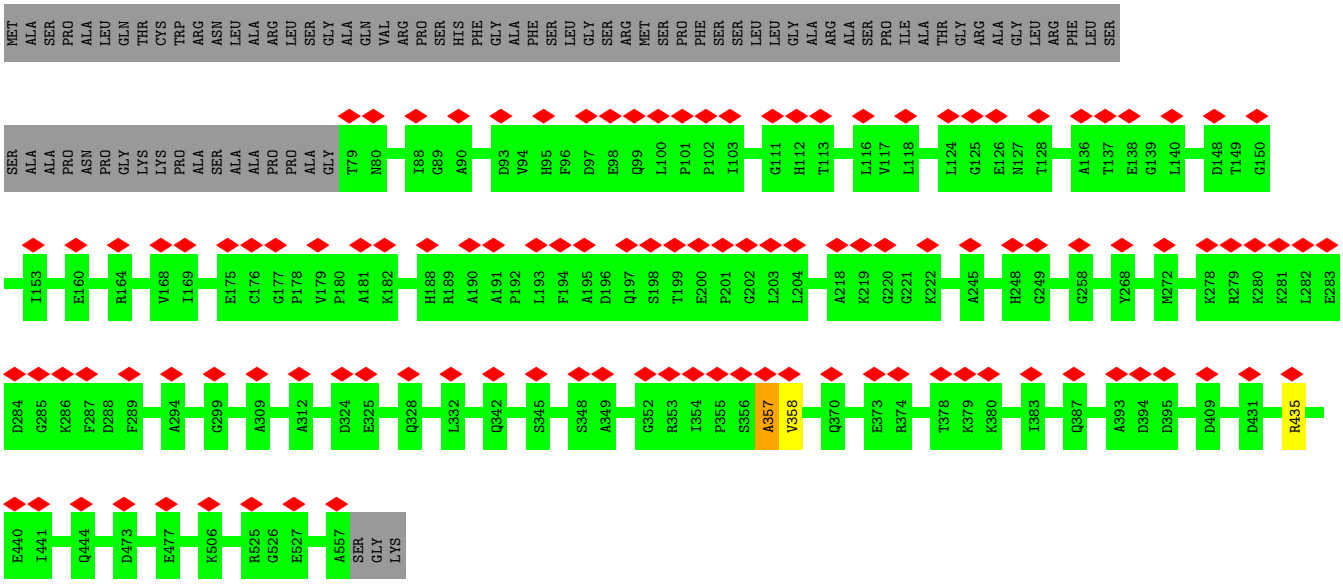
Chain C1:





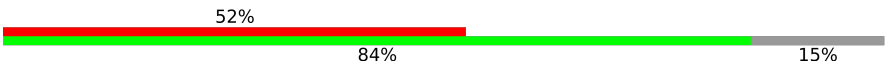
• Molecule 27: ATP synthase subunit beta

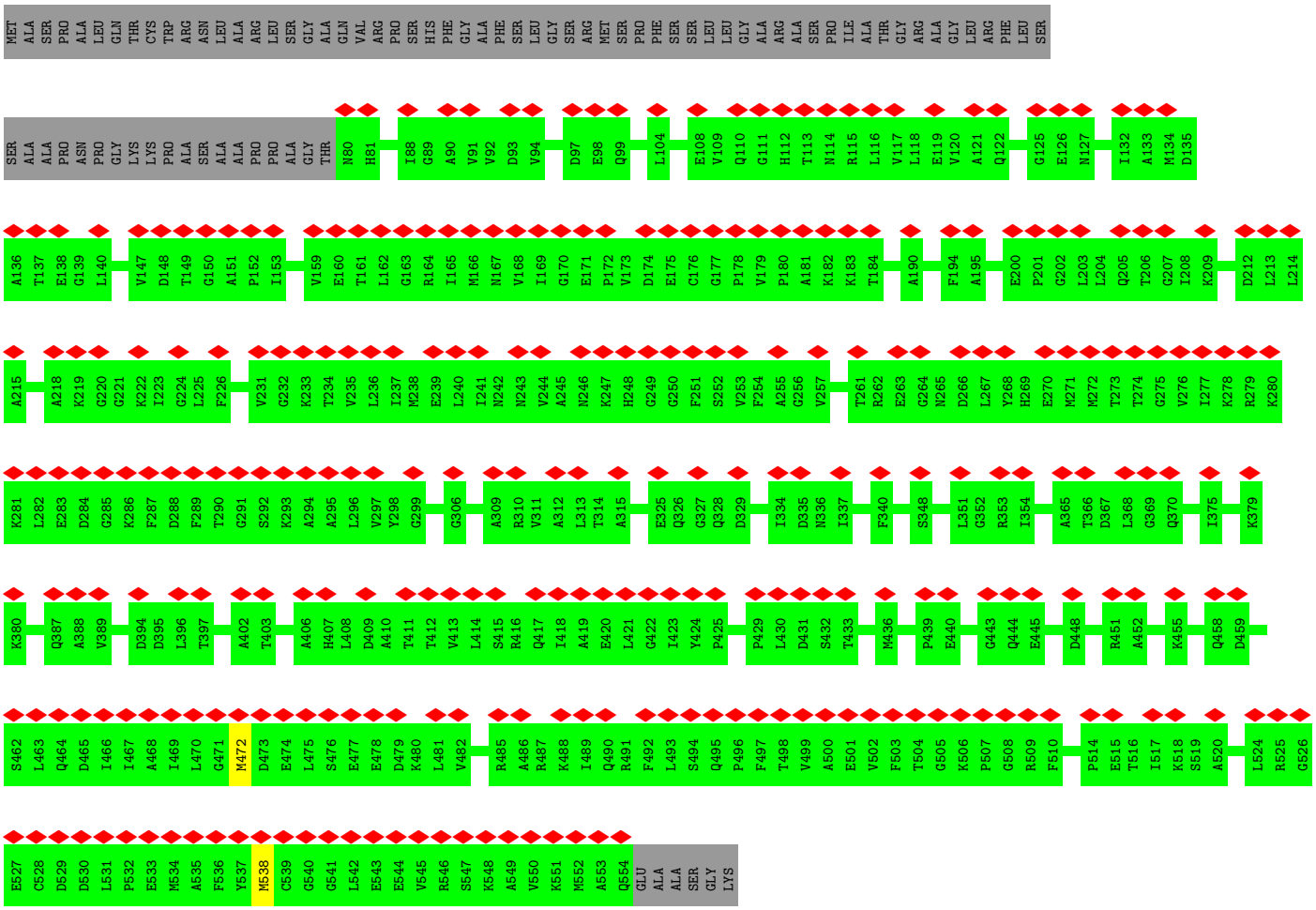
Chain B2:



• Molecule 27: ATP synthase subunit beta

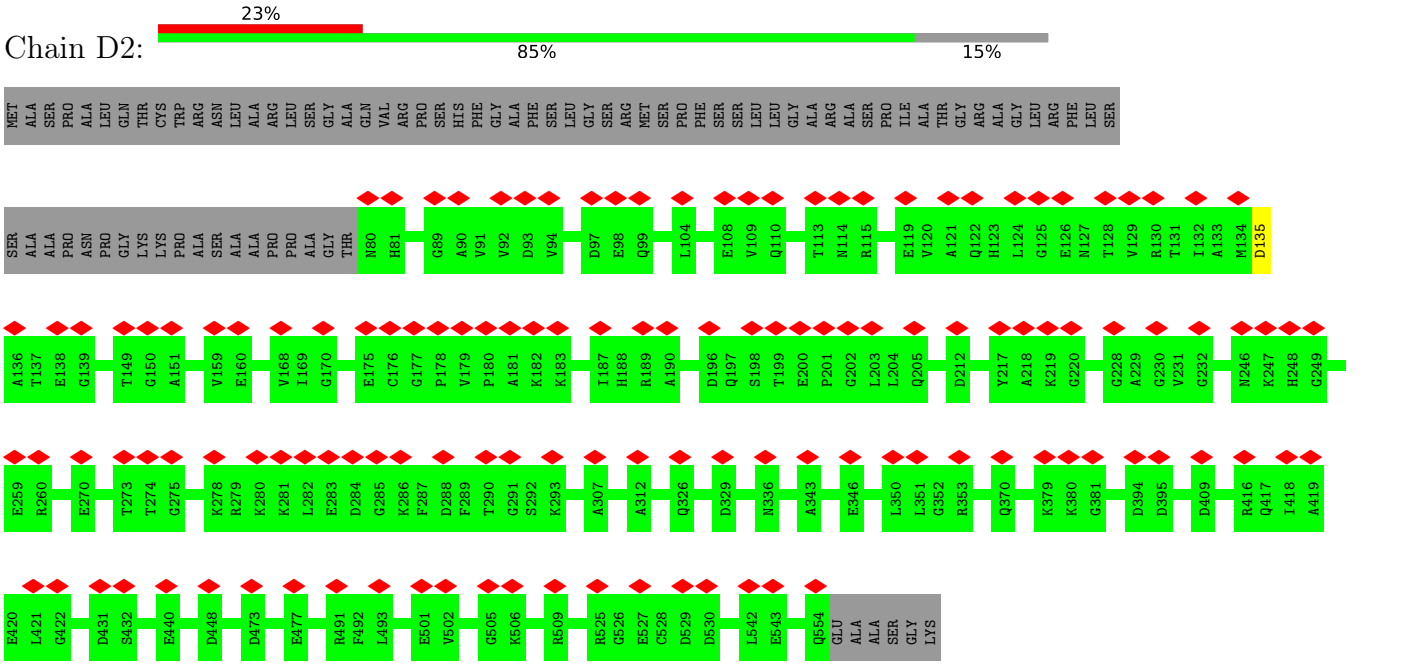
Chain F2:





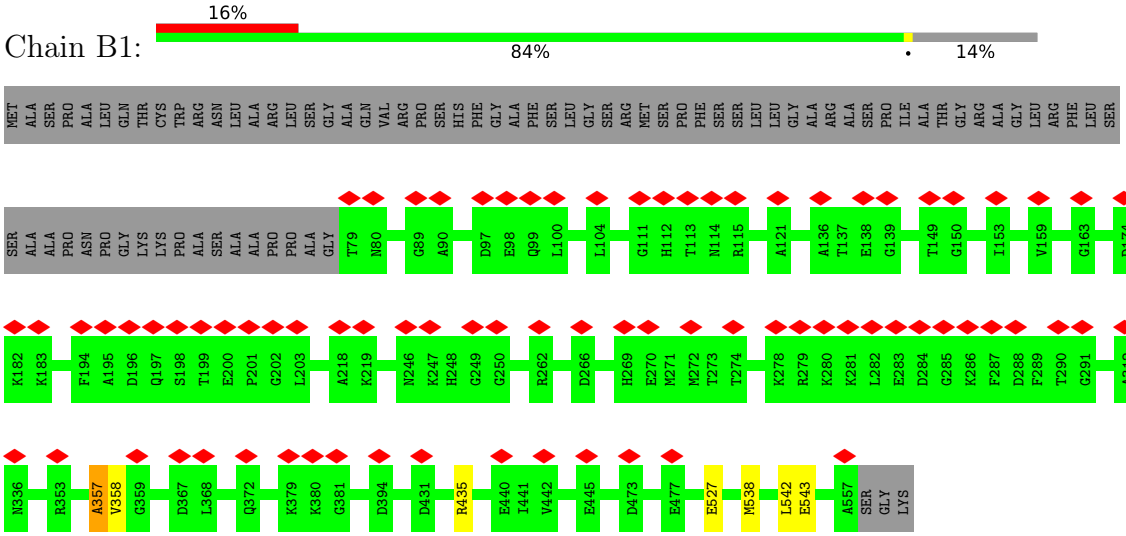
• Molecule 27: ATP synthase subunit beta

Chain D2:



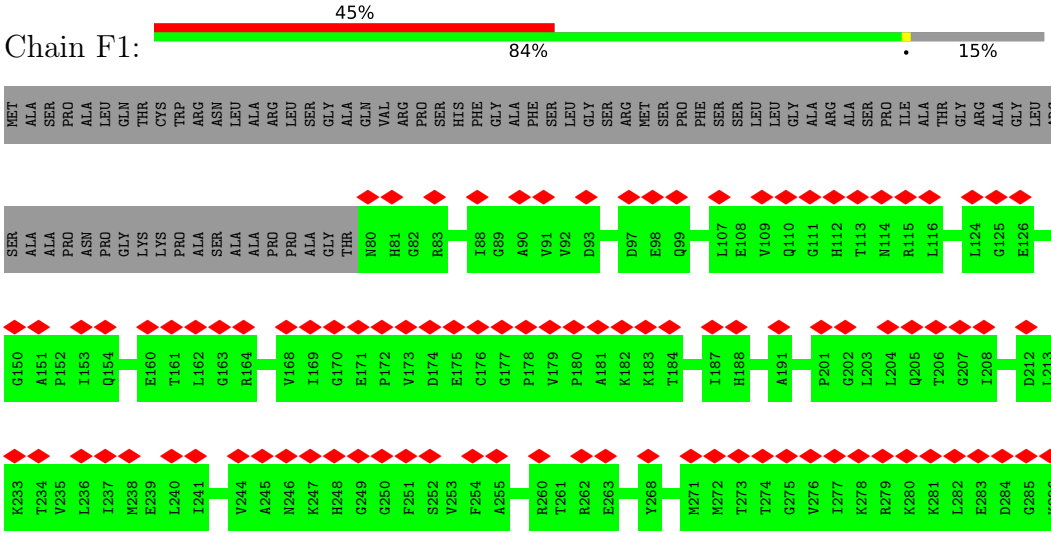
• Molecule 27: ATP synthase subunit beta

Chain B1:



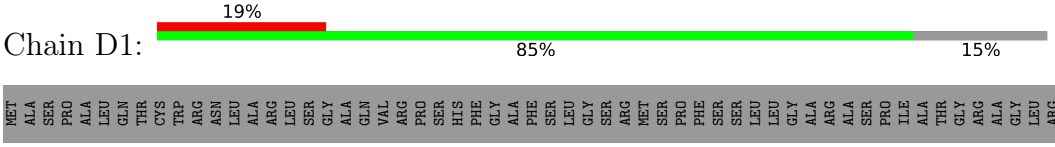
• Molecule 27: ATP synthase subunit beta

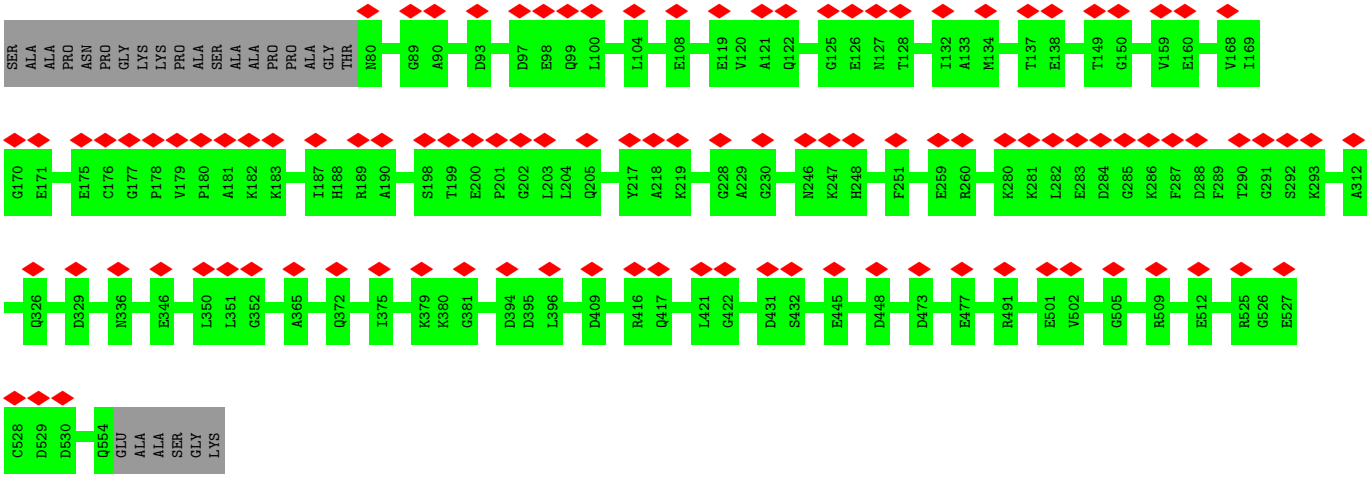
Chain F1:



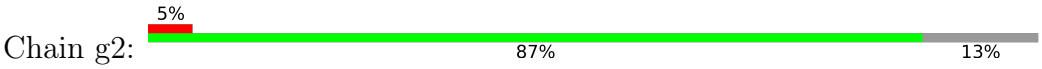
• Molecule 27: ATP synthase subunit beta

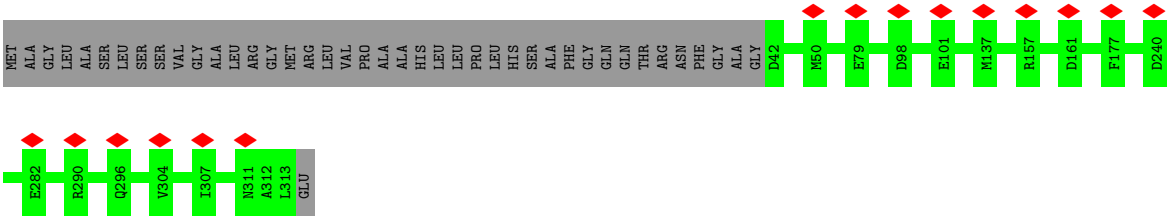
Chain D1:



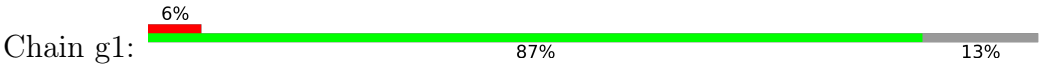


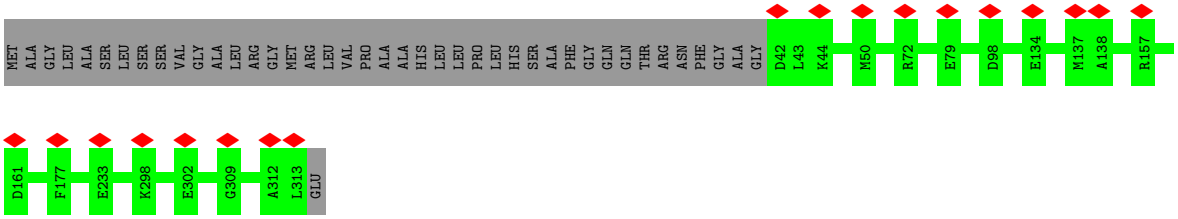
• Molecule 28: ATP synthase subunit gamma



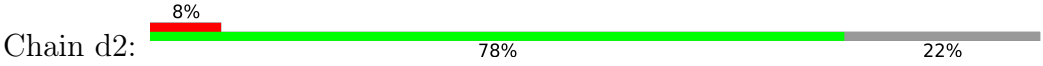


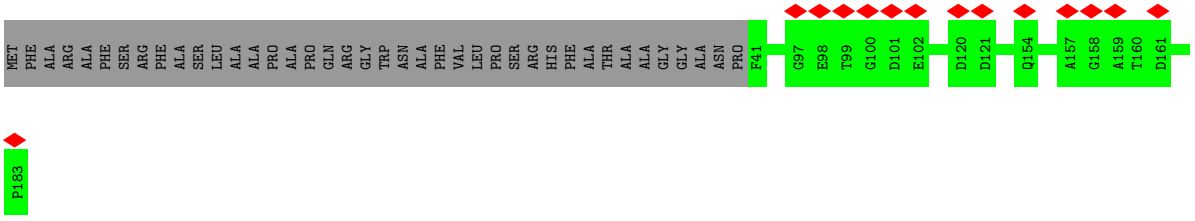
• Molecule 28: ATP synthase subunit gamma





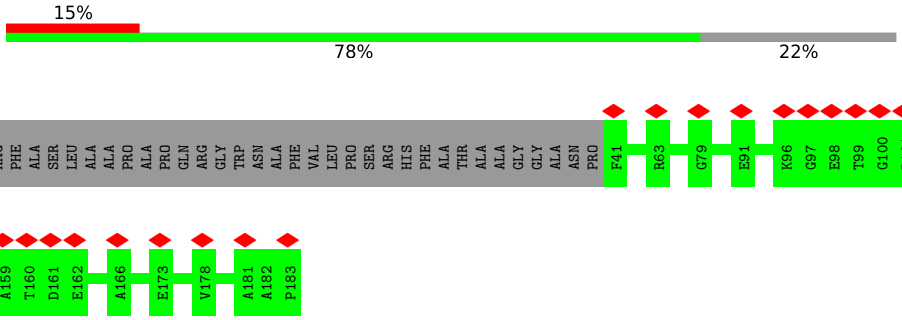
• Molecule 29: ATP synthase subunit delta





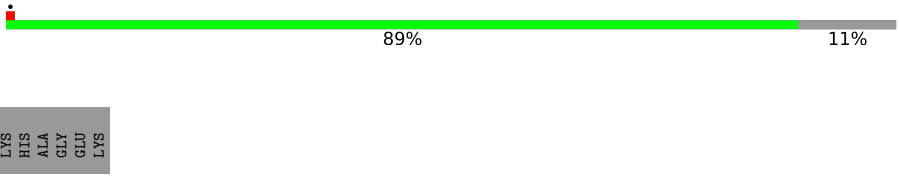
• Molecule 29: ATP synthase subunit delta

Chain d1:



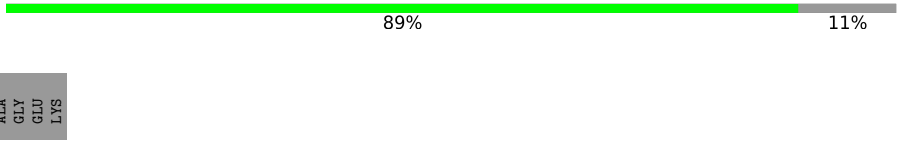
• Molecule 30: ATP synthase subunit epsilon

Chain e2:



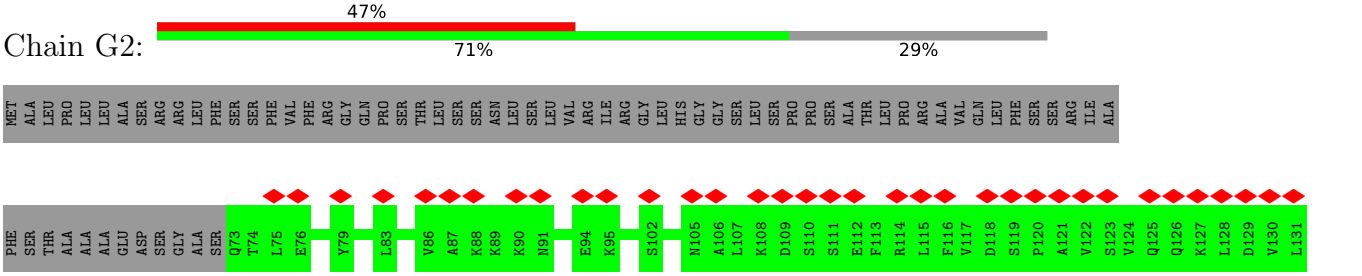
• Molecule 30: ATP synthase subunit epsilon

Chain e1:



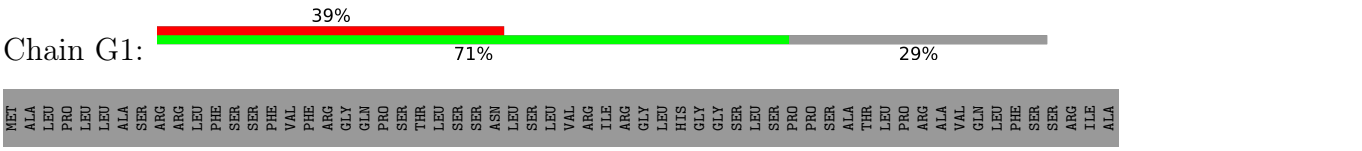
• Molecule 31: Oligomycin sensitivity conferring protein (OSCP)

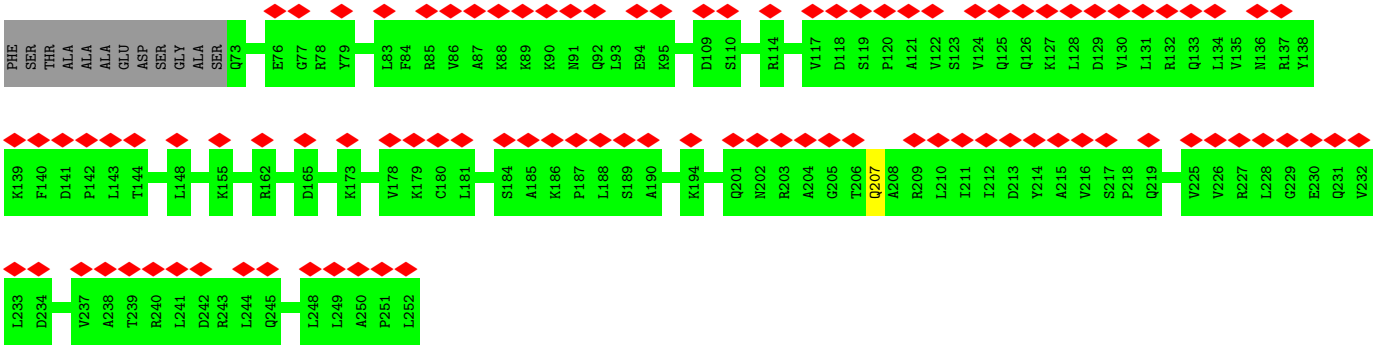
Chain G2:



• Molecule 31: Oligomycin sensitivity conferring protein (OSCP)

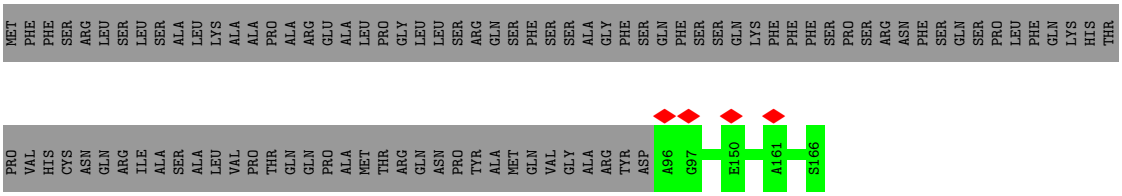
Chain G1:





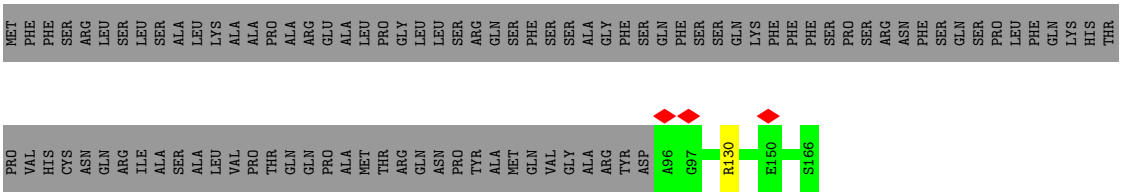
• Molecule 32: subunit c

Chain H2:



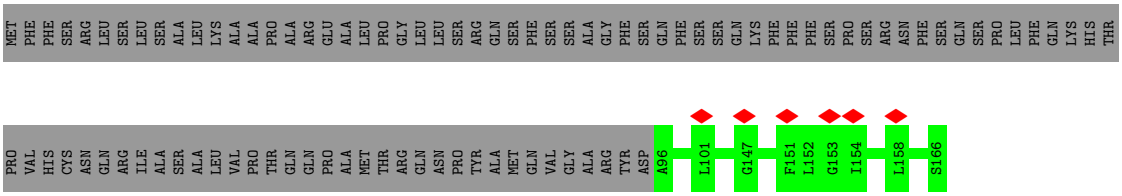
• Molecule 32: subunit c

Chain I2:



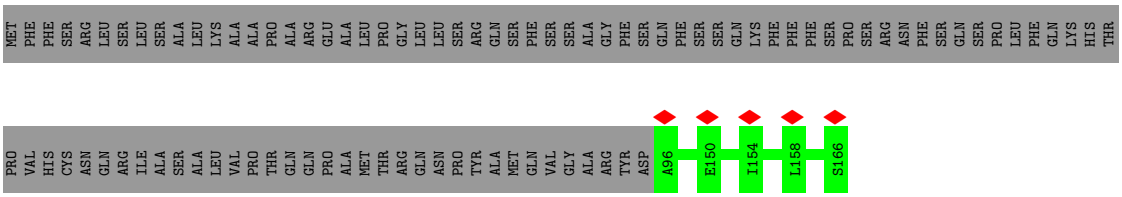
• Molecule 32: subunit c

Chain J2:



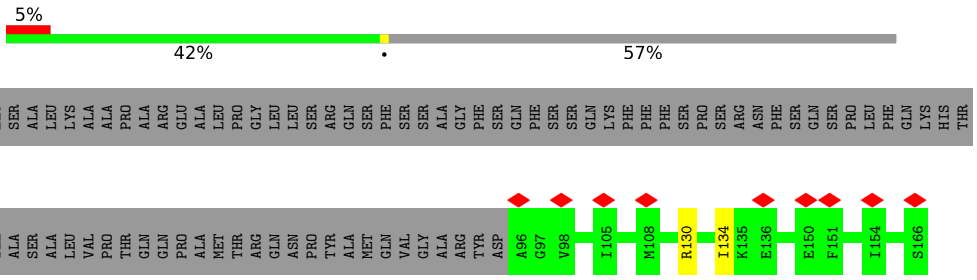
• Molecule 32: subunit c

Chain K2:



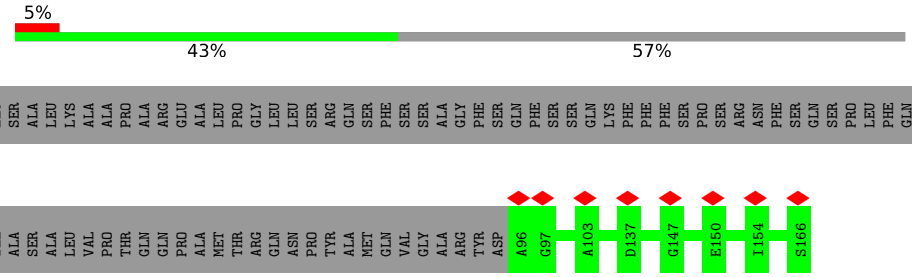
• Molecule 32: subunit c

Chain L2:



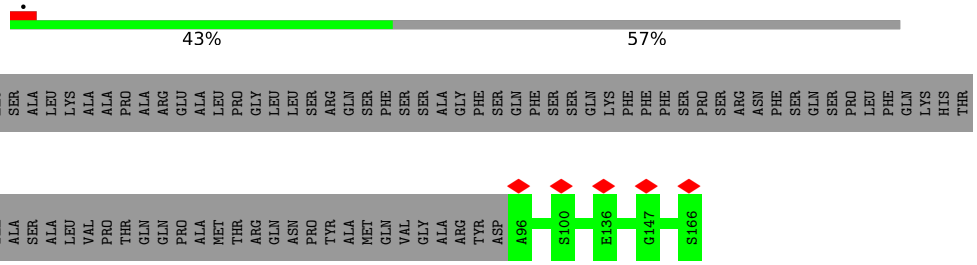
• Molecule 32: subunit c

Chain M2:



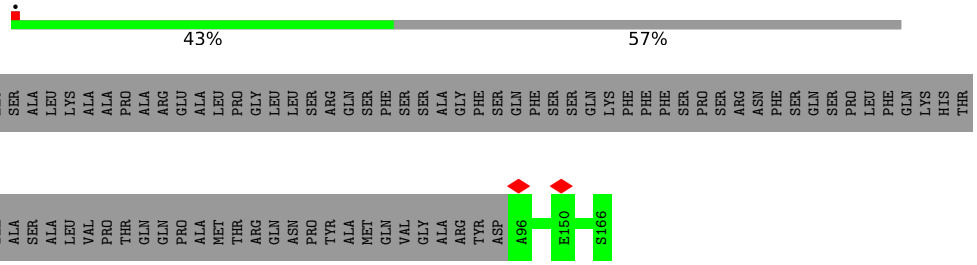
• Molecule 32: subunit c

Chain N2:



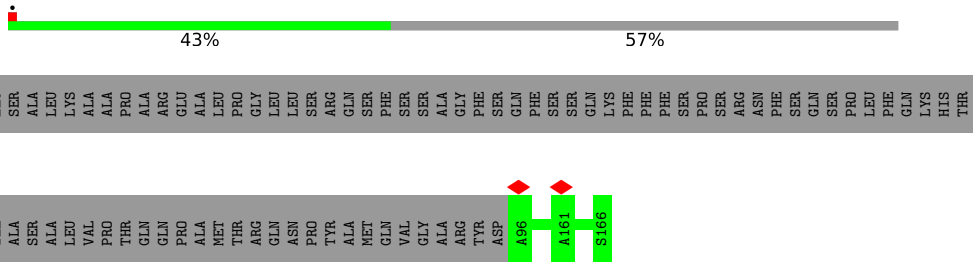
• Molecule 32: subunit c

Chain O2:



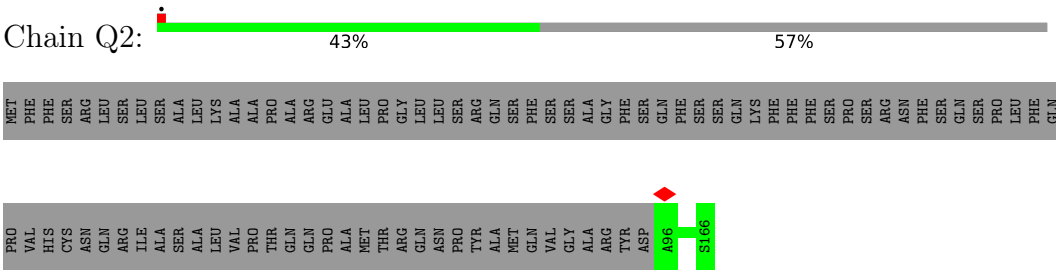
• Molecule 32: subunit c

Chain P2:



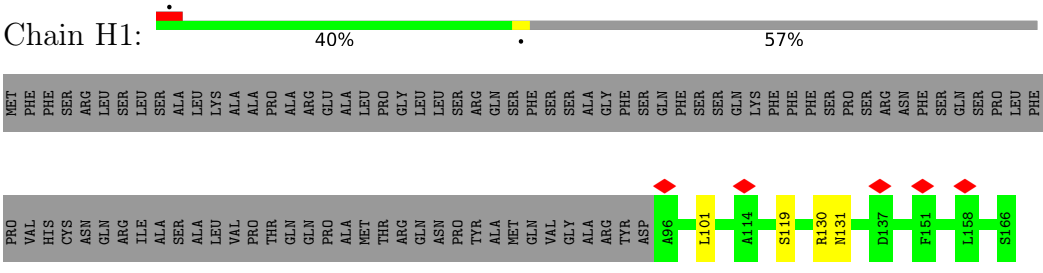
• Molecule 32: subunit c

Chain Q2:



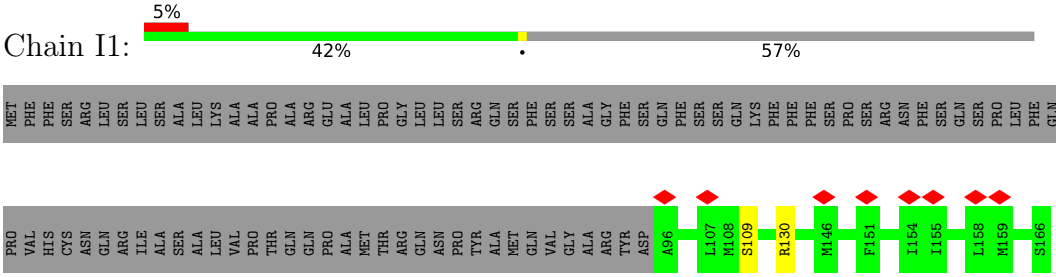
• Molecule 32: subunit c

Chain H1:



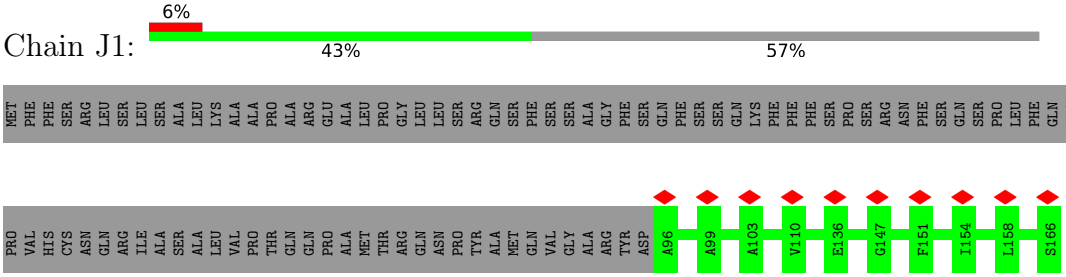
• Molecule 32: subunit c

Chain I1:



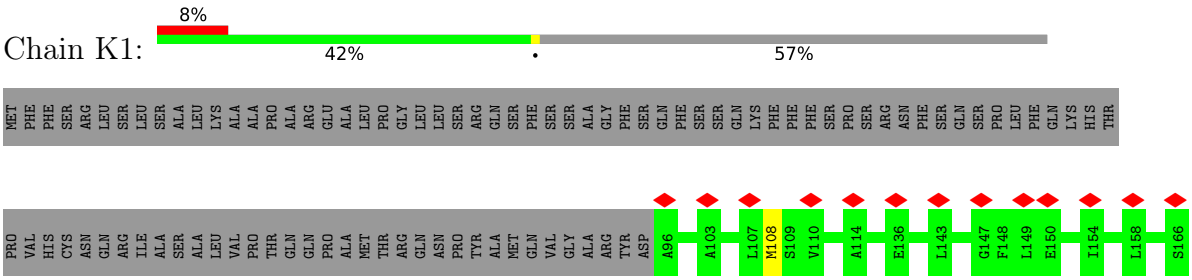
• Molecule 32: subunit c

Chain J1:



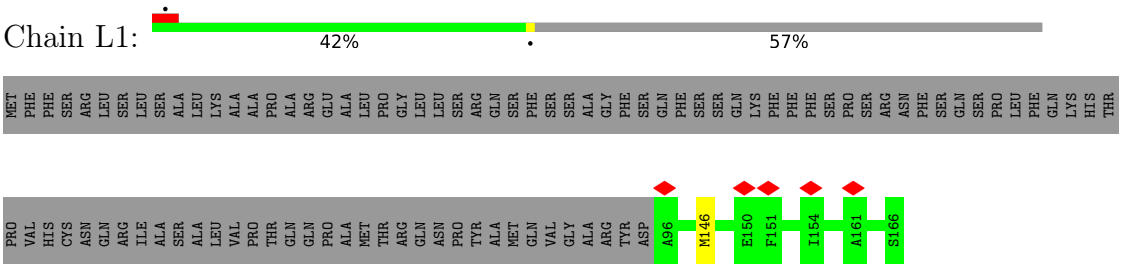
• Molecule 32: subunit c

Chain K1:



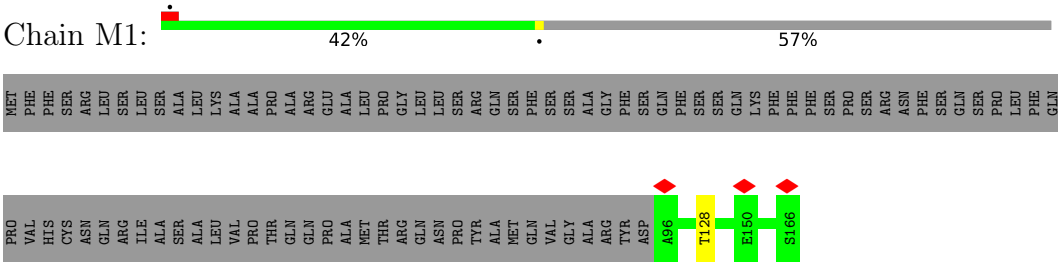
• Molecule 32: subunit c

Chain L1:



• Molecule 32: subunit c

Chain M1:

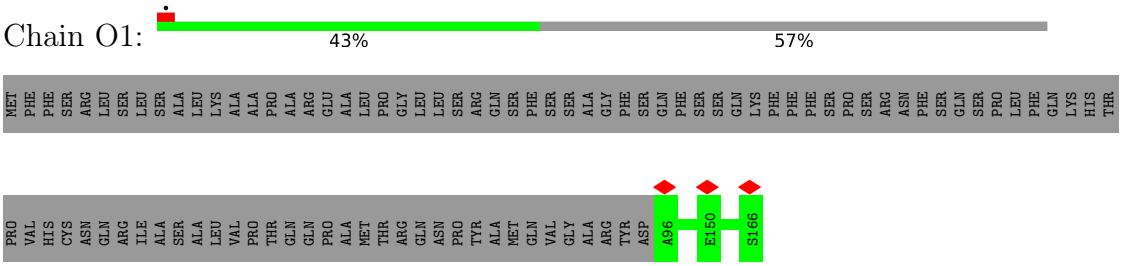


• Molecule 32: subunit c

Chain N1:

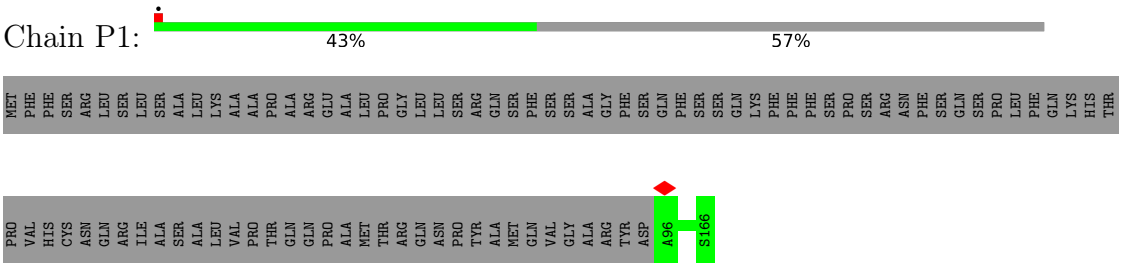
• Molecule 32: subunit c

Chain O1:



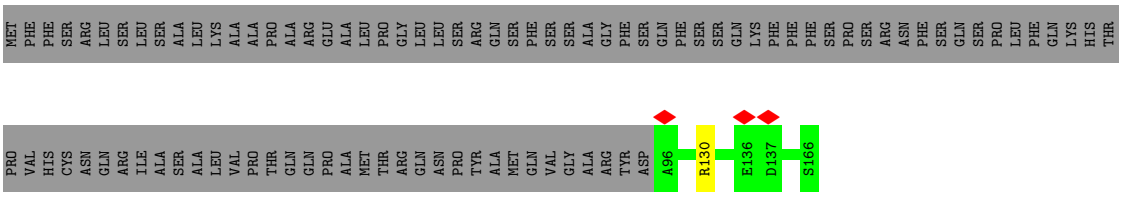
• Molecule 32: subunit c

Chain P1:



• Molecule 32: subunit c

Chain Q1:


MET PHE PHE SER ARG LEU SER LEU SER ALA LEU LYS ALA ALA PRO ALA ARG GLU ALA LEU PRO GLY LEU LEU SER ARG GLN SER PHE SER SER ALA GLY PHE SER GLN PHE SER SER GLN LYS PHE PHE PHE SER PRO SER ARG ASN PHE SER GLN SER PRO LEU PHE GLN LYS HIS THR
PRO VAL HIS CYS ASN GLN ARG ILE ALA SER ALA LEU VAL PRO THR GLN GLN PRO ALA MET THR ARG GLN ASN PRO TYR ALA MET GLN VAL GLY ALA ARG TYR ASP A96 R130 E136 D137 S166

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	101505	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 ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.375	Depositor
Minimum map value	-0.174	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	464.8, 464.8, 464.8	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, PEE, ADP, PC1, LMT, 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	Q	0.32	0/1103	0.43	0/1496
1	q	0.31	0/1103	0.43	0/1496
2	I	0.34	0/719	0.42	0/962
2	i	0.34	0/719	0.42	0/962
3	T	0.32	0/741	0.45	0/1007
3	t	0.32	0/741	0.44	0/1007
4	G	0.34	0/896	0.43	0/1216
4	g	0.34	0/896	0.44	0/1216
5	O	0.41	0/1250	0.46	0/1682
5	o	0.41	0/1250	0.45	0/1682
6	K	0.37	0/981	0.42	0/1321
6	k	0.37	0/981	0.42	0/1321
7	J	0.48	0/1573	0.47	0/2137
7	j	0.48	0/1573	0.47	0/2137
8	S	0.38	0/826	0.44	0/1119
8	s	0.38	0/826	0.44	0/1119
9	U	0.44	0/770	0.45	0/1040
9	u	0.44	0/770	0.46	0/1040
10	H	0.43	0/1902	0.44	0/2575
10	h	0.43	0/1902	0.44	0/2575
11	E	0.42	0/1154	0.45	0/1572
11	e	0.42	0/1154	0.45	0/1572
12	X	0.36	0/678	0.42	0/923
12	x	0.36	0/678	0.42	0/923
13	B	0.35	0/4016	0.43	0/5422
13	b	0.35	0/4016	0.43	0/5422
14	R	0.34	0/1092	0.44	0/1470
14	r	0.34	0/1092	0.46	0/1470
15	P	0.36	0/888	0.39	0/1202
15	p	0.36	0/888	0.40	0/1202
16	V	0.44	0/944	0.47	0/1280
16	v	0.44	0/944	0.47	0/1280

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	L	0.38	0/1651	0.45	0/2227
17	l	0.38	0/1651	0.45	0/2227
18	C	0.42	0/1057	0.46	0/1428
18	c	0.41	0/1057	0.46	0/1428
19	D	0.41	0/2143	0.46	0/2912
19	d	0.41	0/2143	0.46	0/2912
20	M	0.41	0/789	0.45	0/1065
20	m	0.40	0/789	0.45	0/1065
21	N	0.34	0/1280	0.42	0/1734
21	n	0.34	0/1280	0.42	0/1734
22	F	0.35	0/1475	0.44	0/2009
22	f	0.35	0/1475	0.44	0/2009
23	W	0.41	0/784	0.48	0/1064
23	w	0.41	0/784	0.48	0/1064
24	A	0.32	0/3883	0.40	0/5262
24	a	0.32	0/3883	0.40	0/5262
25	i1	0.27	0/343	0.38	0/459
25	i2	0.27	0/343	0.37	0/459
26	A1	0.25	0/3979	0.44	0/5372
26	A2	0.25	0/3979	0.44	0/5372
26	C1	0.25	0/3938	0.44	0/5314
26	C2	0.25	0/3938	0.43	0/5314
26	E1	0.24	0/3942	0.43	0/5322
26	E2	0.24	0/3942	0.43	0/5322
27	B1	0.26	0/3698	0.46	0/5016
27	B2	0.26	0/3698	0.45	0/5016
27	D1	0.25	0/3672	0.44	0/4980
27	D2	0.25	0/3672	0.44	0/4980
27	F1	0.25	0/3672	0.47	1/4980 (0.0%)
27	F2	0.25	0/3672	0.45	0/4980
28	g1	0.26	0/2145	0.40	0/2890
28	g2	0.26	0/2145	0.41	0/2890
29	d1	0.25	0/1083	0.43	0/1466
29	d2	0.26	0/1083	0.44	0/1466
30	e1	0.29	0/547	0.43	0/733
30	e2	0.28	0/547	0.42	0/733
31	G1	0.25	0/1431	0.44	0/1929
31	G2	0.24	0/1431	0.43	0/1929
32	H1	0.30	0/507	0.55	0/686
32	H2	0.27	0/507	0.41	0/686
32	I1	0.30	0/507	0.47	0/686
32	I2	0.26	0/507	0.41	0/686
32	J1	0.29	0/507	0.44	0/686

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	J2	0.27	0/507	0.42	0/686
32	K1	0.28	0/507	0.46	0/686
32	K2	0.26	0/507	0.40	0/686
32	L1	0.29	0/507	0.47	0/686
32	L2	0.28	0/507	0.55	0/686
32	M1	0.28	0/507	0.43	0/686
32	M2	0.26	0/507	0.40	0/686
32	N1	0.27	0/507	0.41	0/686
32	N2	0.26	0/507	0.40	0/686
32	O1	0.28	0/507	0.41	0/686
32	O2	0.28	0/507	0.41	0/686
32	P1	0.31	0/507	0.46	0/686
32	P2	0.30	0/507	0.46	0/686
32	Q1	0.29	0/507	0.46	0/686
32	Q2	0.28	0/507	0.42	0/686
All	All	0.32	0/132230	0.44	1/178892 (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
7	J	0	1
7	j	0	1
26	A1	0	1
26	A2	0	1
27	B1	0	1
27	B2	0	1
27	F1	1	0
All	All	1	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	F1	538	MET	N-CA-CB	6.08	121.55	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	F1	538	MET	CA

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	A1	198	MET	Peptide
26	A2	198	MET	Peptide
27	B2	357	ALA	Peptide
7	J	89	PHE	Peptide
7	j	89	PHE	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	131/134 (98%)	125 (95%)	6 (5%)	0	100	100
1	q	131/134 (98%)	126 (96%)	5 (4%)	0	100	100
2	I	88/236 (37%)	85 (97%)	3 (3%)	0	100	100
2	i	88/236 (37%)	85 (97%)	3 (3%)	0	100	100
3	T	90/133 (68%)	87 (97%)	3 (3%)	0	100	100
3	t	90/133 (68%)	87 (97%)	3 (3%)	0	100	100
4	G	110/252 (44%)	102 (93%)	8 (7%)	0	100	100
4	g	110/252 (44%)	102 (93%)	8 (7%)	0	100	100
5	O	147/157 (94%)	141 (96%)	6 (4%)	0	100	100
5	o	147/157 (94%)	141 (96%)	6 (4%)	0	100	100
6	K	115/224 (51%)	112 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	k	115/224 (51%)	111 (96%)	4 (4%)	0	100	100
7	J	174/229 (76%)	166 (95%)	8 (5%)	0	100	100
7	j	174/229 (76%)	166 (95%)	8 (5%)	0	100	100
8	S	93/128 (73%)	92 (99%)	1 (1%)	0	100	100
8	s	93/128 (73%)	92 (99%)	1 (1%)	0	100	100
9	U	92/126 (73%)	90 (98%)	2 (2%)	0	100	100
9	u	92/126 (73%)	90 (98%)	2 (2%)	0	100	100
10	H	224/239 (94%)	216 (96%)	8 (4%)	0	100	100
10	h	224/239 (94%)	214 (96%)	10 (4%)	0	100	100
11	E	138/325 (42%)	135 (98%)	3 (2%)	0	100	100
11	e	138/325 (42%)	135 (98%)	3 (2%)	0	100	100
12	X	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
12	x	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
13	B	480/571 (84%)	466 (97%)	14 (3%)	0	100	100
13	b	480/571 (84%)	465 (97%)	15 (3%)	0	100	100
14	R	131/134 (98%)	122 (93%)	9 (7%)	0	100	100
14	r	131/134 (98%)	124 (95%)	7 (5%)	0	100	100
15	P	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
15	p	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
16	V	108/111 (97%)	108 (100%)	0	0	100	100
16	v	108/111 (97%)	108 (100%)	0	0	100	100
17	L	205/208 (99%)	201 (98%)	4 (2%)	0	100	100
17	l	205/208 (99%)	201 (98%)	4 (2%)	0	100	100
18	C	120/398 (30%)	114 (95%)	6 (5%)	0	100	100
18	c	120/398 (30%)	114 (95%)	6 (5%)	0	100	100
19	D	251/310 (81%)	246 (98%)	5 (2%)	0	100	100
19	d	251/310 (81%)	246 (98%)	5 (2%)	0	100	100
20	M	94/205 (46%)	91 (97%)	3 (3%)	0	100	100
20	m	94/205 (46%)	91 (97%)	3 (3%)	0	100	100
21	N	158/166 (95%)	156 (99%)	2 (1%)	0	100	100
21	n	158/166 (95%)	156 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	F	184/267 (69%)	173 (94%)	11 (6%)	0	100	100
22	f	184/267 (69%)	173 (94%)	11 (6%)	0	100	100
23	W	93/106 (88%)	87 (94%)	6 (6%)	0	100	100
23	w	93/106 (88%)	88 (95%)	5 (5%)	0	100	100
24	A	461/536 (86%)	445 (96%)	16 (4%)	0	100	100
24	a	461/536 (86%)	445 (96%)	16 (4%)	0	100	100
25	i1	38/145 (26%)	38 (100%)	0	0	100	100
25	i2	38/145 (26%)	38 (100%)	0	0	100	100
26	A1	510/565 (90%)	488 (96%)	22 (4%)	0	100	100
26	A2	510/565 (90%)	489 (96%)	21 (4%)	0	100	100
26	C1	503/565 (89%)	487 (97%)	16 (3%)	0	100	100
26	C2	503/565 (89%)	485 (96%)	18 (4%)	0	100	100
26	E1	505/565 (89%)	482 (95%)	23 (5%)	0	100	100
26	E2	505/565 (89%)	485 (96%)	20 (4%)	0	100	100
27	B1	477/560 (85%)	453 (95%)	22 (5%)	2 (0%)	30	60
27	B2	477/560 (85%)	454 (95%)	21 (4%)	2 (0%)	30	60
27	D1	473/560 (84%)	455 (96%)	18 (4%)	0	100	100
27	D2	473/560 (84%)	452 (96%)	21 (4%)	0	100	100
27	F1	473/560 (84%)	455 (96%)	18 (4%)	0	100	100
27	F2	473/560 (84%)	455 (96%)	18 (4%)	0	100	100
28	g1	270/314 (86%)	260 (96%)	10 (4%)	0	100	100
28	g2	270/314 (86%)	260 (96%)	10 (4%)	0	100	100
29	d1	141/183 (77%)	136 (96%)	5 (4%)	0	100	100
29	d2	141/183 (77%)	137 (97%)	4 (3%)	0	100	100
30	e1	63/73 (86%)	59 (94%)	4 (6%)	0	100	100
30	e2	63/73 (86%)	59 (94%)	4 (6%)	0	100	100
31	G1	178/252 (71%)	159 (89%)	19 (11%)	0	100	100
31	G2	178/252 (71%)	159 (89%)	19 (11%)	0	100	100
32	H1	69/166 (42%)	69 (100%)	0	0	100	100
32	H2	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	I1	69/166 (42%)	68 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	I2	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	J1	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	J2	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	K1	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	K2	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	L1	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	L2	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	M1	69/166 (42%)	63 (91%)	6 (9%)	0	100	100
32	M2	69/166 (42%)	64 (93%)	5 (7%)	0	100	100
32	N1	69/166 (42%)	69 (100%)	0	0	100	100
32	N2	69/166 (42%)	69 (100%)	0	0	100	100
32	O1	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	O2	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	P1	69/166 (42%)	66 (96%)	3 (4%)	0	100	100
32	P2	69/166 (42%)	66 (96%)	3 (4%)	0	100	100
32	Q1	69/166 (42%)	69 (100%)	0	0	100	100
32	Q2	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
All	All	16388/22836 (72%)	15771 (96%)	613 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	B1	358	VAL
27	B2	357	ALA
27	B2	358	VAL
27	B1	357	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Q	119/120 (99%)	117 (98%)	2 (2%)	56 83
1	q	119/120 (99%)	119 (100%)	0	100 100
2	I	71/197 (36%)	71 (100%)	0	100 100
2	i	71/197 (36%)	71 (100%)	0	100 100
3	T	77/106 (73%)	77 (100%)	0	100 100
3	t	77/106 (73%)	77 (100%)	0	100 100
4	G	93/214 (44%)	93 (100%)	0	100 100
4	g	93/214 (44%)	93 (100%)	0	100 100
5	O	127/129 (98%)	127 (100%)	0	100 100
5	o	127/129 (98%)	127 (100%)	0	100 100
6	K	100/175 (57%)	100 (100%)	0	100 100
6	k	100/175 (57%)	100 (100%)	0	100 100
7	J	160/195 (82%)	160 (100%)	0	100 100
7	j	160/195 (82%)	160 (100%)	0	100 100
8	S	86/113 (76%)	86 (100%)	0	100 100
8	s	86/113 (76%)	86 (100%)	0	100 100
9	U	76/98 (78%)	76 (100%)	0	100 100
9	u	76/98 (78%)	76 (100%)	0	100 100
10	H	197/204 (97%)	196 (100%)	1 (0%)	86 96
10	h	197/204 (97%)	196 (100%)	1 (0%)	86 96
11	E	118/258 (46%)	118 (100%)	0	100 100
11	e	118/258 (46%)	118 (100%)	0	100 100
12	X	70/71 (99%)	70 (100%)	0	100 100
12	x	70/71 (99%)	70 (100%)	0	100 100
13	B	428/491 (87%)	427 (100%)	1 (0%)	92 98
13	b	428/491 (87%)	427 (100%)	1 (0%)	92 98
14	R	116/117 (99%)	116 (100%)	0	100 100
14	r	116/117 (99%)	116 (100%)	0	100 100
15	P	91/113 (80%)	91 (100%)	0	100 100
15	p	91/113 (80%)	91 (100%)	0	100 100
16	V	86/87 (99%)	86 (100%)	0	100 100
16	v	86/87 (99%)	86 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	L	177/178 (99%)	177 (100%)	0	100	100
17	l	177/178 (99%)	177 (100%)	0	100	100
18	C	107/338 (32%)	107 (100%)	0	100	100
18	c	107/338 (32%)	107 (100%)	0	100	100
19	D	218/259 (84%)	218 (100%)	0	100	100
19	d	218/259 (84%)	217 (100%)	1 (0%)	86	96
20	M	77/156 (49%)	77 (100%)	0	100	100
20	m	77/156 (49%)	77 (100%)	0	100	100
21	N	138/144 (96%)	137 (99%)	1 (1%)	81	94
21	n	138/144 (96%)	137 (99%)	1 (1%)	81	94
22	F	155/218 (71%)	155 (100%)	0	100	100
22	f	155/218 (71%)	155 (100%)	0	100	100
23	W	84/89 (94%)	83 (99%)	1 (1%)	67	89
23	w	84/89 (94%)	83 (99%)	1 (1%)	67	89
24	A	392/447 (88%)	391 (100%)	1 (0%)	91	97
24	a	392/447 (88%)	390 (100%)	2 (0%)	86	96
25	i1	37/125 (30%)	37 (100%)	0	100	100
25	i2	37/125 (30%)	37 (100%)	0	100	100
26	A1	421/454 (93%)	421 (100%)	0	100	100
26	A2	421/454 (93%)	421 (100%)	0	100	100
26	C1	415/454 (91%)	415 (100%)	0	100	100
26	C2	415/454 (91%)	415 (100%)	0	100	100
26	E1	416/454 (92%)	416 (100%)	0	100	100
26	E2	416/454 (92%)	416 (100%)	0	100	100
27	B1	390/447 (87%)	384 (98%)	6 (2%)	60	85
27	B2	390/447 (87%)	389 (100%)	1 (0%)	91	97
27	D1	388/447 (87%)	388 (100%)	0	100	100
27	D2	388/447 (87%)	387 (100%)	1 (0%)	91	97
27	F1	388/447 (87%)	383 (99%)	5 (1%)	65	88
27	F2	388/447 (87%)	386 (100%)	2 (0%)	86	96
28	g1	228/257 (89%)	228 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	g2	228/257 (89%)	228 (100%)	0	100	100
29	d1	118/144 (82%)	118 (100%)	0	100	100
29	d2	118/144 (82%)	118 (100%)	0	100	100
30	e1	57/61 (93%)	57 (100%)	0	100	100
30	e2	57/61 (93%)	57 (100%)	0	100	100
31	G1	154/212 (73%)	153 (99%)	1 (1%)	84	95
31	G2	154/212 (73%)	153 (99%)	1 (1%)	84	95
32	H1	52/133 (39%)	48 (92%)	4 (8%)	10	31
32	H2	52/133 (39%)	52 (100%)	0	100	100
32	I1	52/133 (39%)	50 (96%)	2 (4%)	28	63
32	I2	52/133 (39%)	51 (98%)	1 (2%)	52	81
32	J1	52/133 (39%)	52 (100%)	0	100	100
32	J2	52/133 (39%)	52 (100%)	0	100	100
32	K1	52/133 (39%)	51 (98%)	1 (2%)	52	81
32	K2	52/133 (39%)	52 (100%)	0	100	100
32	L1	52/133 (39%)	51 (98%)	1 (2%)	52	81
32	L2	52/133 (39%)	50 (96%)	2 (4%)	28	63
32	M1	52/133 (39%)	51 (98%)	1 (2%)	52	81
32	M2	52/133 (39%)	52 (100%)	0	100	100
32	N1	52/133 (39%)	52 (100%)	0	100	100
32	N2	52/133 (39%)	52 (100%)	0	100	100
32	O1	52/133 (39%)	52 (100%)	0	100	100
32	O2	52/133 (39%)	52 (100%)	0	100	100
32	P1	52/133 (39%)	52 (100%)	0	100	100
32	P2	52/133 (39%)	52 (100%)	0	100	100
32	Q1	52/133 (39%)	51 (98%)	1 (2%)	52	81
32	Q2	52/133 (39%)	52 (100%)	0	100	100
All	All	13790/18698 (74%)	13746 (100%)	44 (0%)	90	97

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	F1	528	CYS

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Mol	Chain	Res	Type
32	H1	119	SER
27	F1	536	PHE
27	F1	542	LEU
32	H1	131	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
32	N2	115	GLN
27	B1	80	ASN
26	C1	490	ASN
27	B1	99	GLN
24	A	321	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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)

54 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
38	ADP	B2	601	-	24,29,29	3.67	9 (37%)	29,45,45	3.70	8 (27%)
35	CDL	B	601	-	99,99,99	0.87	7 (7%)	105,111,111	1.00	3 (2%)
38	ADP	D2	601	-	24,29,29	3.68	9 (37%)	29,45,45	3.46	6 (20%)
34	LMT	D	401	-	36,36,36	1.15	2 (5%)	47,47,47	0.86	1 (2%)
34	LMT	D	403	-	36,36,36	1.11	2 (5%)	47,47,47	0.89	1 (2%)
35	CDL	D	402	-	99,99,99	0.88	8 (8%)	105,111,111	1.02	3 (2%)
35	CDL	v	202	-	99,99,99	0.88	7 (7%)	105,111,111	0.98	4 (3%)
35	CDL	E	401	-	99,99,99	0.88	8 (8%)	105,111,111	1.01	4 (3%)
36	PEE	C	403	-	50,50,50	1.15	5 (10%)	53,55,55	1.00	2 (3%)
34	LMT	x	101	-	36,36,36	1.16	2 (5%)	47,47,47	1.03	3 (6%)
37	ATP	A1	601	-	26,33,33	4.81	7 (26%)	31,52,52	2.43	8 (25%)
36	PEE	J	301	-	50,50,50	1.12	6 (12%)	53,55,55	1.07	3 (5%)
38	ADP	B1	601	-	24,29,29	3.67	9 (37%)	29,45,45	3.44	6 (20%)
34	LMT	C	402	-	36,36,36	1.10	2 (5%)	47,47,47	1.00	1 (2%)
35	CDL	O	203	-	99,99,99	0.88	7 (7%)	105,111,111	1.00	5 (4%)
33	PC1	O	201	-	53,53,53	0.96	3 (5%)	59,61,61	1.05	3 (5%)
35	CDL	C	401	-	99,99,99	0.88	6 (6%)	105,111,111	0.85	3 (2%)
33	PC1	O	204	5	53,53,53	0.95	4 (7%)	59,61,61	1.04	2 (3%)
35	CDL	U	201	-	99,99,99	0.88	7 (7%)	105,111,111	1.00	4 (3%)
36	PEE	c	403	-	50,50,50	1.15	5 (10%)	53,55,55	1.01	2 (3%)
34	LMT	o	202	-	36,36,36	1.12	2 (5%)	47,47,47	0.91	1 (2%)
36	PEE	j	302	-	50,50,50	1.14	6 (12%)	53,55,55	1.08	3 (5%)
33	PC1	o	201	-	53,53,53	0.96	4 (7%)	59,61,61	1.04	3 (5%)
34	LMT	O	202	-	36,36,36	1.12	2 (5%)	47,47,47	0.94	1 (2%)
35	CDL	c	401	-	99,99,99	0.88	6 (6%)	105,111,111	0.91	4 (3%)
34	LMT	d	401	-	36,36,36	1.15	2 (5%)	47,47,47	0.90	1 (2%)
35	CDL	d	402	-	99,99,99	0.88	8 (8%)	105,111,111	1.02	3 (2%)
35	CDL	h	302	-	99,99,99	0.87	6 (6%)	105,111,111	0.98	4 (3%)
36	PEE	j	301	-	50,50,50	1.12	6 (12%)	53,55,55	1.08	3 (5%)
35	CDL	H	302	-	99,99,99	0.87	7 (7%)	105,111,111	0.98	4 (3%)
34	LMT	c	402	-	36,36,36	1.10	2 (5%)	47,47,47	1.01	1 (2%)
35	CDL	b	602	-	99,99,99	0.88	8 (8%)	105,111,111	0.98	4 (3%)
35	CDL	B	602	-	99,99,99	0.88	8 (8%)	105,111,111	0.98	4 (3%)
34	LMT	c	404	-	36,36,36	1.11	2 (5%)	47,47,47	1.07	2 (4%)
35	CDL	o	203	-	99,99,99	0.88	7 (7%)	105,111,111	1.00	5 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	CDL	b	601	-	99,99,99	0.87	8 (8%)	105,111,111	1.00	4 (3%)
34	LMT	d	403	-	36,36,36	1.12	2 (5%)	47,47,47	0.85	1 (2%)
37	ATP	C1	601	-	26,33,33	4.78	9 (34%)	31,52,52	2.52	9 (29%)
38	ADP	D1	601	-	24,29,29	3.69	8 (33%)	29,45,45	3.58	7 (24%)
33	PC1	V	201	-	53,53,53	0.99	3 (5%)	59,61,61	0.98	2 (3%)
34	LMT	H	301	-	36,36,36	1.13	2 (5%)	47,47,47	1.03	2 (4%)
37	ATP	E2	601	-	26,33,33	4.80	8 (30%)	31,52,52	2.47	9 (29%)
33	PC1	o	204	5	53,53,53	0.96	4 (7%)	59,61,61	1.04	2 (3%)
35	CDL	e	401	-	99,99,99	0.88	8 (8%)	105,111,111	1.01	4 (3%)
35	CDL	u	201	-	99,99,99	0.88	7 (7%)	105,111,111	1.01	4 (3%)
37	ATP	C2	601	-	26,33,33	4.82	8 (30%)	31,52,52	2.47	8 (25%)
35	CDL	V	202	-	99,99,99	0.88	7 (7%)	105,111,111	0.97	4 (3%)
37	ATP	E1	601	-	26,33,33	4.81	8 (30%)	31,52,52	2.49	8 (25%)
33	PC1	v	201	-	53,53,53	0.99	3 (5%)	59,61,61	0.99	2 (3%)
36	PEE	J	302	-	50,50,50	1.14	6 (12%)	53,55,55	1.15	3 (5%)
34	LMT	X	101	-	36,36,36	1.16	2 (5%)	47,47,47	1.03	3 (6%)
37	ATP	A2	601	-	26,33,33	4.80	7 (26%)	31,52,52	2.49	8 (25%)
34	LMT	h	301	-	36,36,36	1.13	2 (5%)	47,47,47	1.03	2 (4%)
34	LMT	C	404	-	36,36,36	1.11	2 (5%)	47,47,47	1.14	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	ADP	B2	601	-	-	4/12/32/32	0/3/3/3
35	CDL	B	601	-	-	39/110/110/110	-
38	ADP	D2	601	-	-	2/12/32/32	0/3/3/3
34	LMT	D	401	-	-	11/21/61/61	0/2/2/2
34	LMT	D	403	-	-	5/21/61/61	0/2/2/2
35	CDL	D	402	-	-	46/110/110/110	-
35	CDL	v	202	-	-	40/110/110/110	-
35	CDL	E	401	-	-	49/110/110/110	-
36	PEE	C	403	-	-	22/54/54/54	-
34	LMT	x	101	-	-	12/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	ATP	A1	601	-	-	0/18/38/38	0/3/3/3
36	PEE	J	301	-	-	22/54/54/54	-
38	ADP	B1	601	-	-	4/12/32/32	0/3/3/3
34	LMT	C	402	-	-	8/21/61/61	0/2/2/2
35	CDL	O	203	-	-	40/110/110/110	-
33	PC1	O	201	-	-	22/57/57/57	-
35	CDL	C	401	-	-	60/110/110/110	-
33	PC1	O	204	5	-	25/57/57/57	-
35	CDL	U	201	-	-	38/110/110/110	-
36	PEE	c	403	-	-	22/54/54/54	-
34	LMT	o	202	-	-	4/21/61/61	0/2/2/2
36	PEE	j	302	-	-	20/54/54/54	-
33	PC1	o	201	-	-	23/57/57/57	-
34	LMT	O	202	-	-	4/21/61/61	0/2/2/2
35	CDL	c	401	-	-	64/110/110/110	-
34	LMT	d	401	-	-	9/21/61/61	0/2/2/2
35	CDL	d	402	-	-	45/110/110/110	-
35	CDL	h	302	-	-	45/110/110/110	-
36	PEE	j	301	-	-	22/54/54/54	-
35	CDL	H	302	-	-	45/110/110/110	-
34	LMT	c	402	-	-	8/21/61/61	0/2/2/2
35	CDL	b	602	-	-	50/110/110/110	-
35	CDL	B	602	-	-	48/110/110/110	-
34	LMT	c	404	-	-	7/21/61/61	0/2/2/2
35	CDL	o	203	-	-	40/110/110/110	-
35	CDL	b	601	-	-	39/110/110/110	-
34	LMT	d	403	-	-	5/21/61/61	0/2/2/2
37	ATP	C1	601	-	-	5/18/38/38	0/3/3/3
38	ADP	D1	601	-	-	0/12/32/32	0/3/3/3
33	PC1	V	201	-	-	31/57/57/57	-
34	LMT	H	301	-	-	9/21/61/61	0/2/2/2
37	ATP	E2	601	-	-	3/18/38/38	0/3/3/3
33	PC1	o	204	5	-	25/57/57/57	-
35	CDL	e	401	-	-	49/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	CDL	u	201	-	-	37/110/110/110	-
37	ATP	C2	601	-	-	4/18/38/38	0/3/3/3
35	CDL	V	202	-	-	39/110/110/110	-
37	ATP	E1	601	-	-	3/18/38/38	0/3/3/3
33	PC1	v	201	-	-	31/57/57/57	-
36	PEE	J	302	-	-	19/54/54/54	-
34	LMT	X	101	-	-	12/21/61/61	0/2/2/2
37	ATP	A2	601	-	-	0/18/38/38	0/3/3/3
34	LMT	h	301	-	-	9/21/61/61	0/2/2/2
34	LMT	C	404	-	-	7/21/61/61	0/2/2/2

The worst 5 of 295 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	C2	601	ATP	C2'-C1'	-17.47	1.27	1.53
37	A2	601	ATP	C2'-C1'	-17.41	1.27	1.53
37	A1	601	ATP	C2'-C1'	-17.40	1.27	1.53
37	E1	601	ATP	C2'-C1'	-17.34	1.27	1.53
37	E2	601	ATP	C2'-C1'	-17.33	1.27	1.53

The worst 5 of 200 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	B2	601	ADP	C1'-N9-C4	15.61	154.07	126.64
38	D1	601	ADP	C1'-N9-C4	14.69	152.45	126.64
38	D2	601	ADP	C1'-N9-C4	14.02	151.28	126.64
38	B1	601	ADP	C1'-N9-C4	13.90	151.06	126.64
37	E1	601	ATP	C5-C6-N6	7.56	131.84	120.35

There are no chirality outliers.

5 of 1232 torsion outliers are listed below:

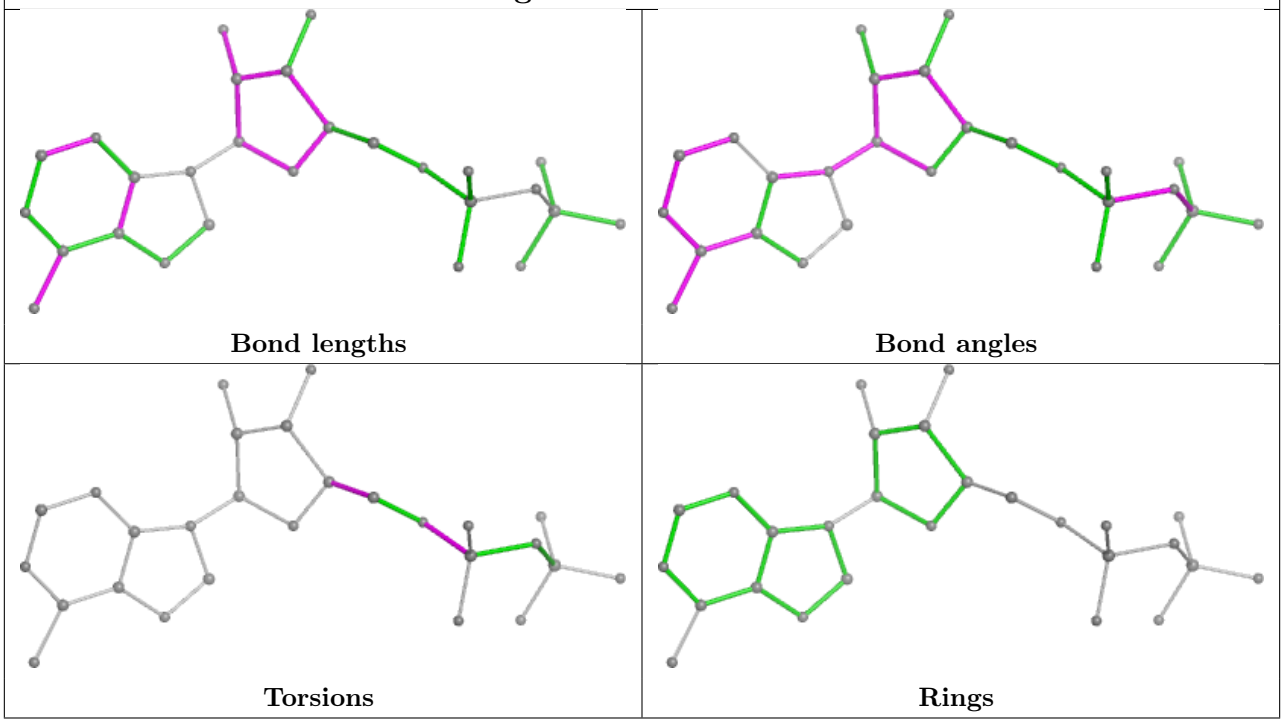
Mol	Chain	Res	Type	Atoms
33	o	201	PC1	C1-O11-P-O14
33	o	201	PC1	O13-C11-C12-N
33	o	201	PC1	C22-C21-O21-C2
33	o	204	PC1	C11-O13-P-O14
33	o	204	PC1	C22-C21-O21-C2

There are no ring outliers.

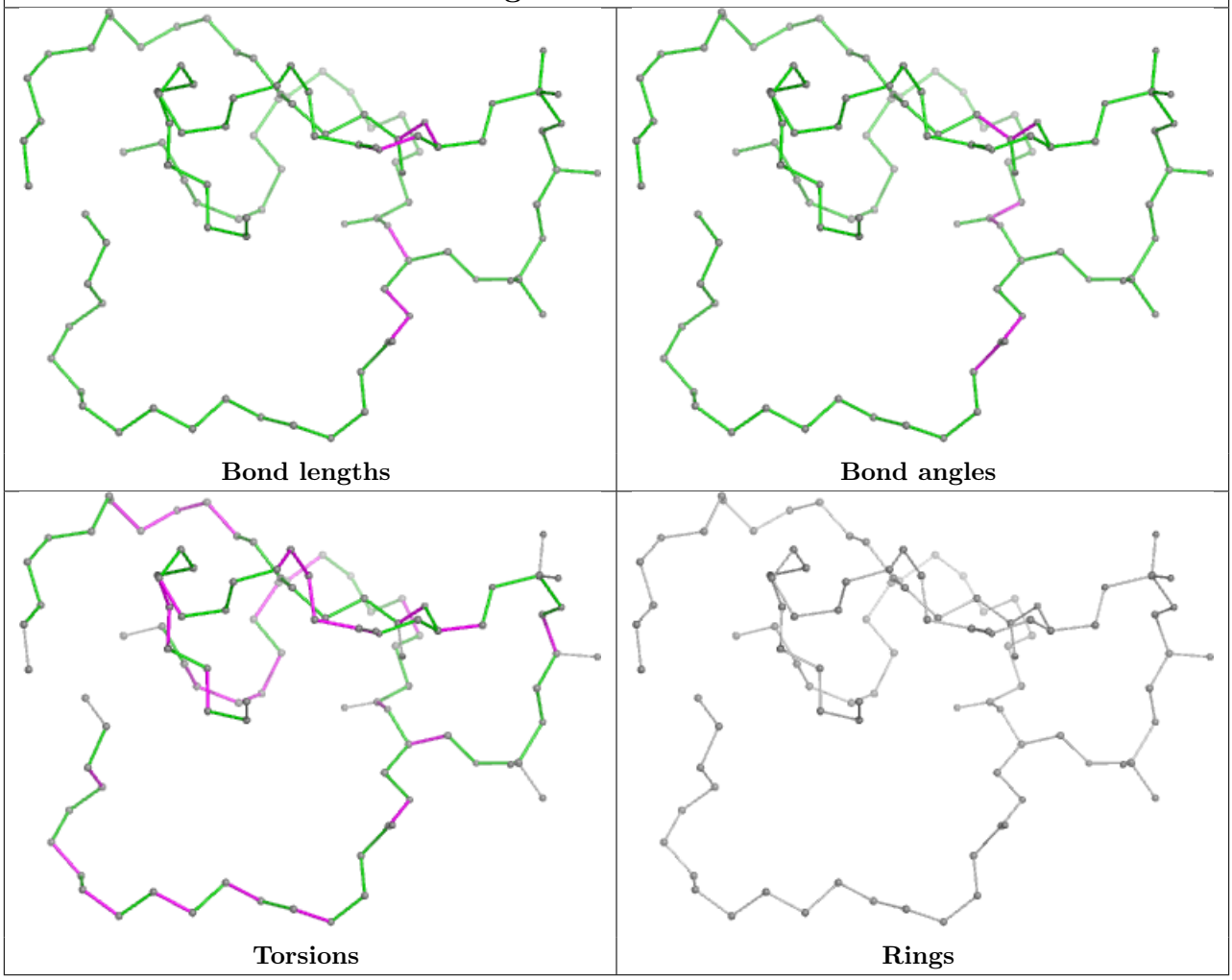
No monomer is involved in short contacts.

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

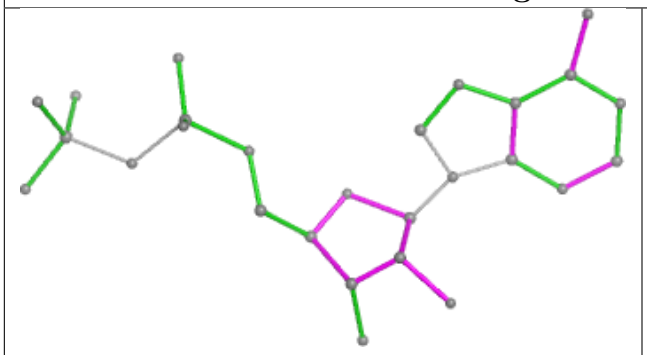
Ligand ADP B2 601



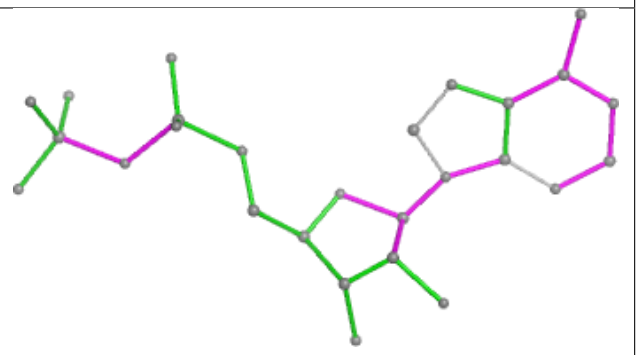
Ligand CDL B 601



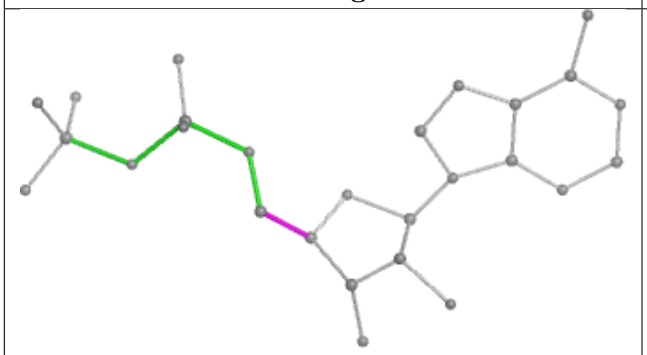
Ligand ADP D2 601



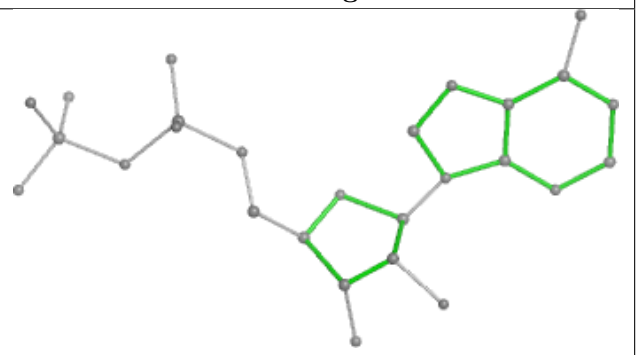
Bond lengths



Bond angles

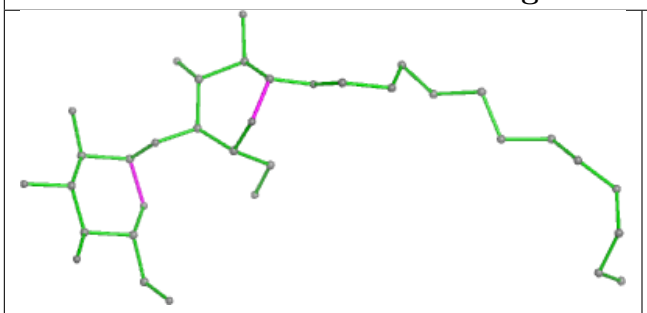


Torsions

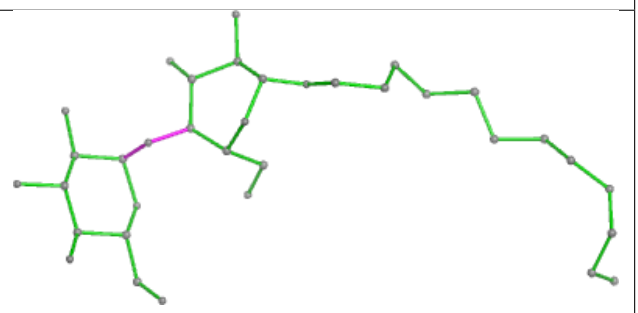


Rings

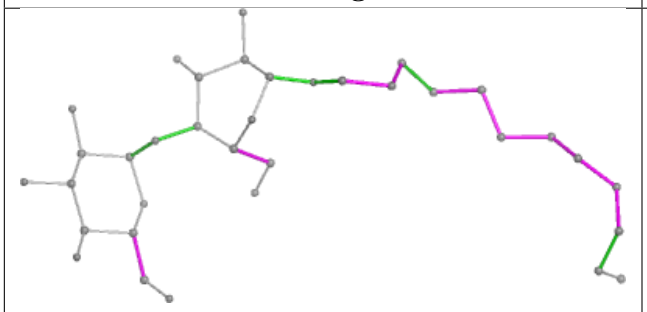
Ligand LMT D 401



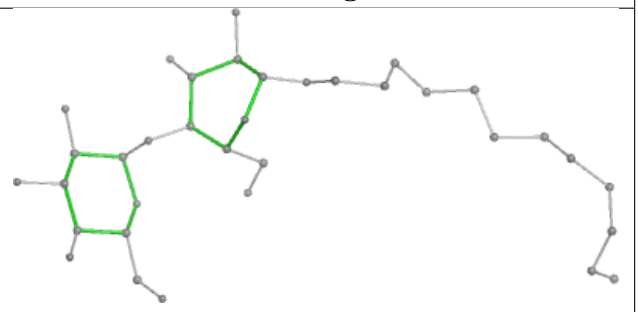
Bond lengths



Bond angles

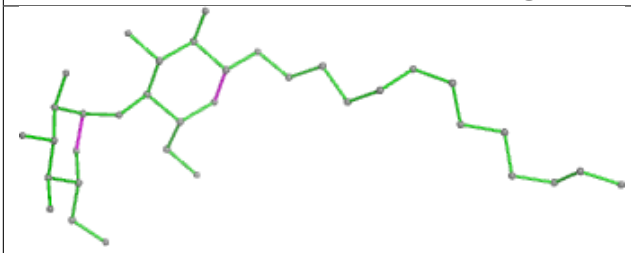


Torsions

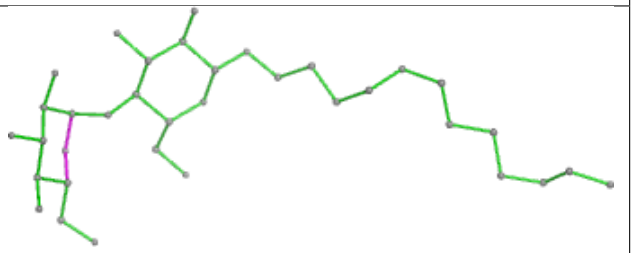


Rings

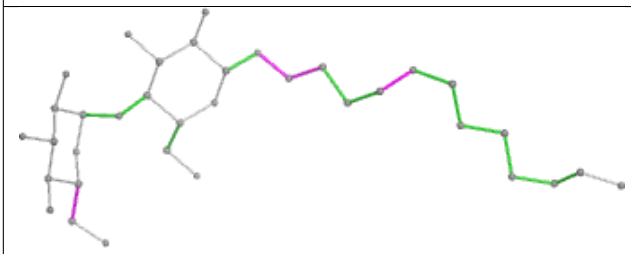
Ligand LMT D 403



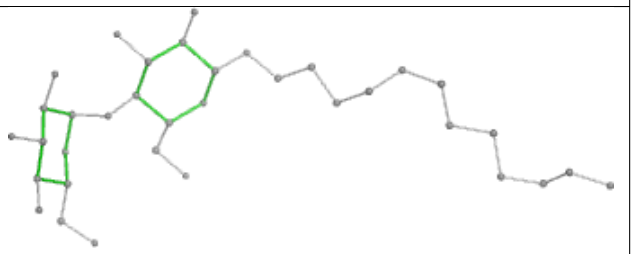
Bond lengths



Bond angles

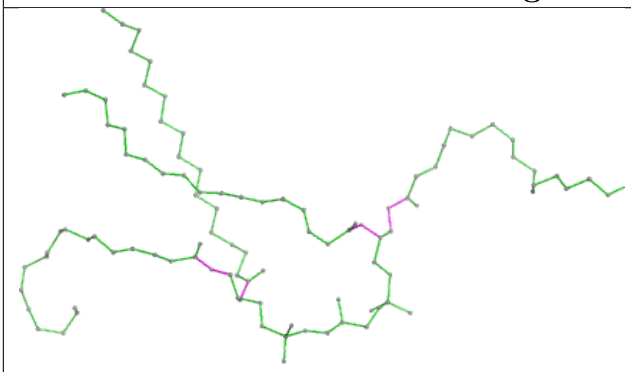


Torsions

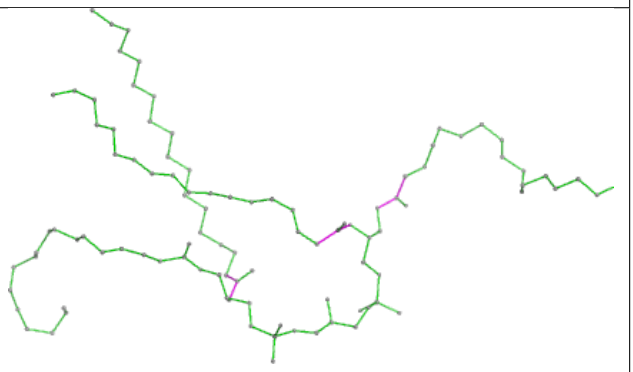


Rings

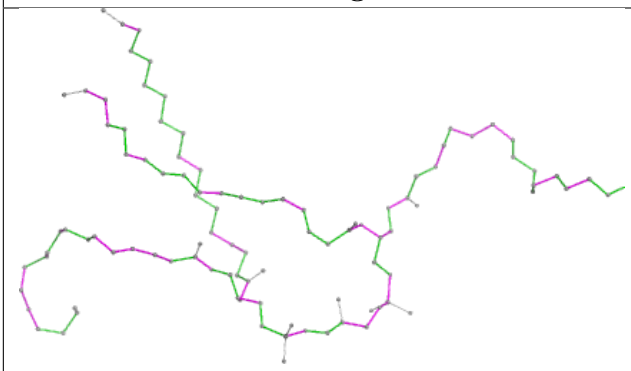
Ligand CDL D 402



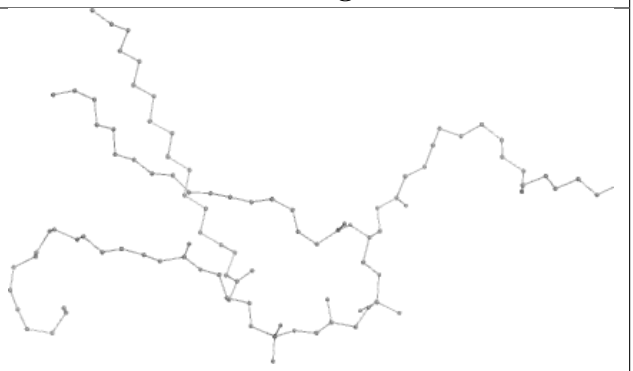
Bond lengths



Bond angles

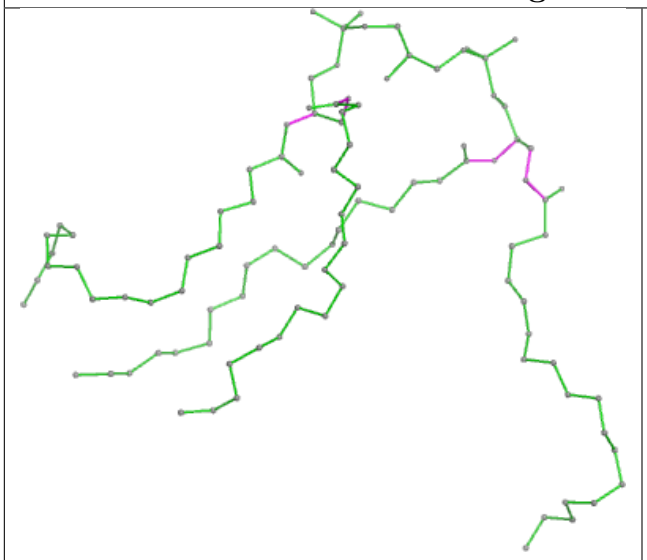


Torsions

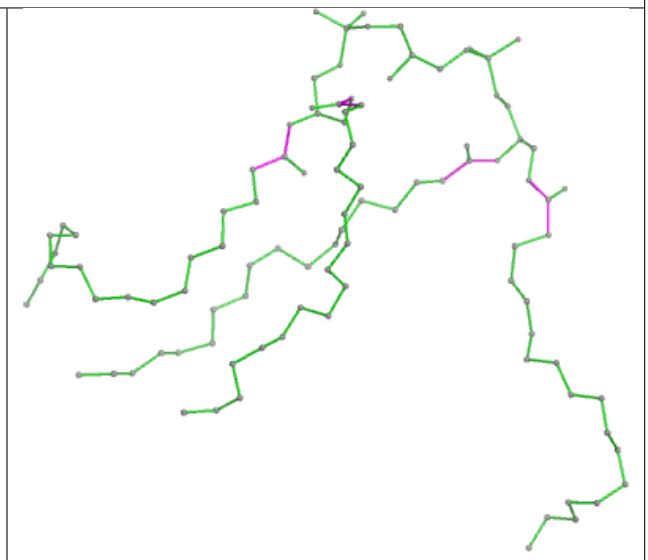


Rings

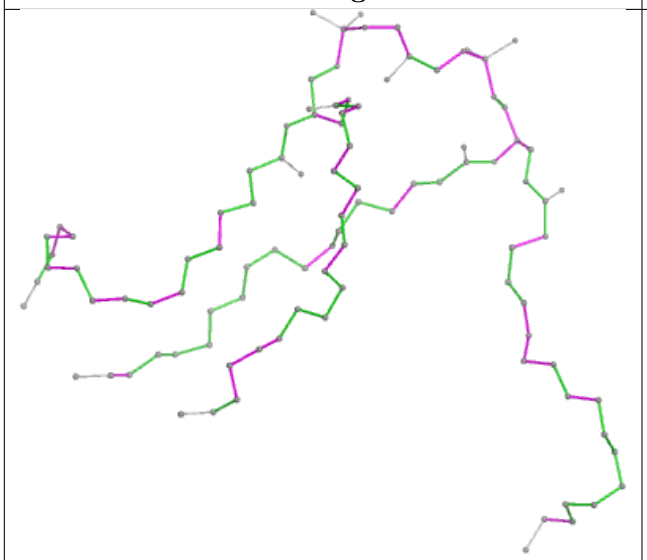
Ligand CDL v 202



Bond lengths



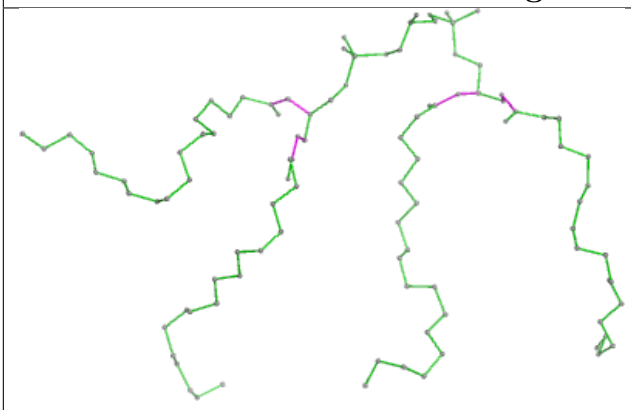
Bond angles



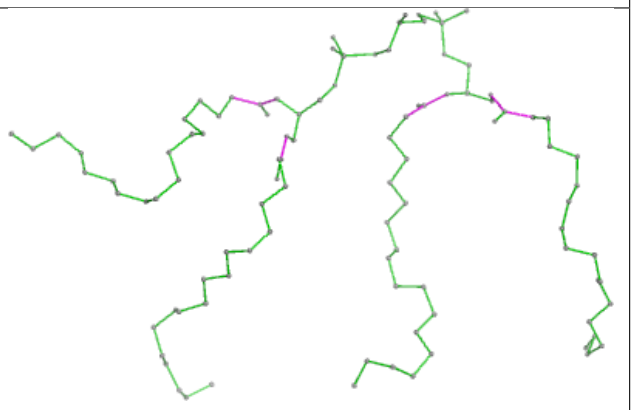
Torsions

Rings

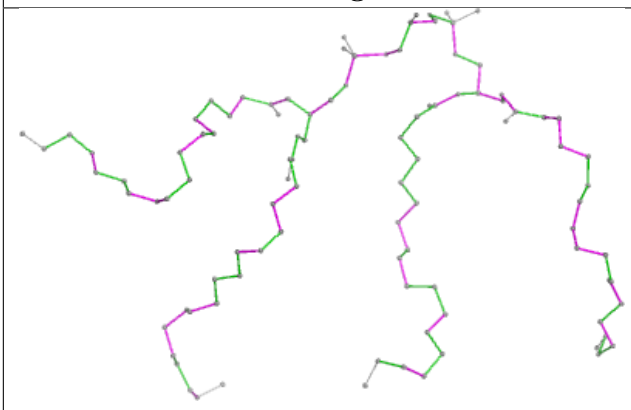
Ligand CDL E 401



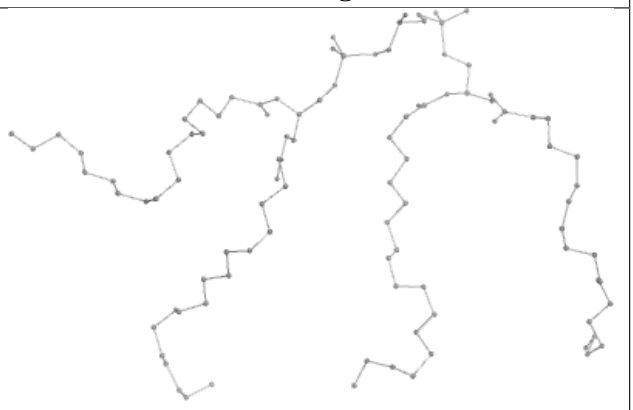
Bond lengths



Bond angles

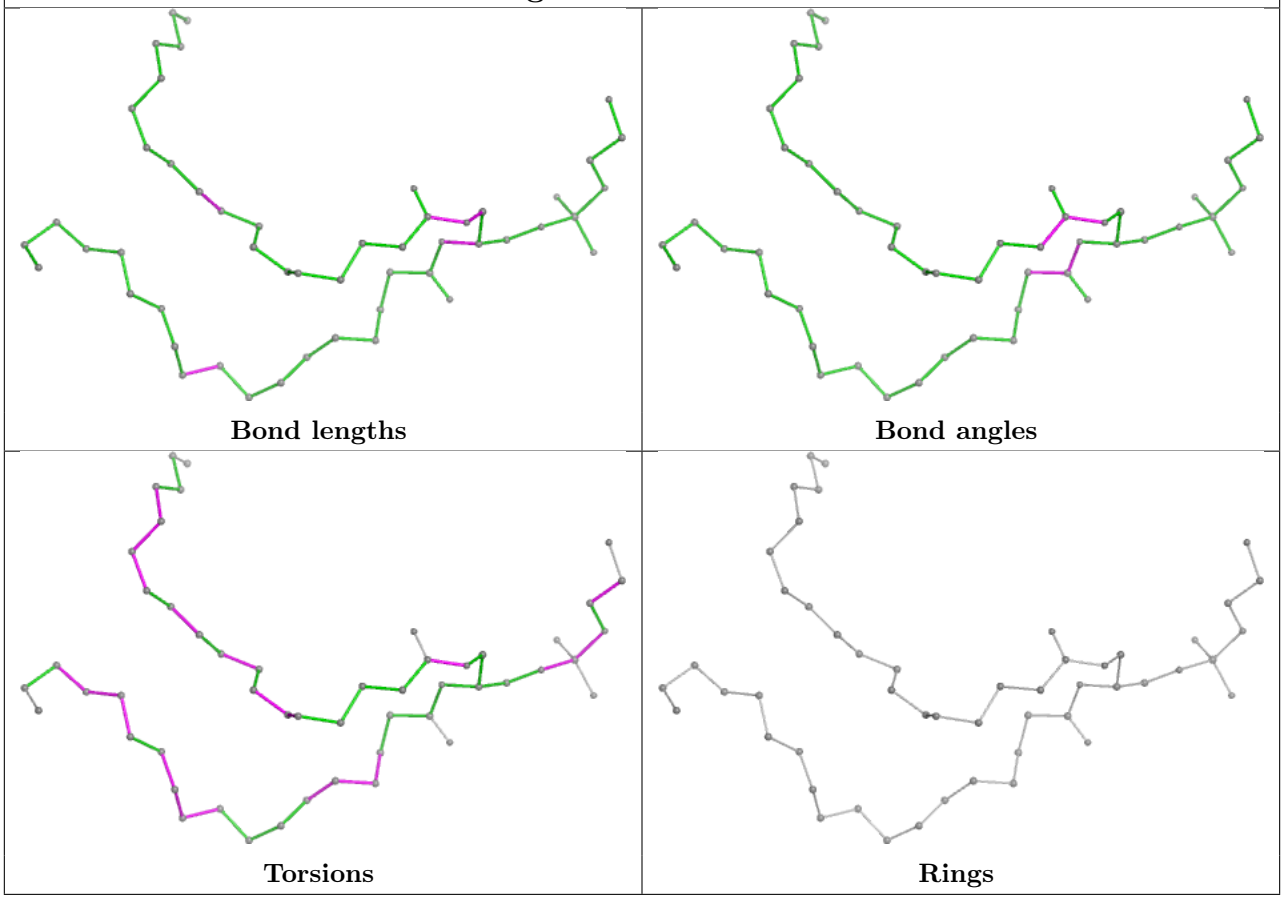


Torsions

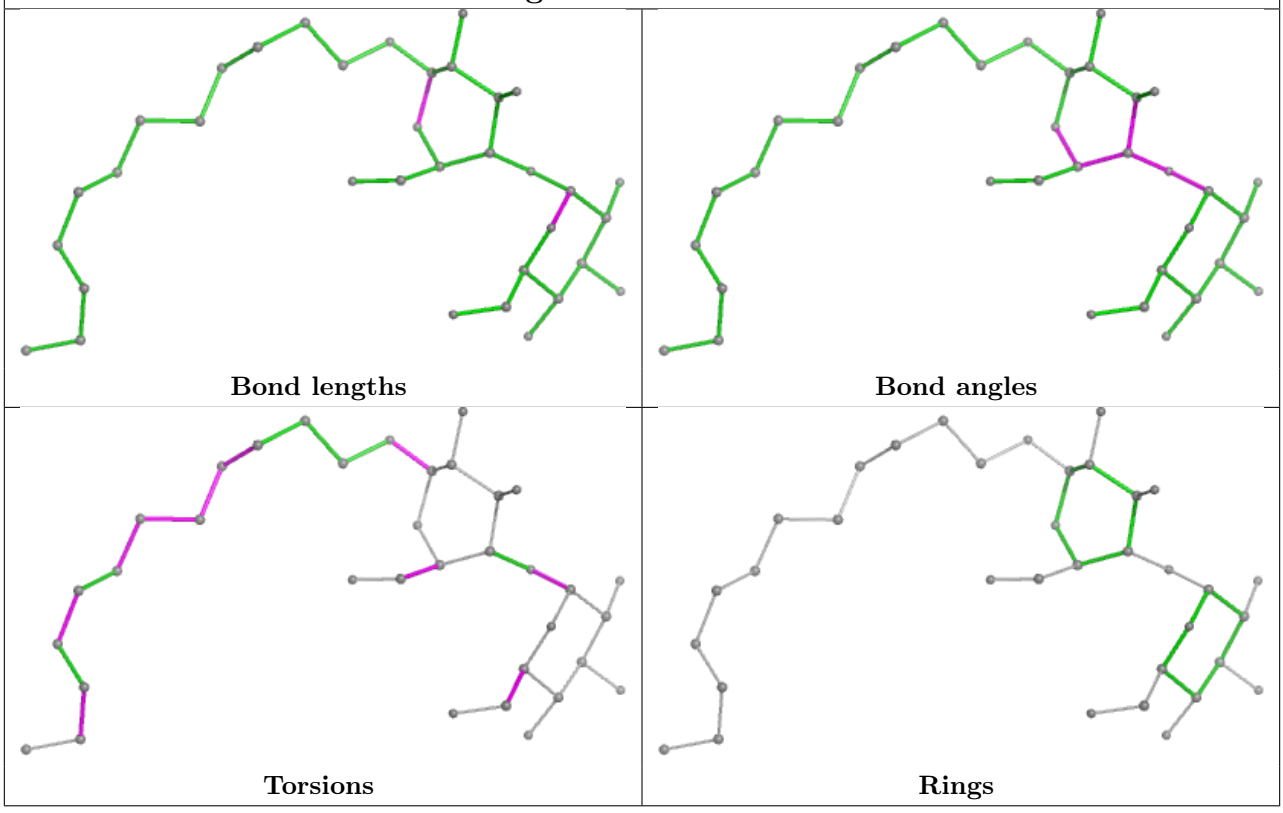


Rings

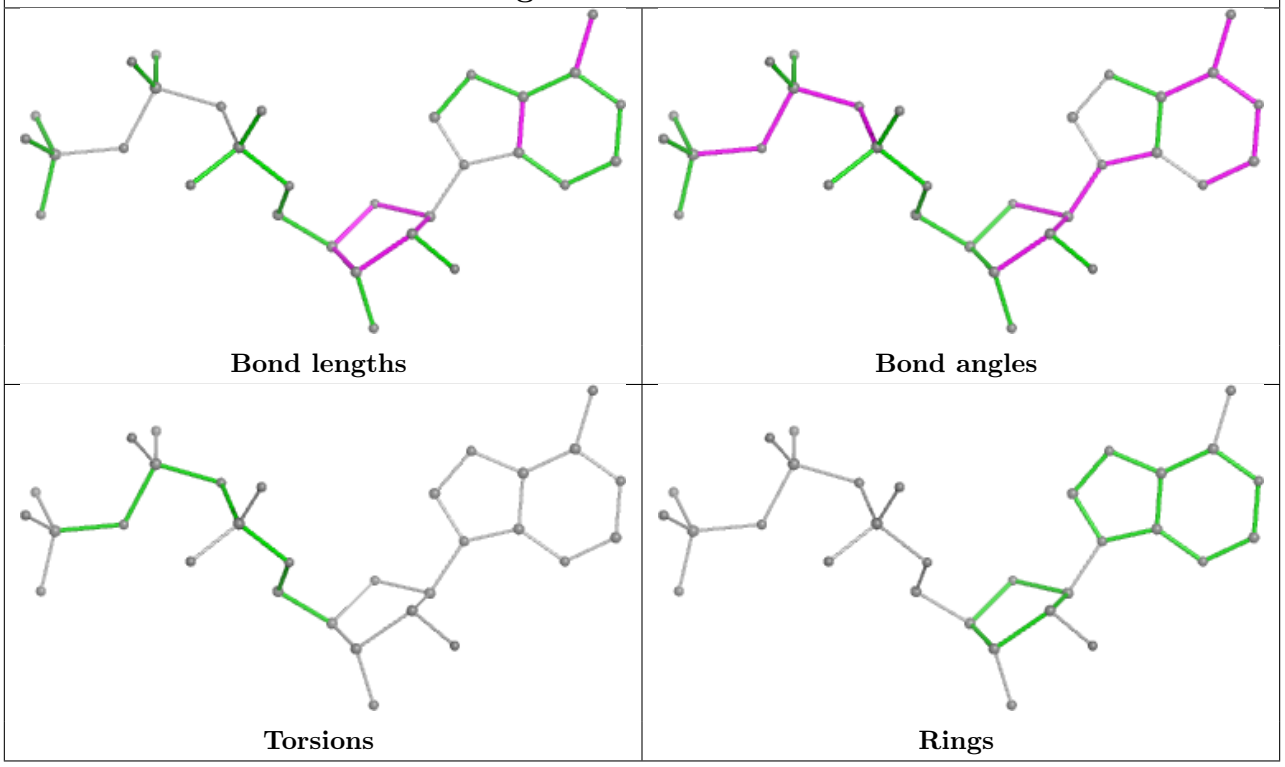
Ligand PEE C 403



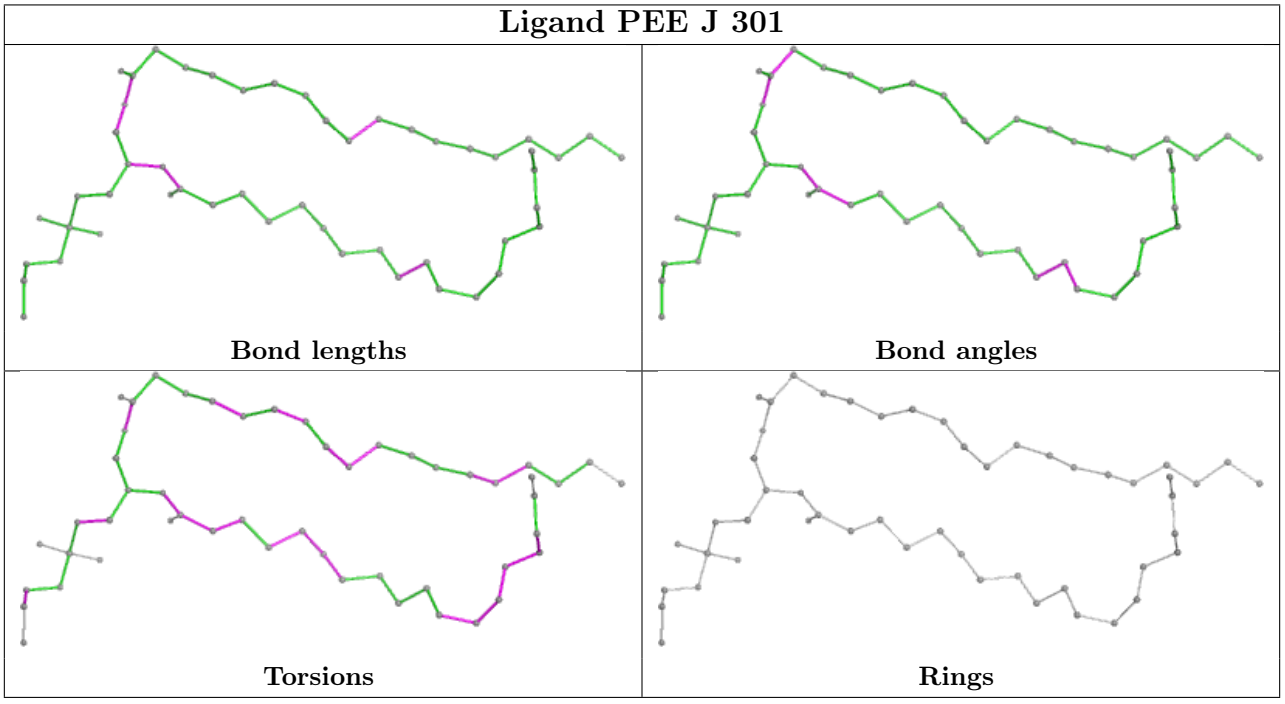
Ligand LMT x 101



Ligand ATP A1 601



Ligand PEE J 301



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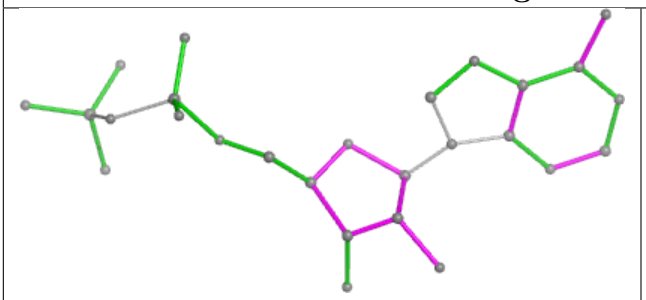

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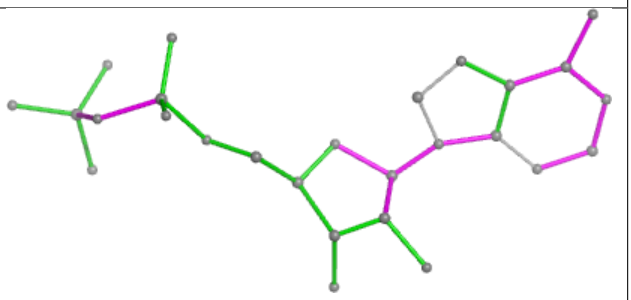
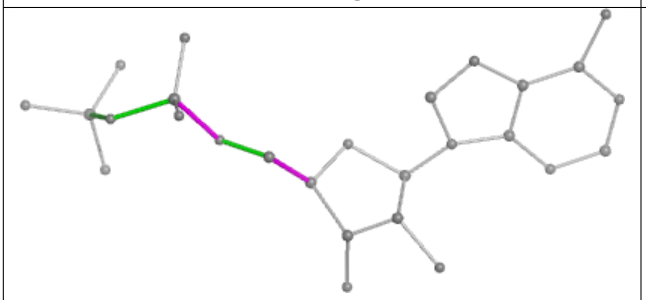
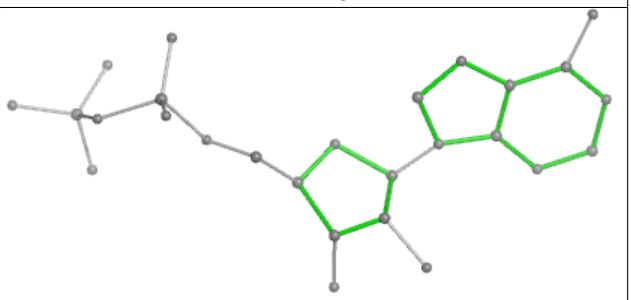


Bond angles

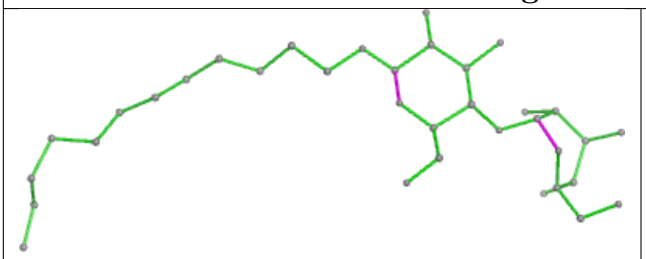


Torsions



Rings

Ligand LMT C 402



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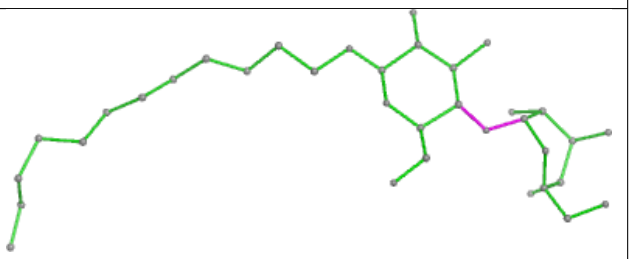
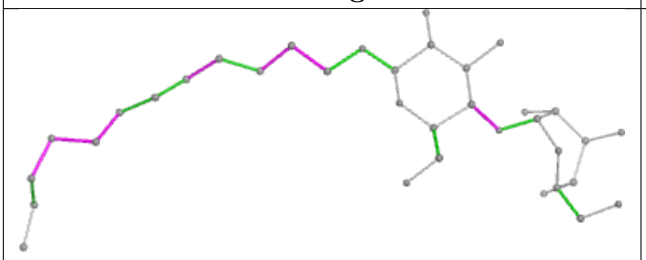


Bond angles



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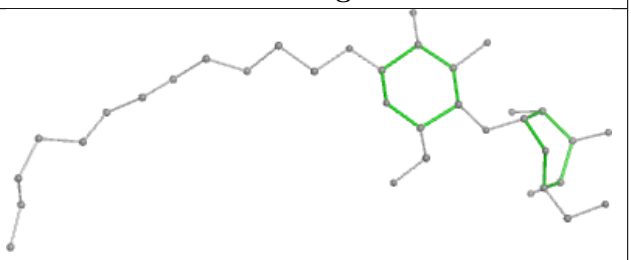
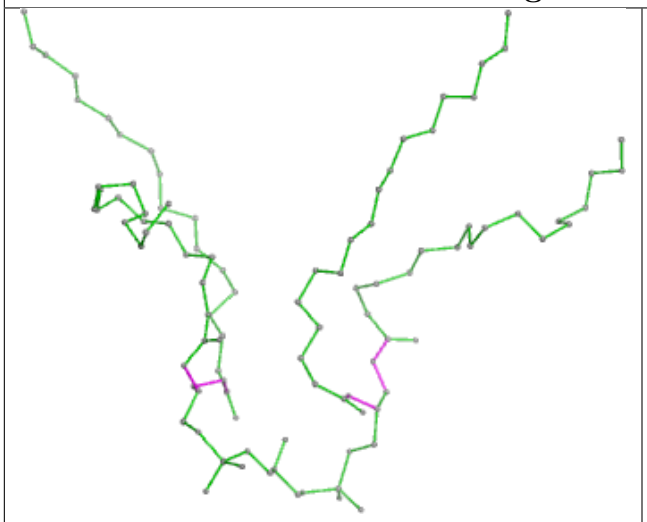


Rings

Ligand CDL O 203



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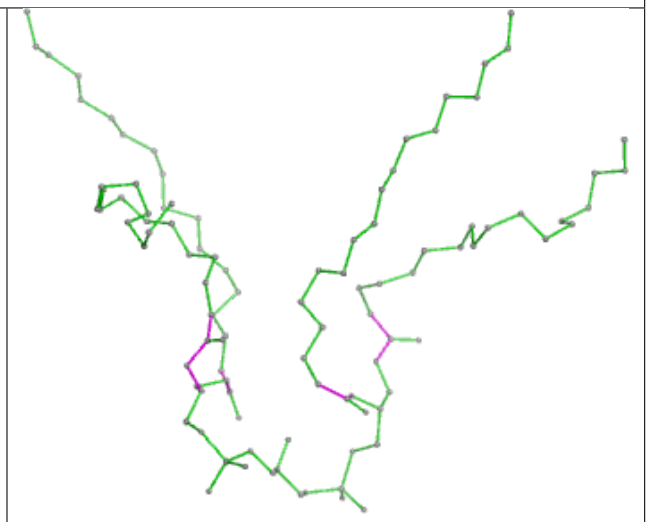
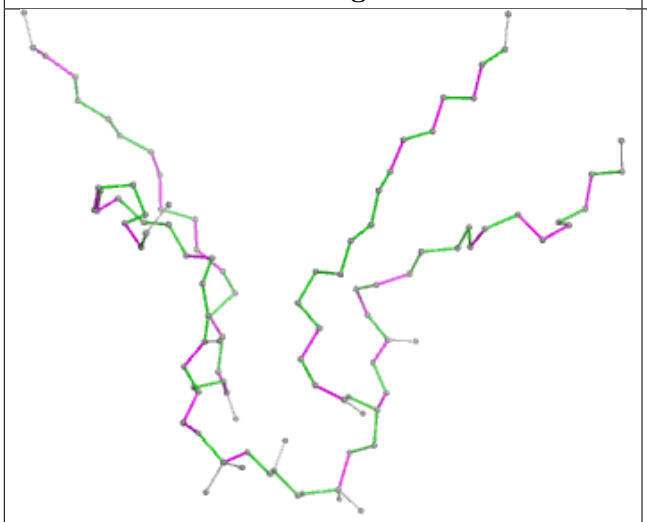


Bond angles



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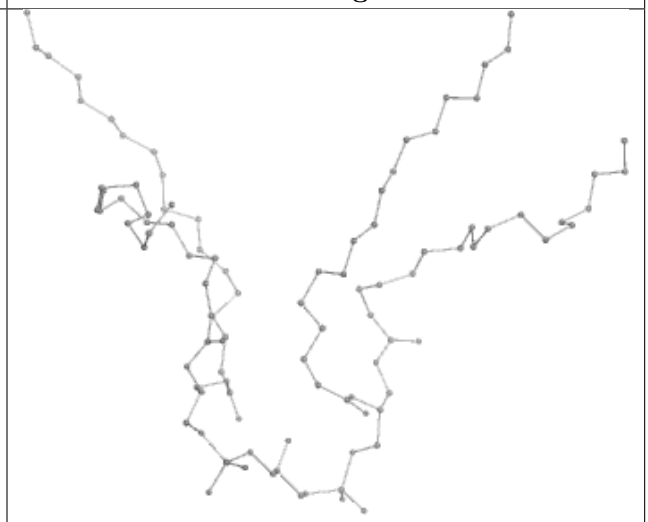
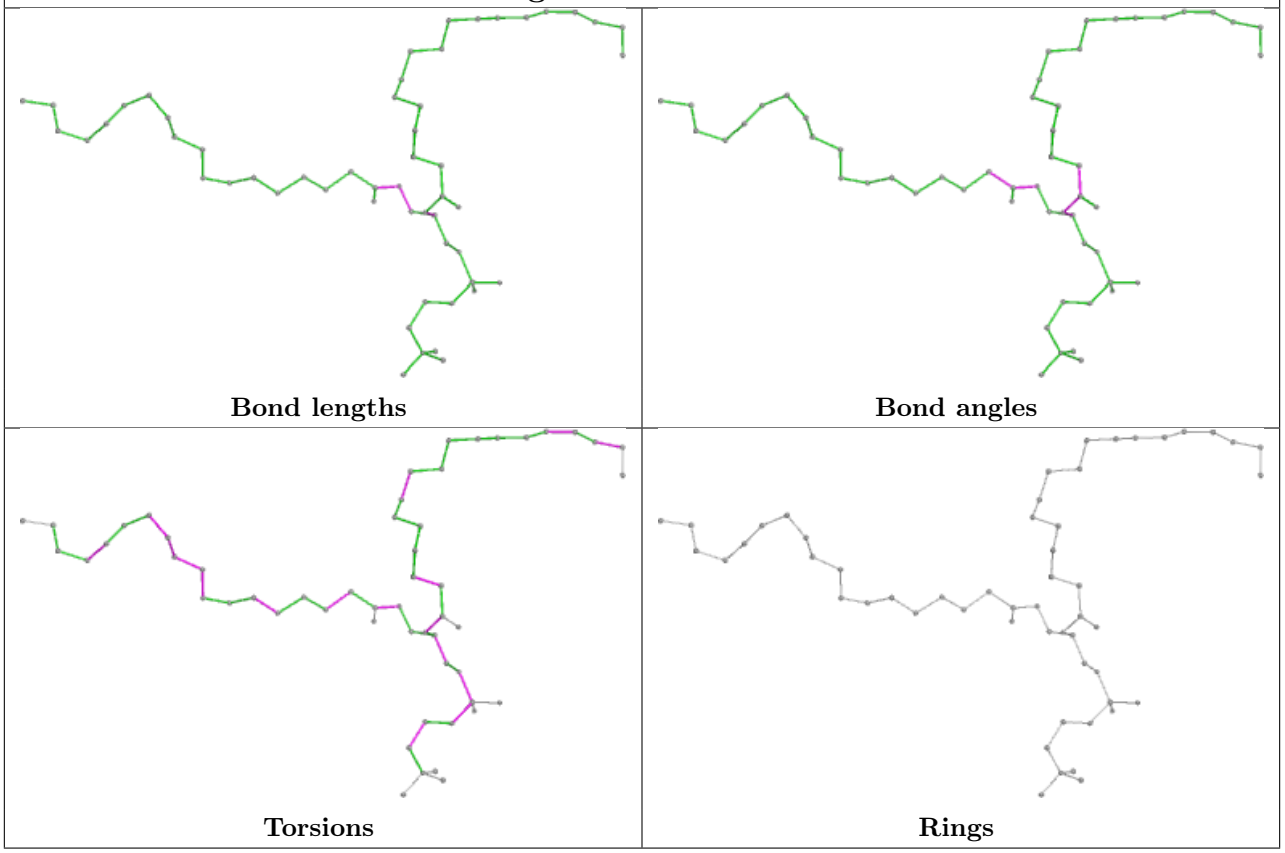


Rings

Ligand PC1 O 201



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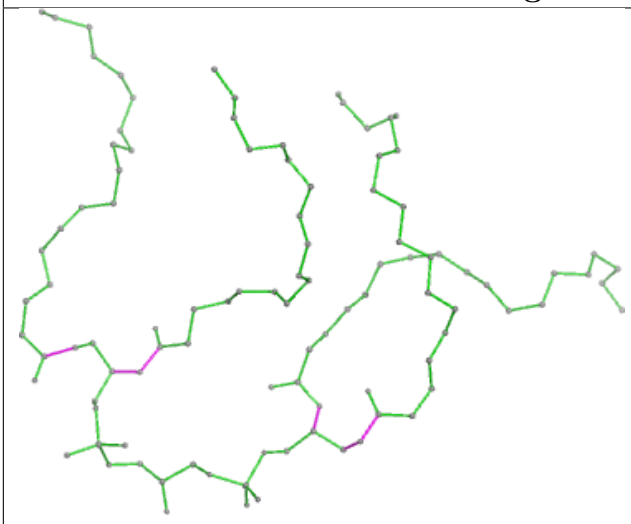

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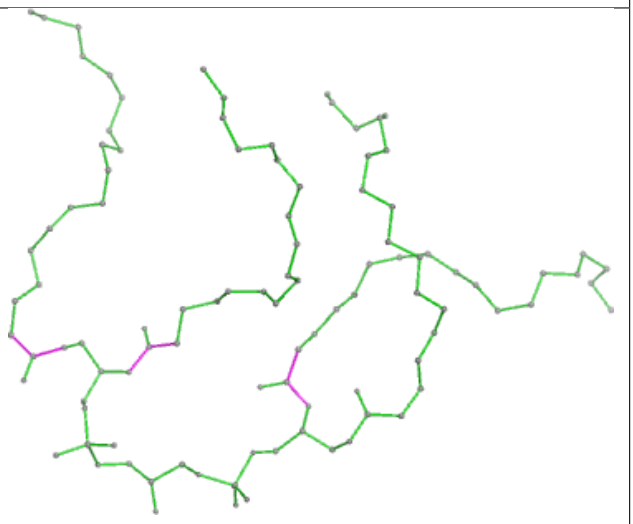
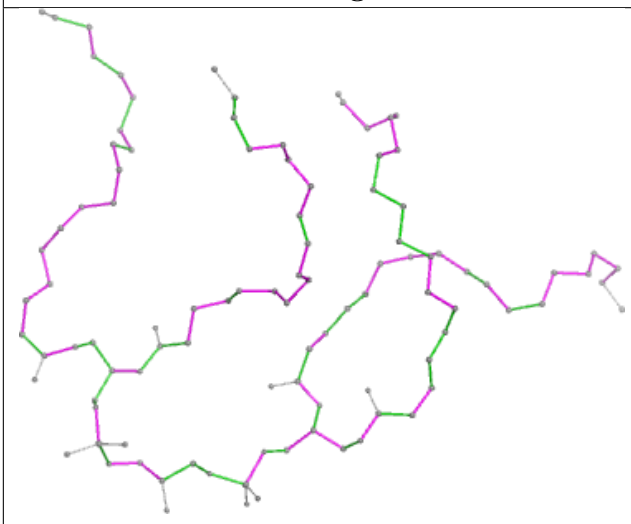


Bond angles



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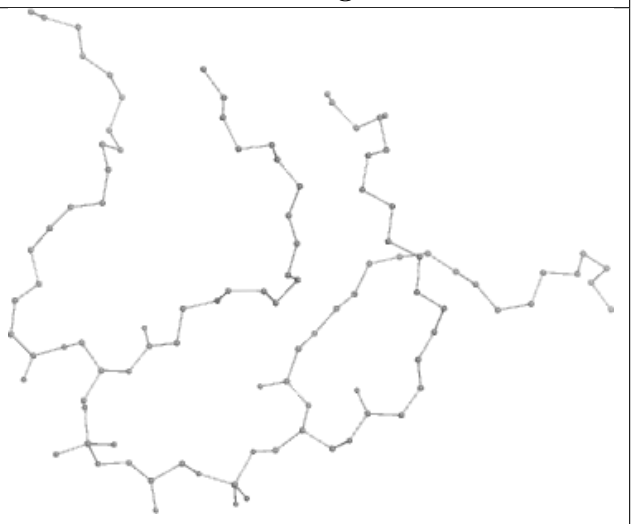
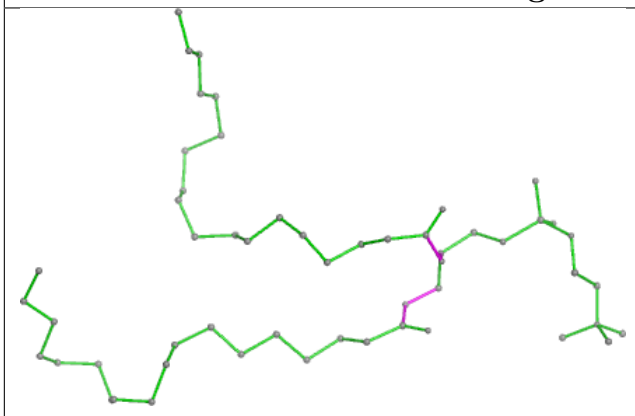


Rings

Ligand PC1 O 204



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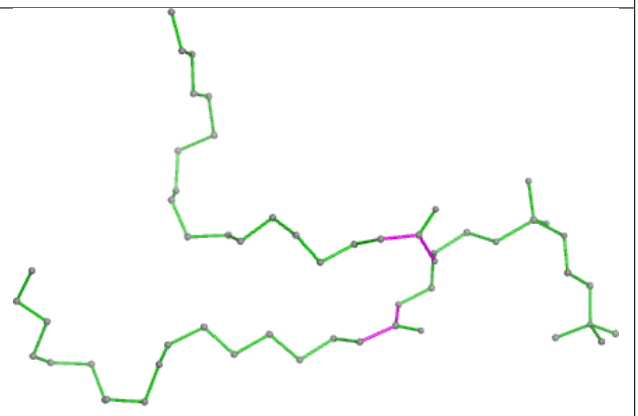
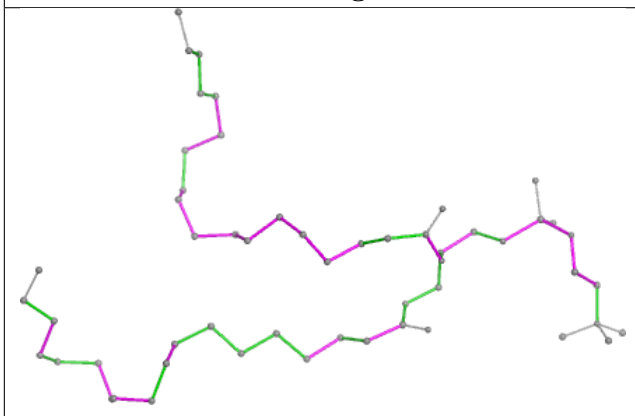


Bond angles



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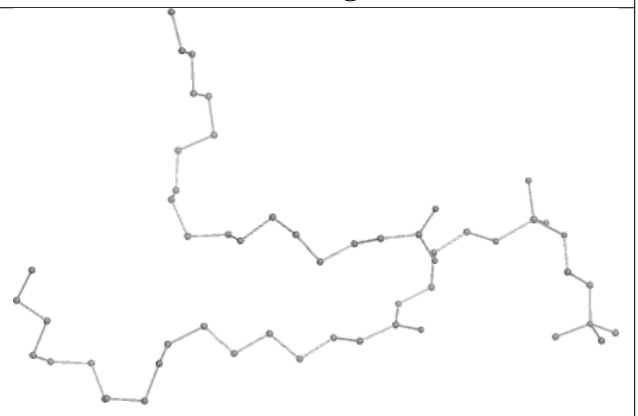
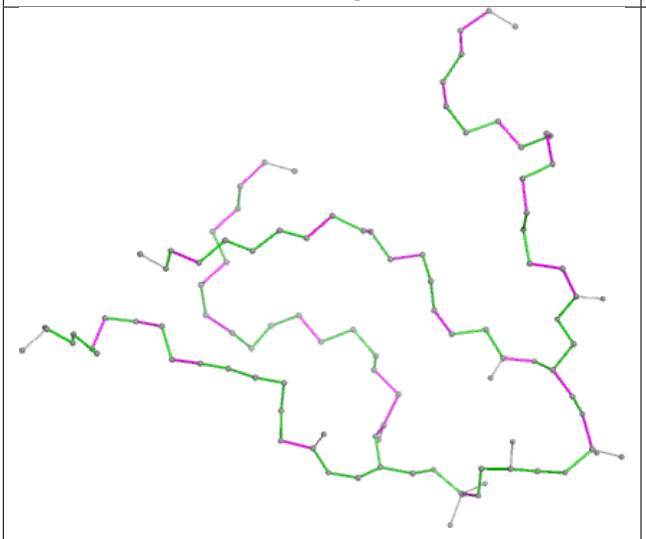


Rings

Ligand CDL U 201

Bond lengths

Bond angles



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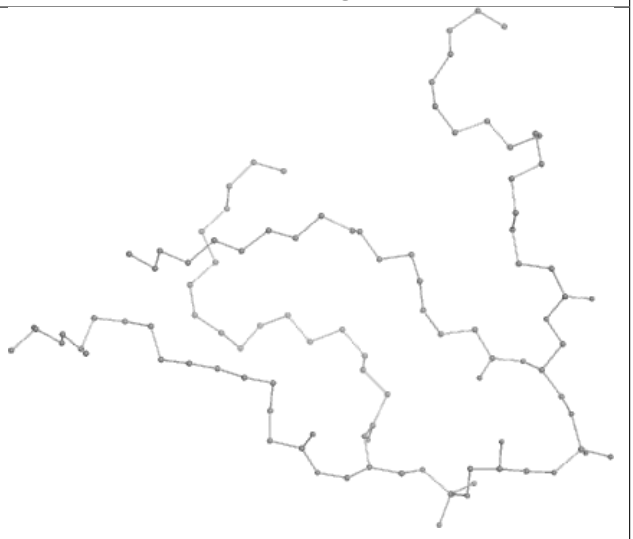
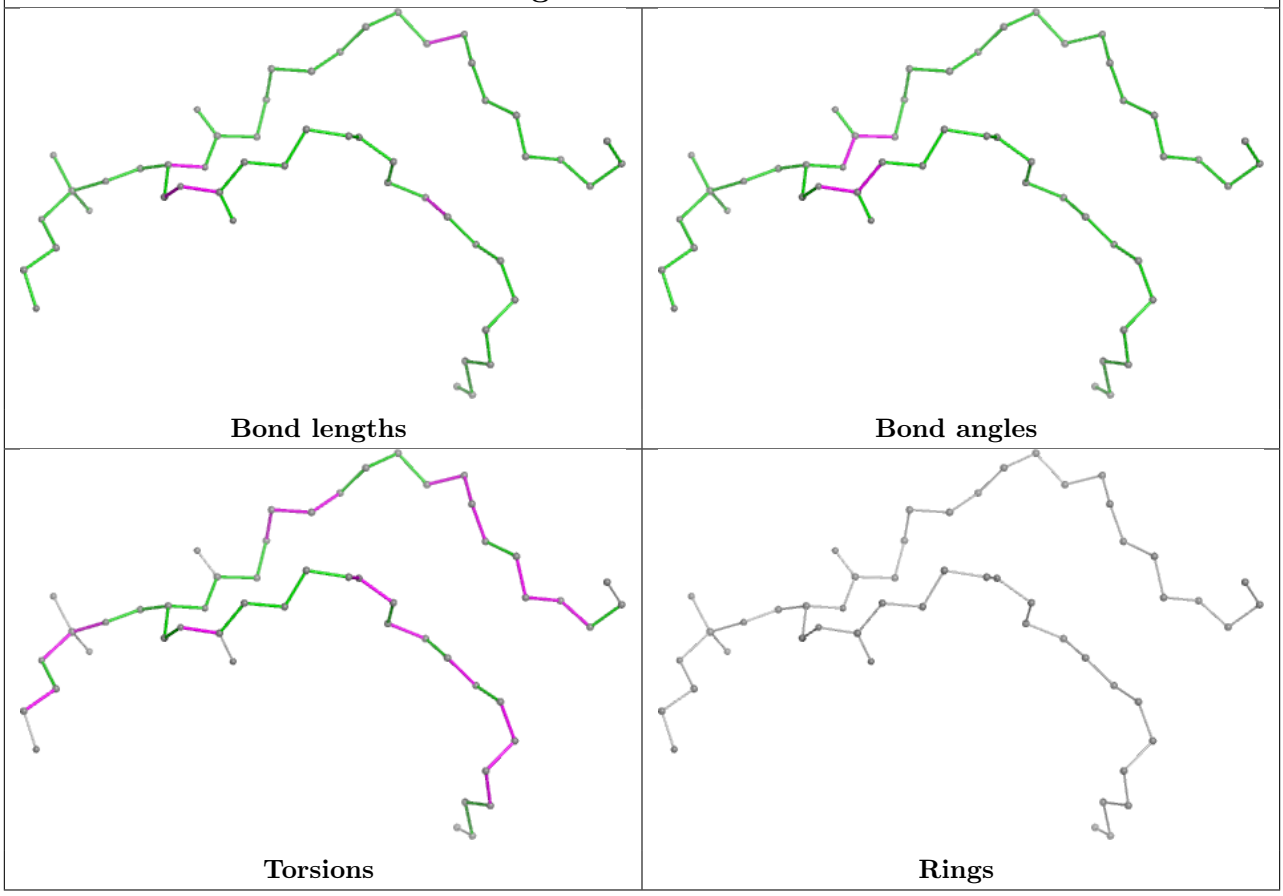
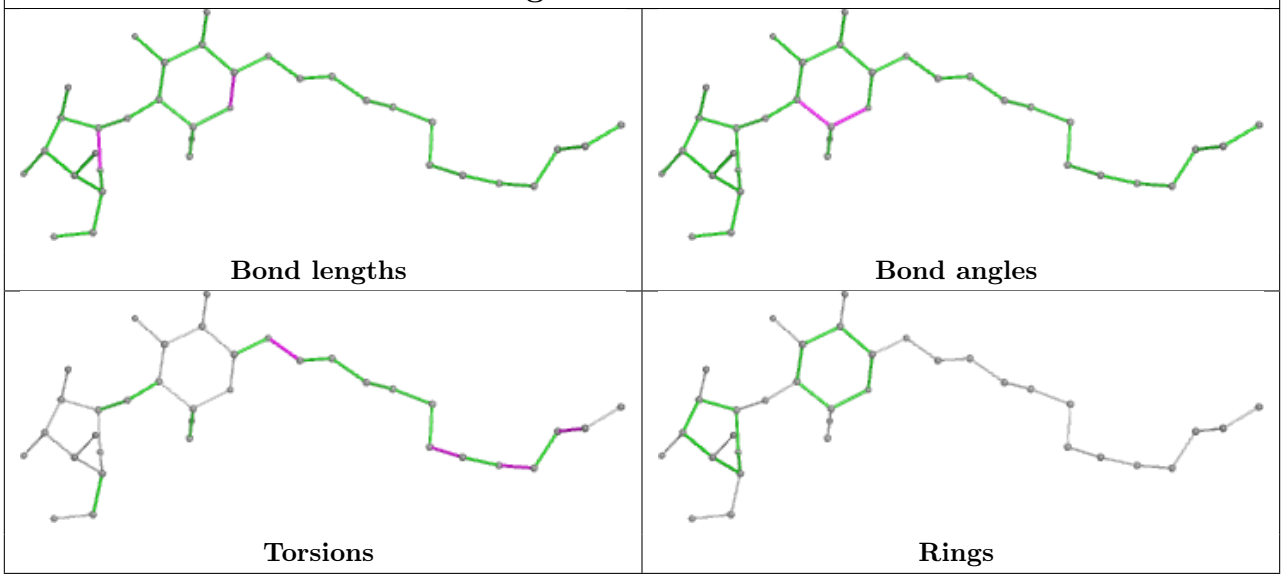


Rings

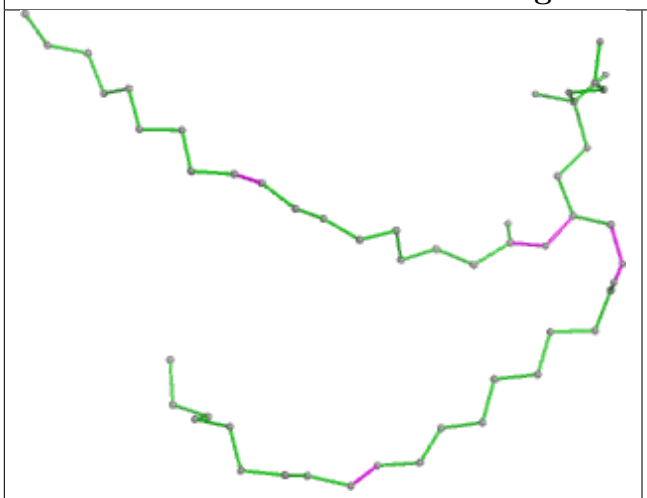
Ligand PEE c 403



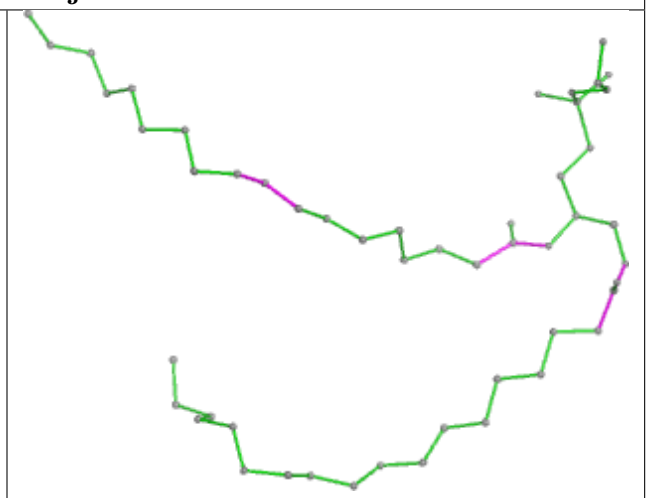
Ligand LMT o 202



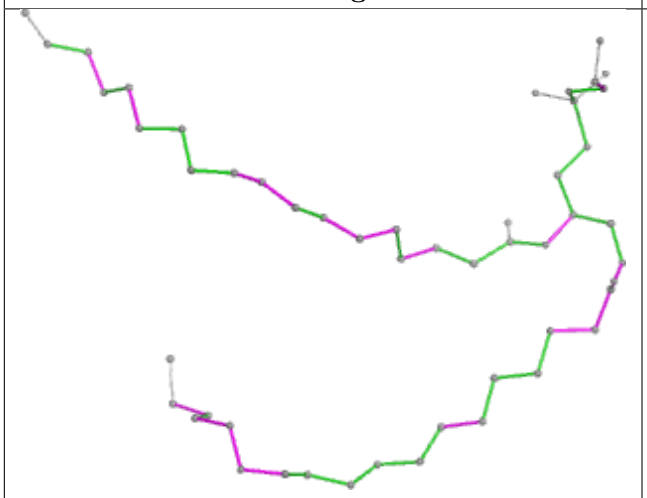
Ligand PEE j 302



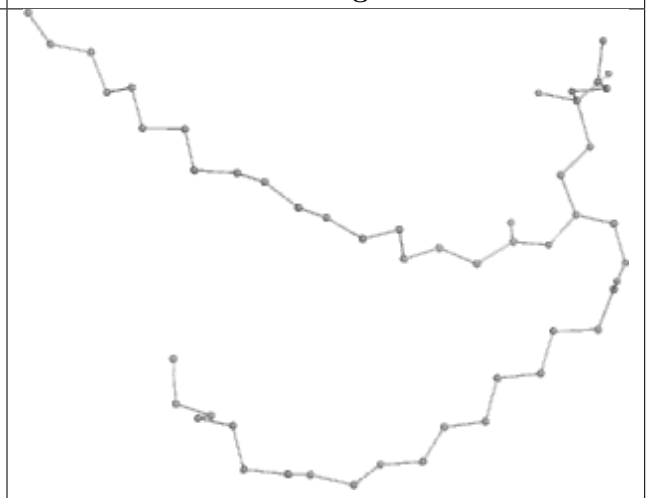
Bond lengths



Bond angles

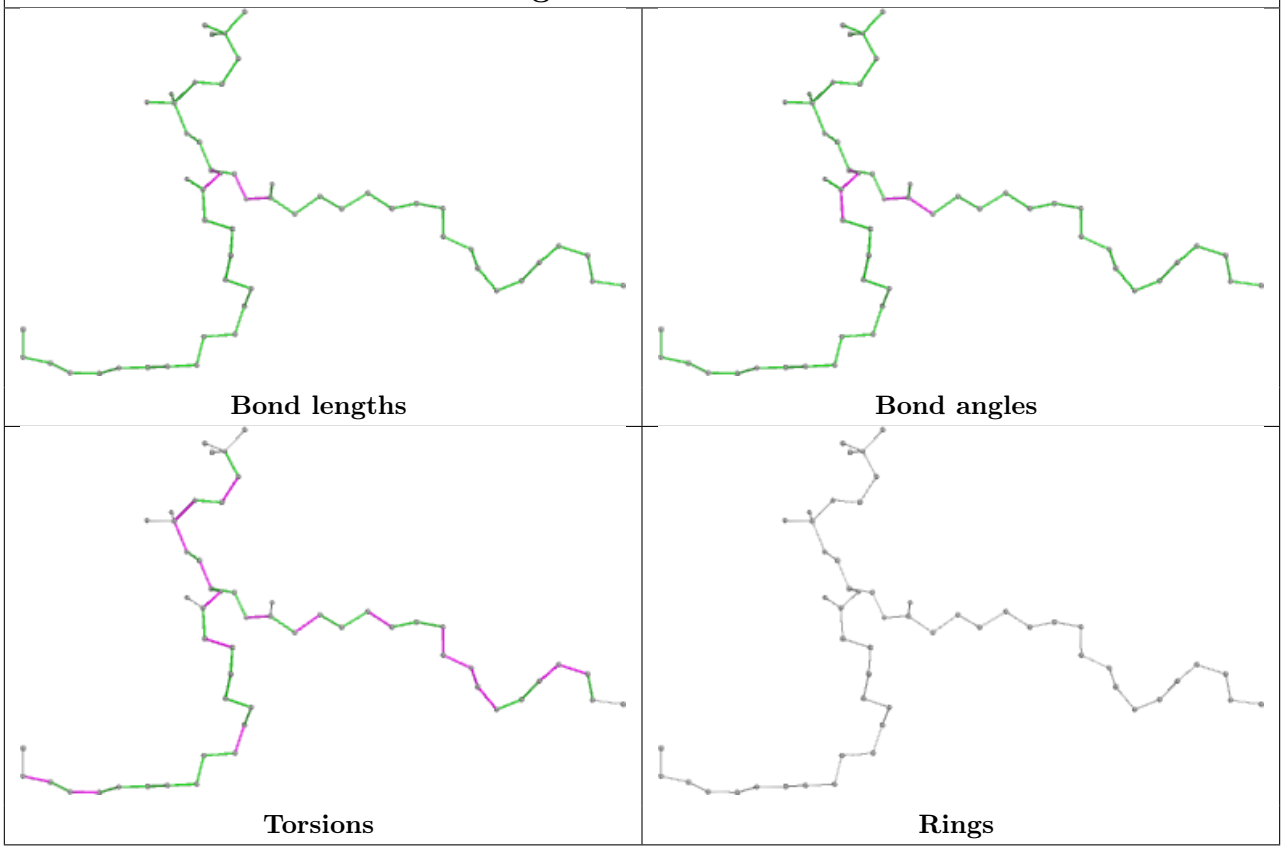


Torsions

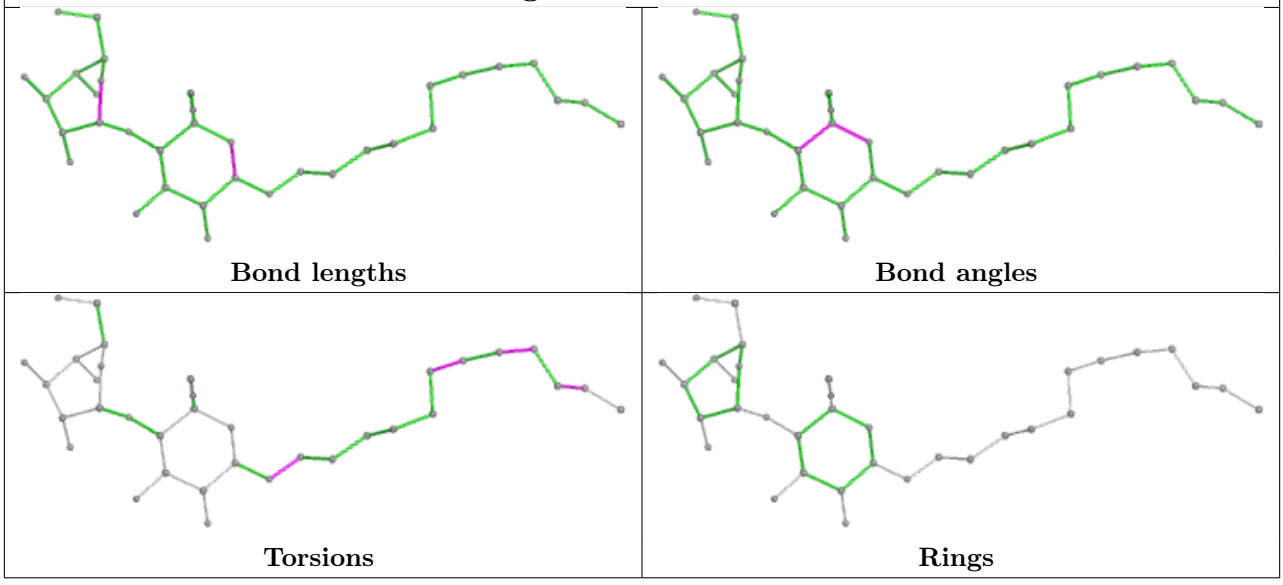


Rings

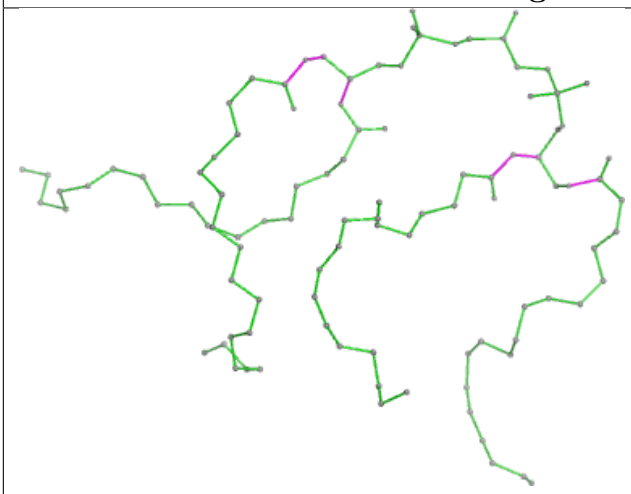
Ligand PC1 o 201



Ligand LMT O 202



Ligand CDL c 401



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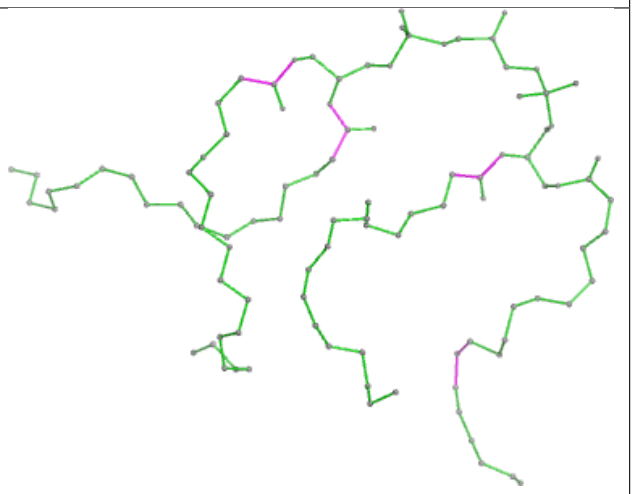
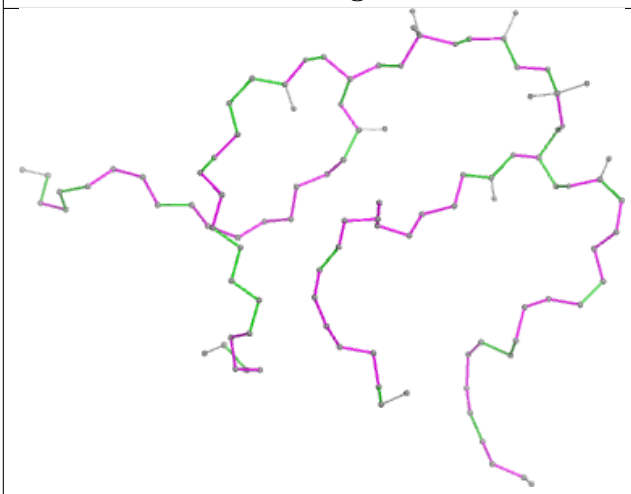


Bond angles



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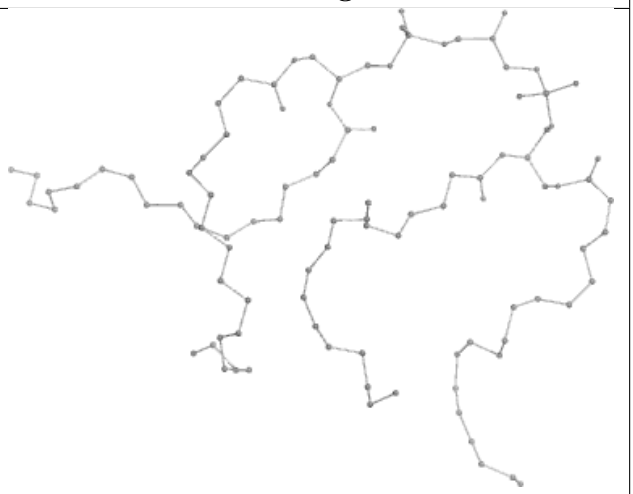
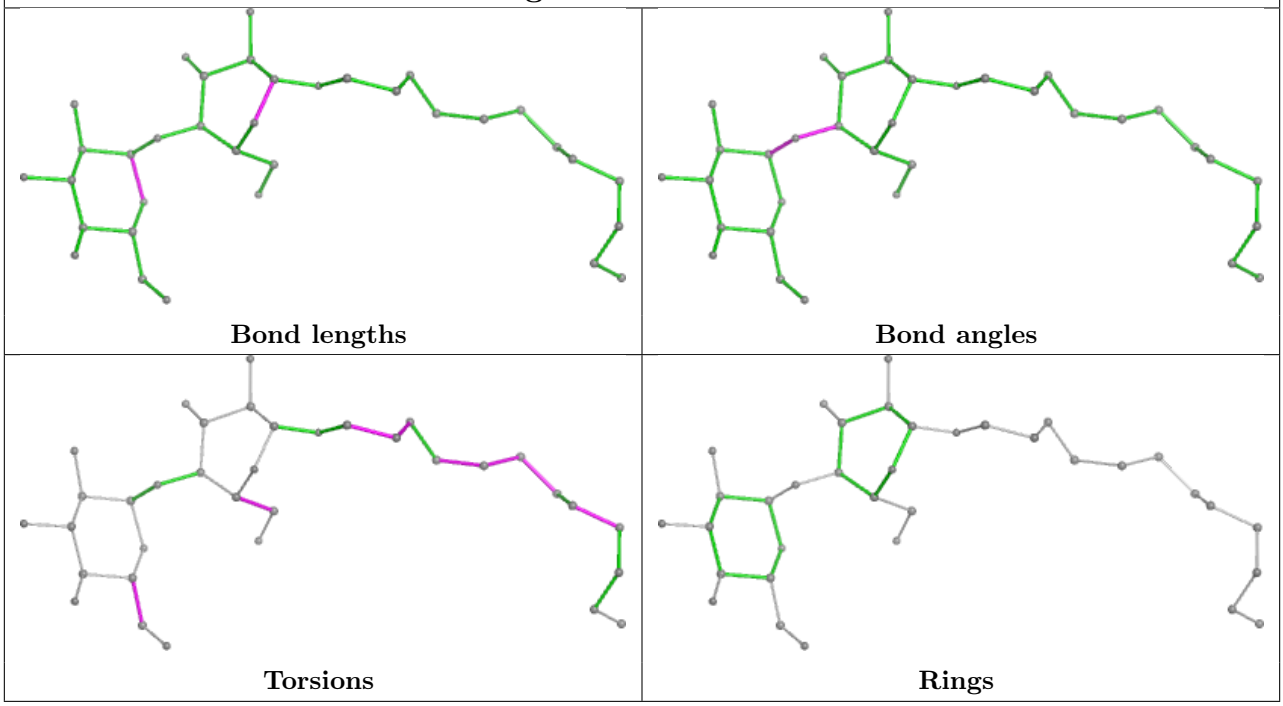


Rings

Ligand LMT d 401



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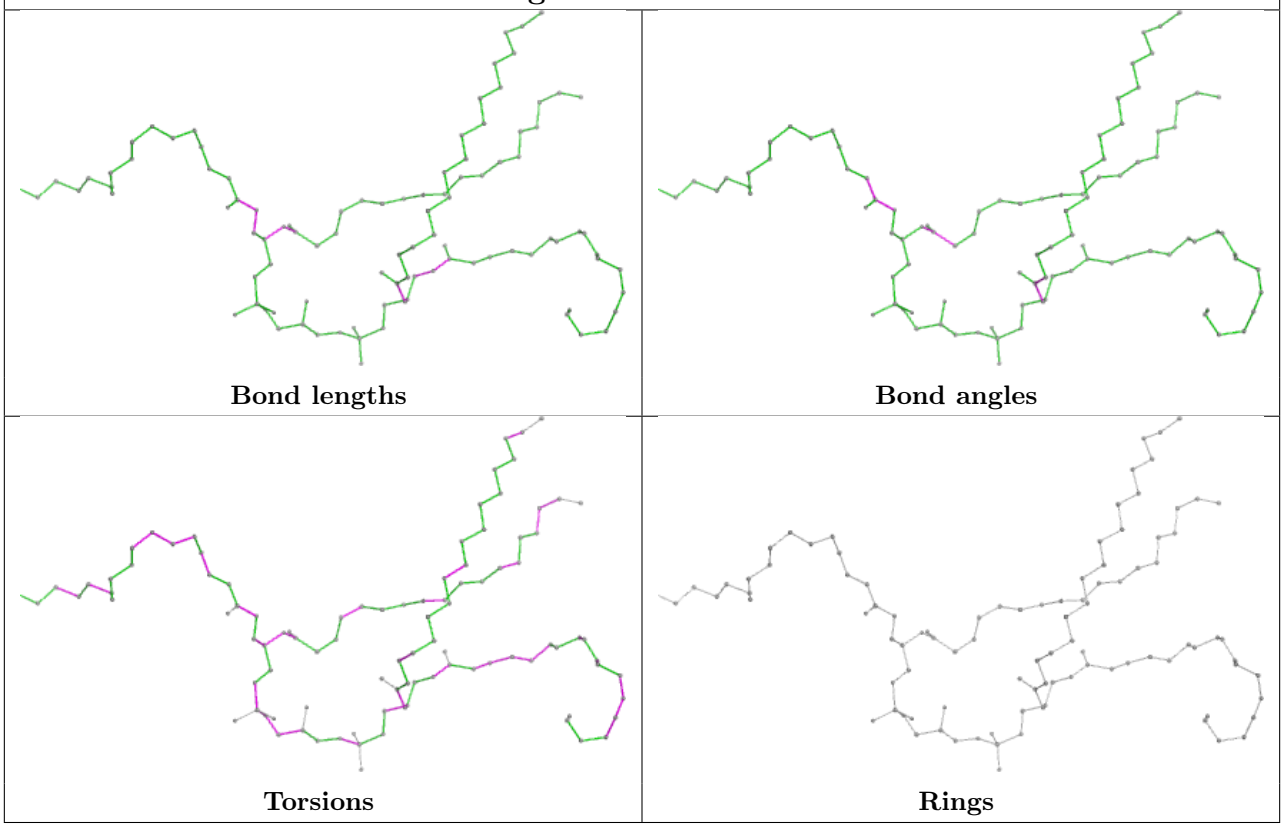
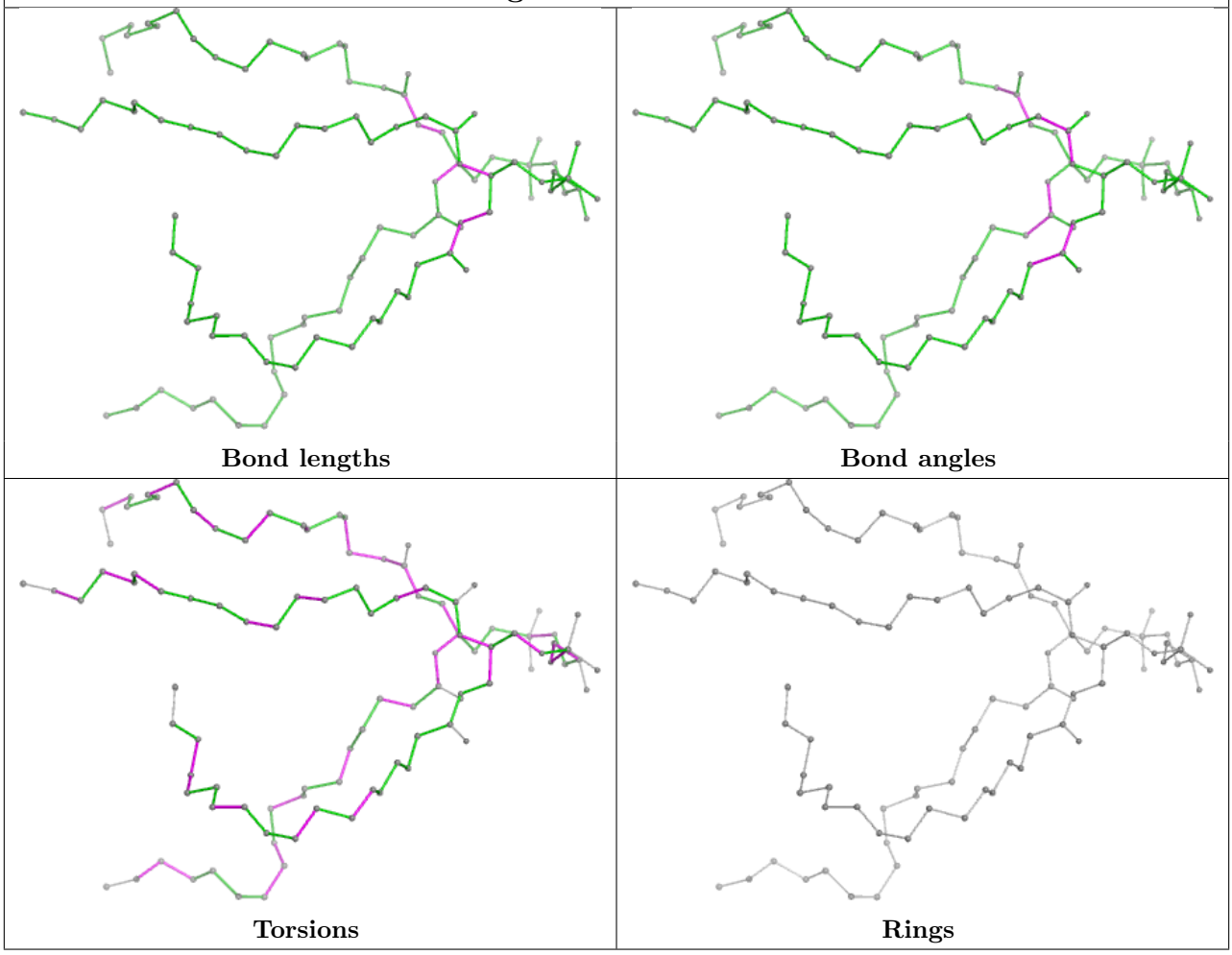
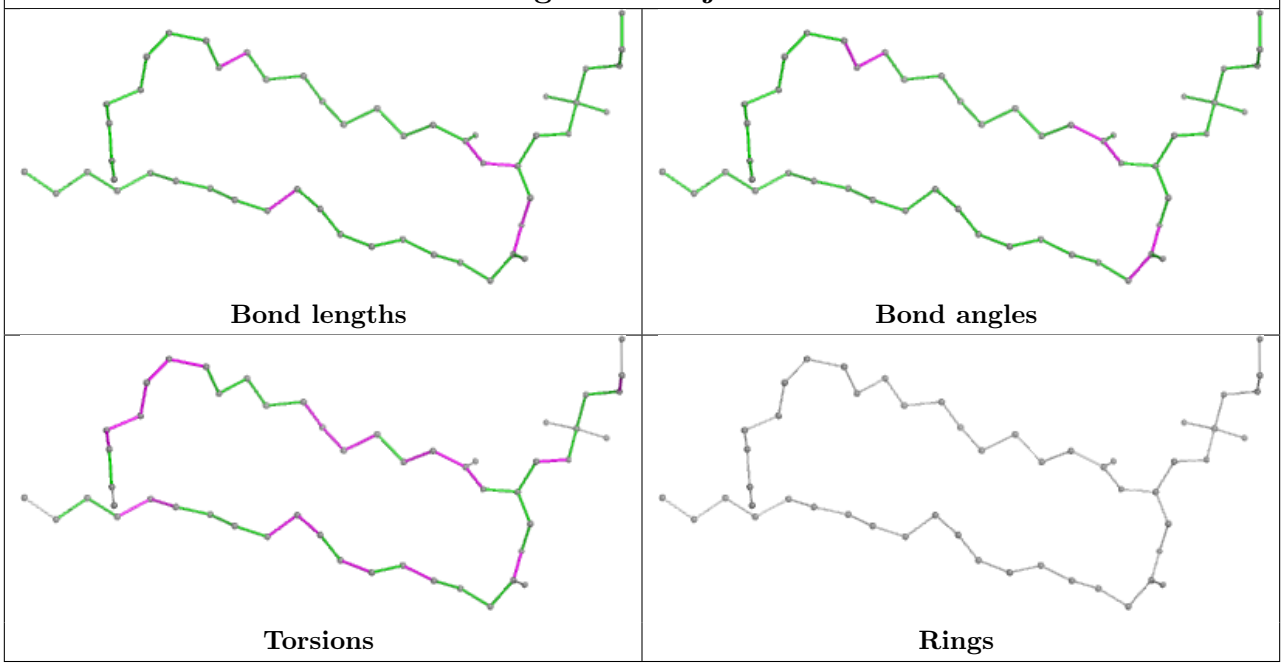


Ligand CDL h 302



Ligand PEE j 301



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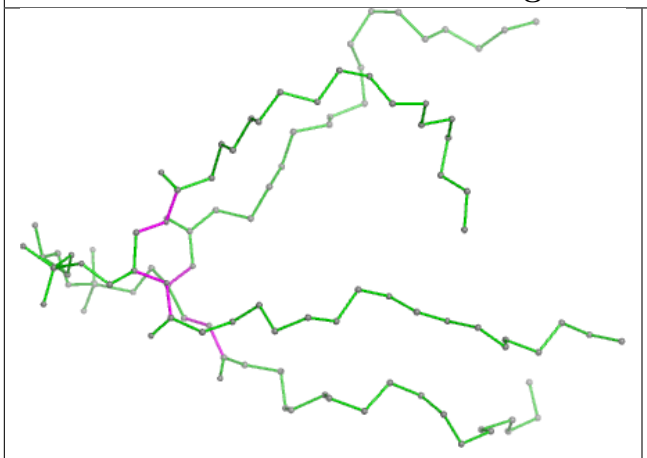
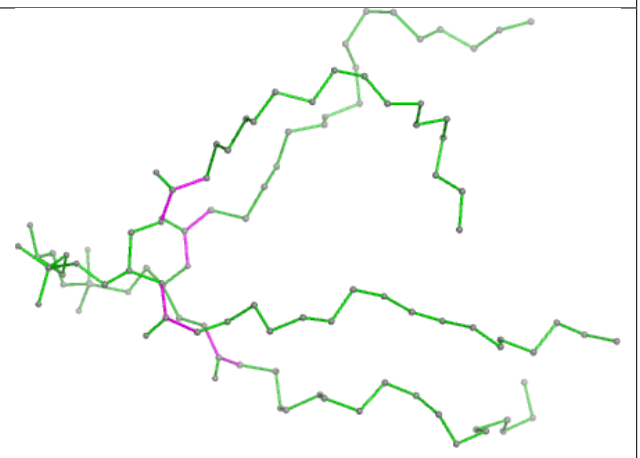
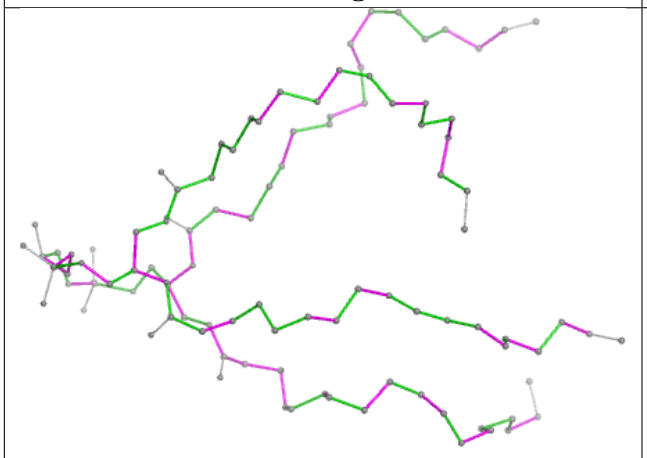


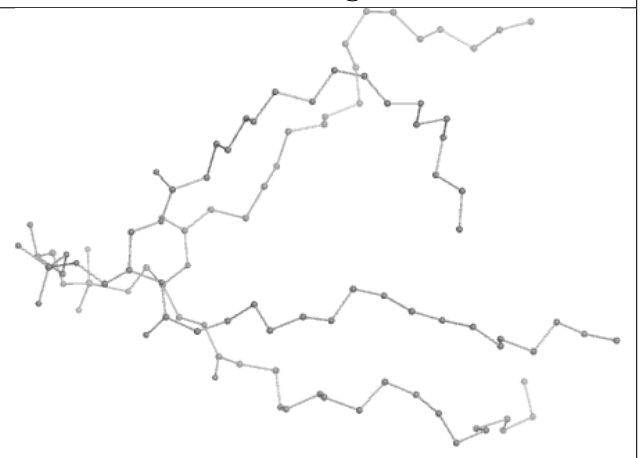
Bond lengths



Bond angles

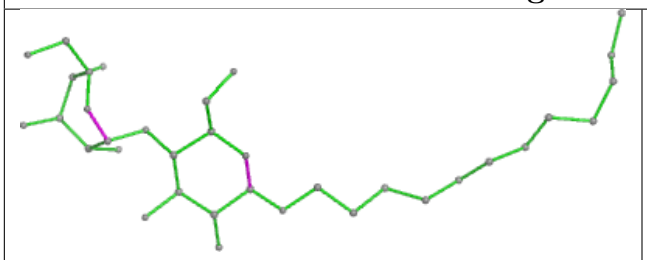


Torsions



Rings

Ligand LMT c 402



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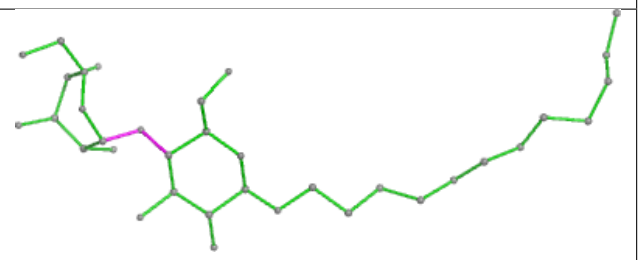
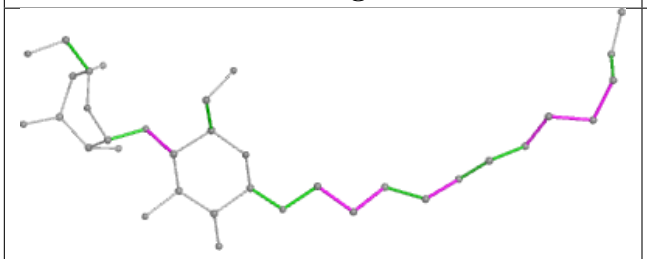
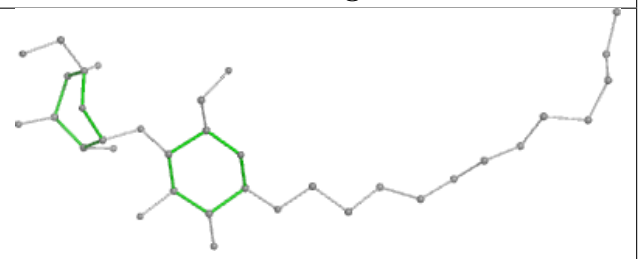


Bond angles

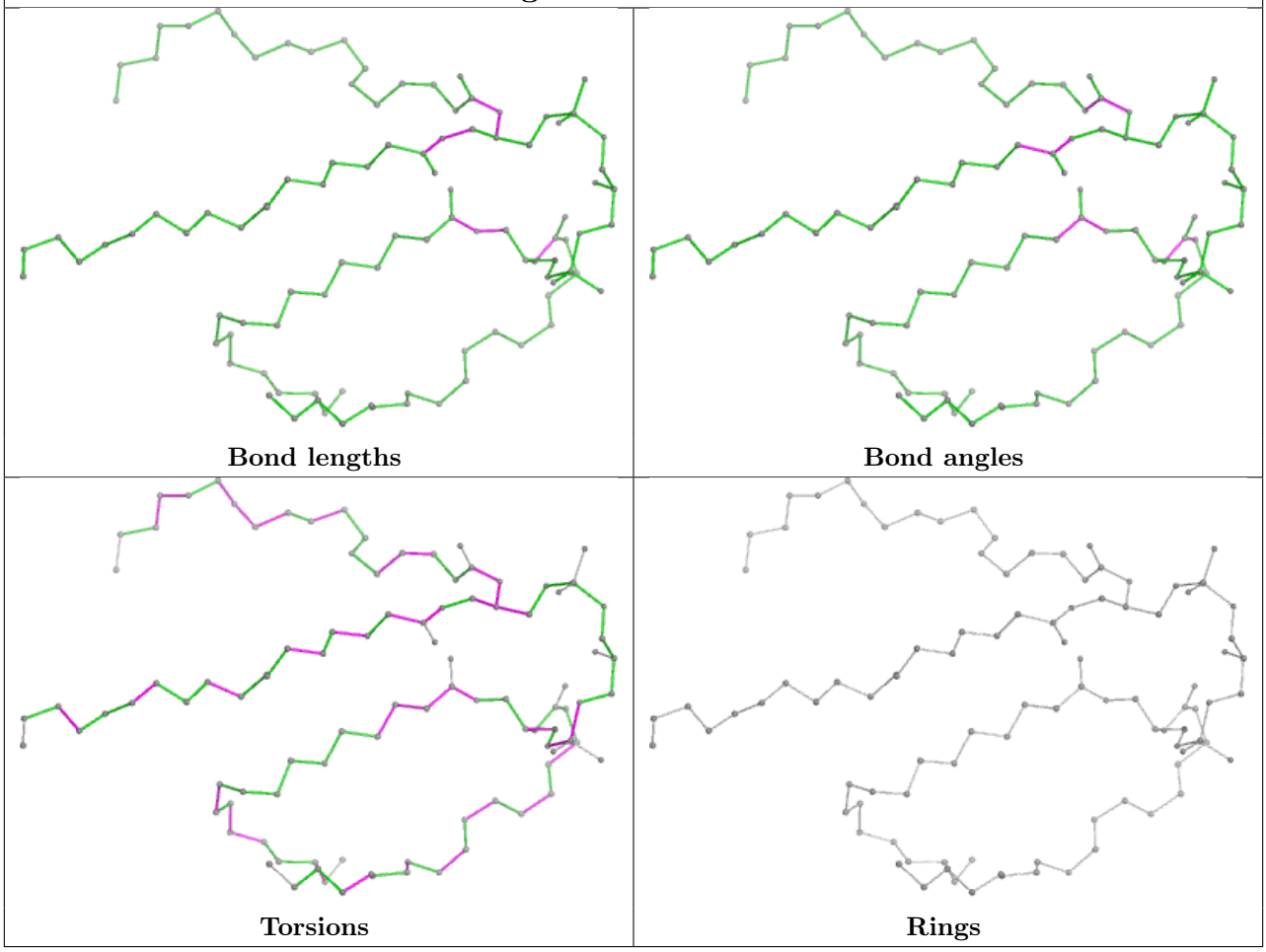


Torsions

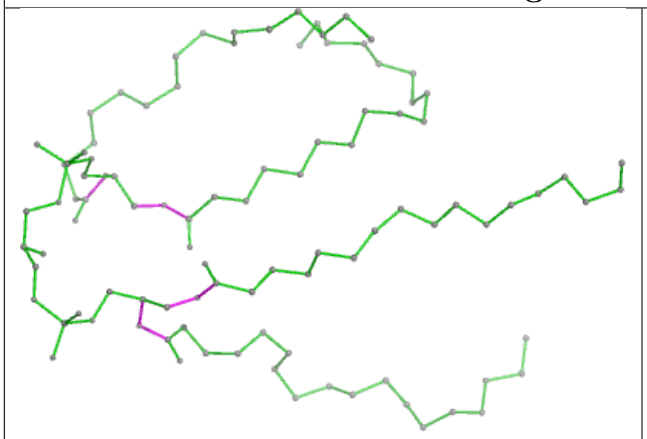


Rings

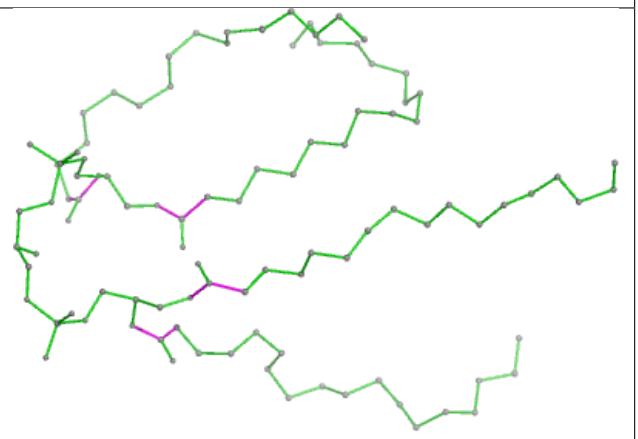
Ligand CDL b 602



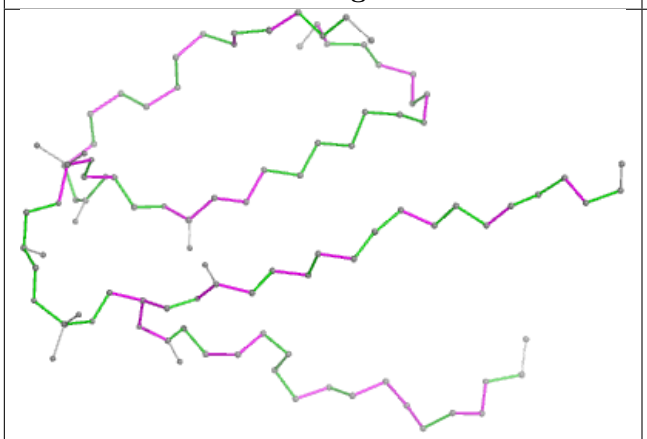
Ligand CDL B 602



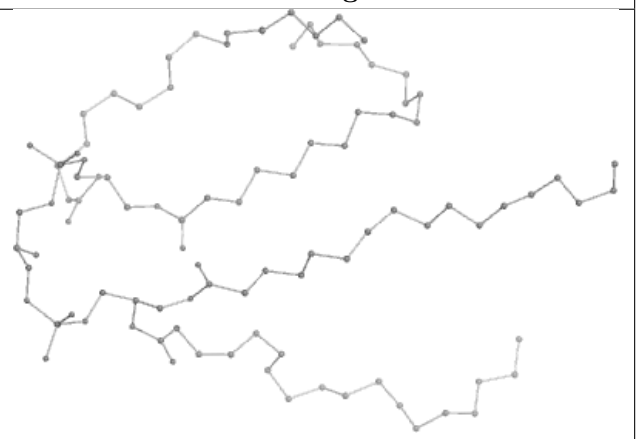
Bond lengths



Bond angles

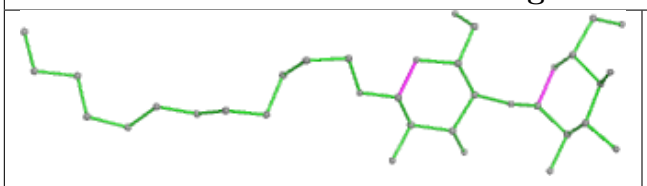


Torsions

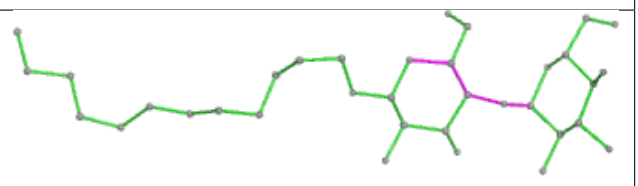


Rings

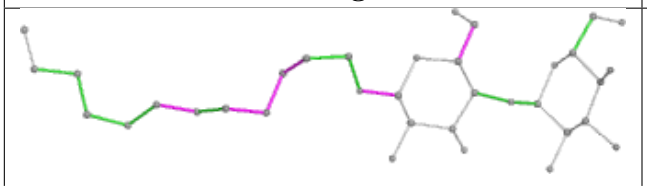
Ligand LMT c 404



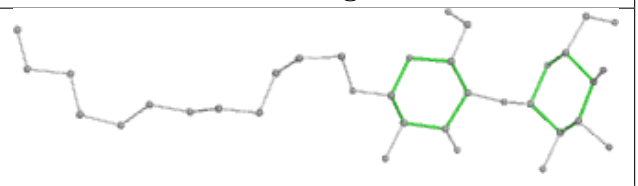
Bond lengths



Bond angles

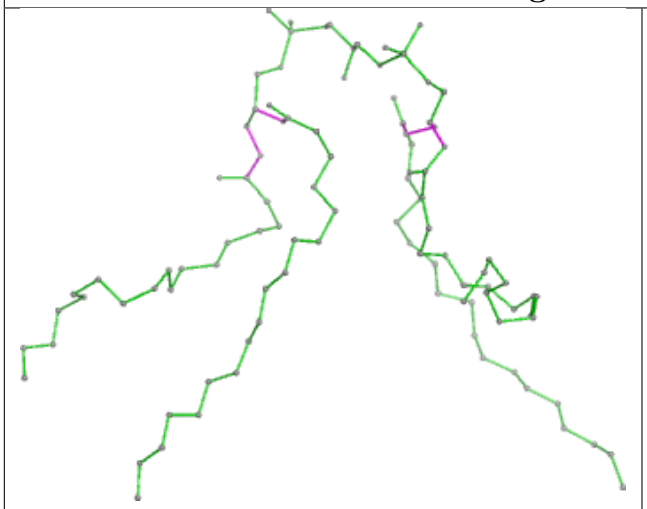


Torsions

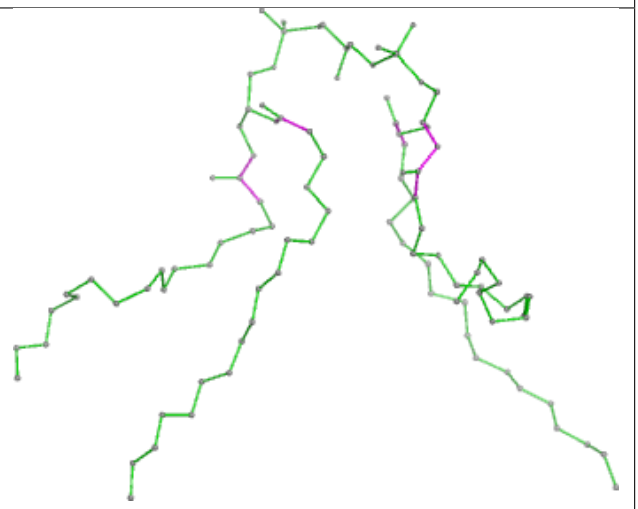


Rings

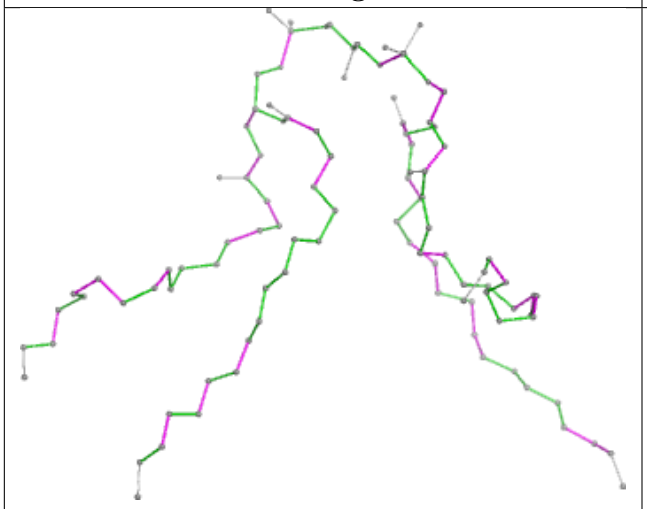
Ligand CDL o 203



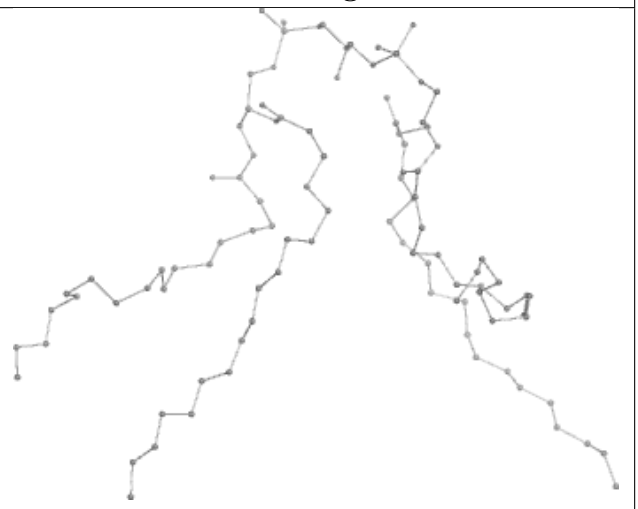
Bond lengths



Bond angles

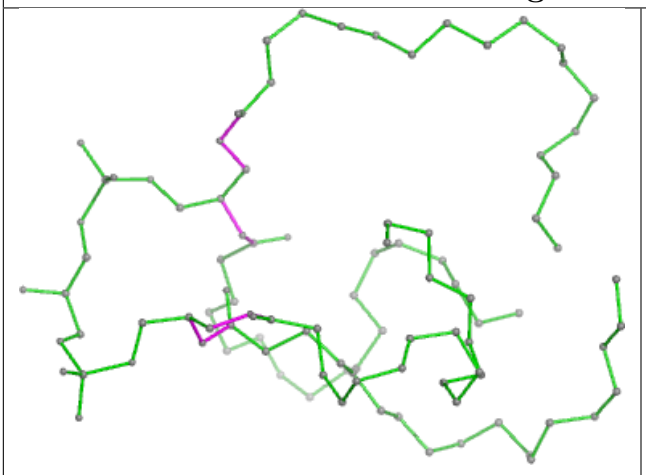


Torsions

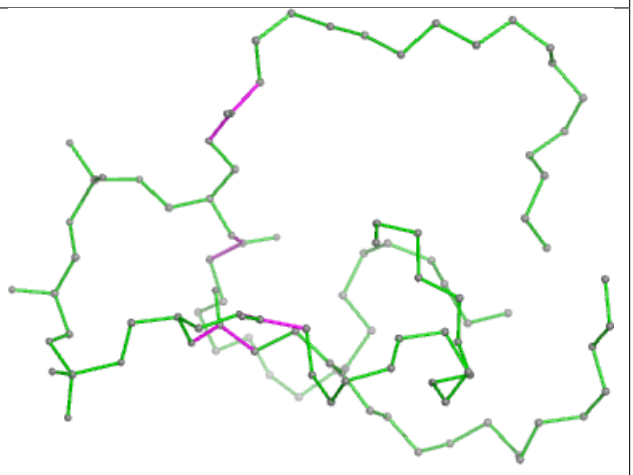


Rings

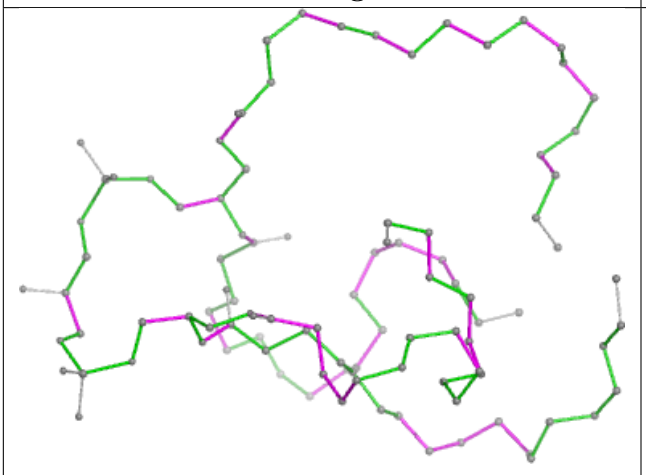
Ligand CDL b 601



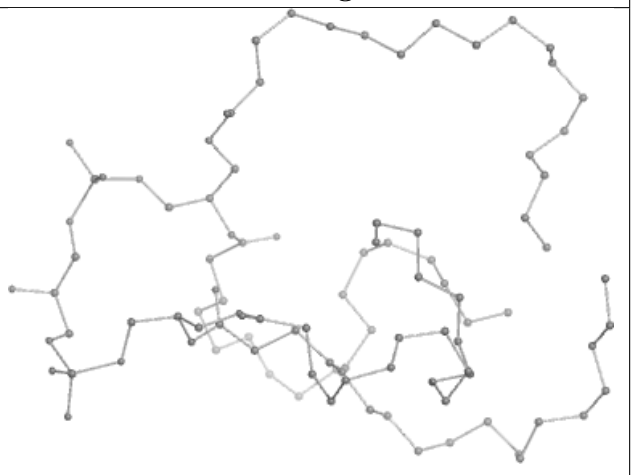
Bond lengths



Bond angles

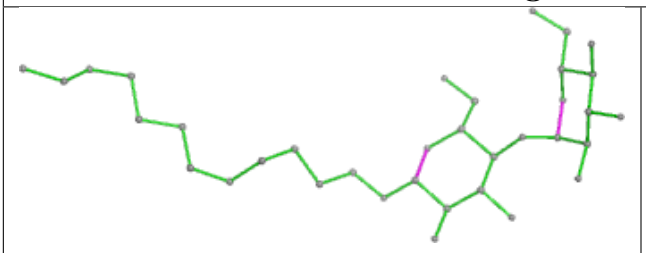


Torsions

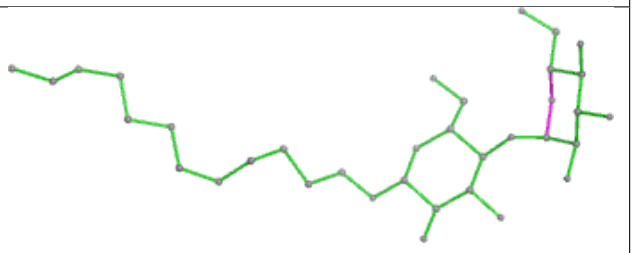


Rings

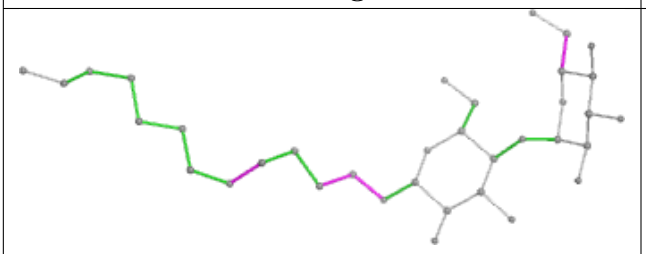
Ligand LMT d 403



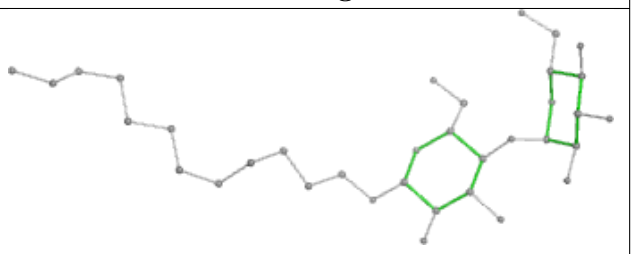
Bond lengths



Bond angles

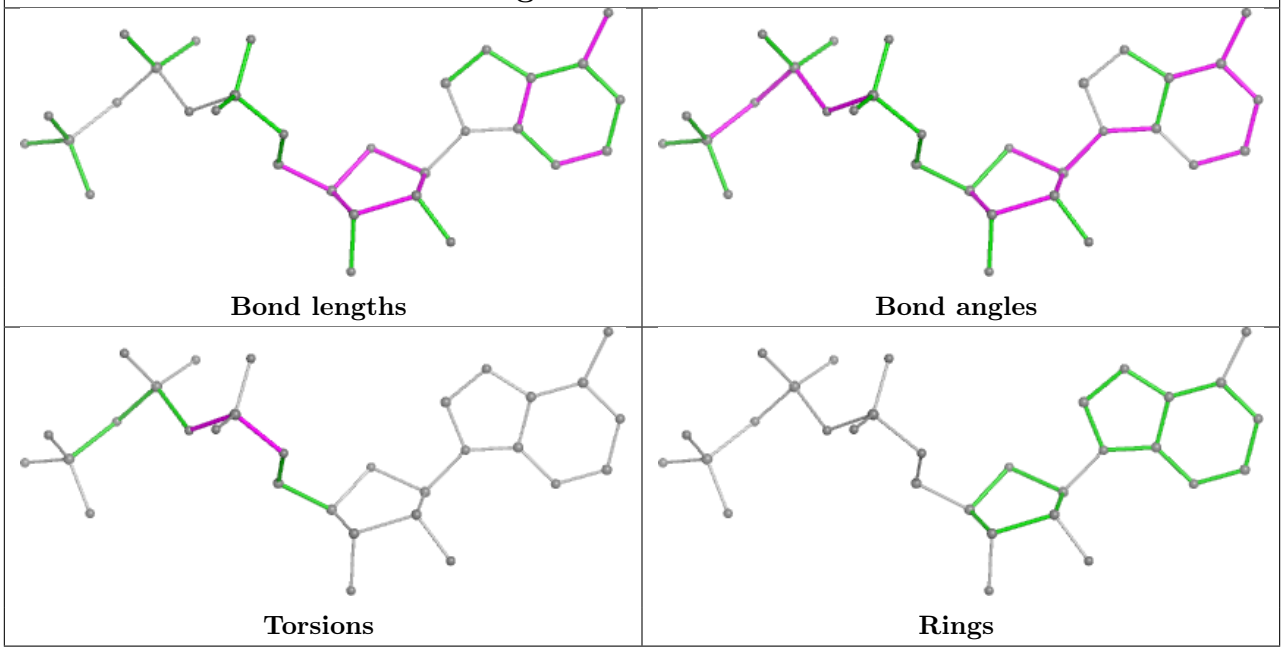


Torsions

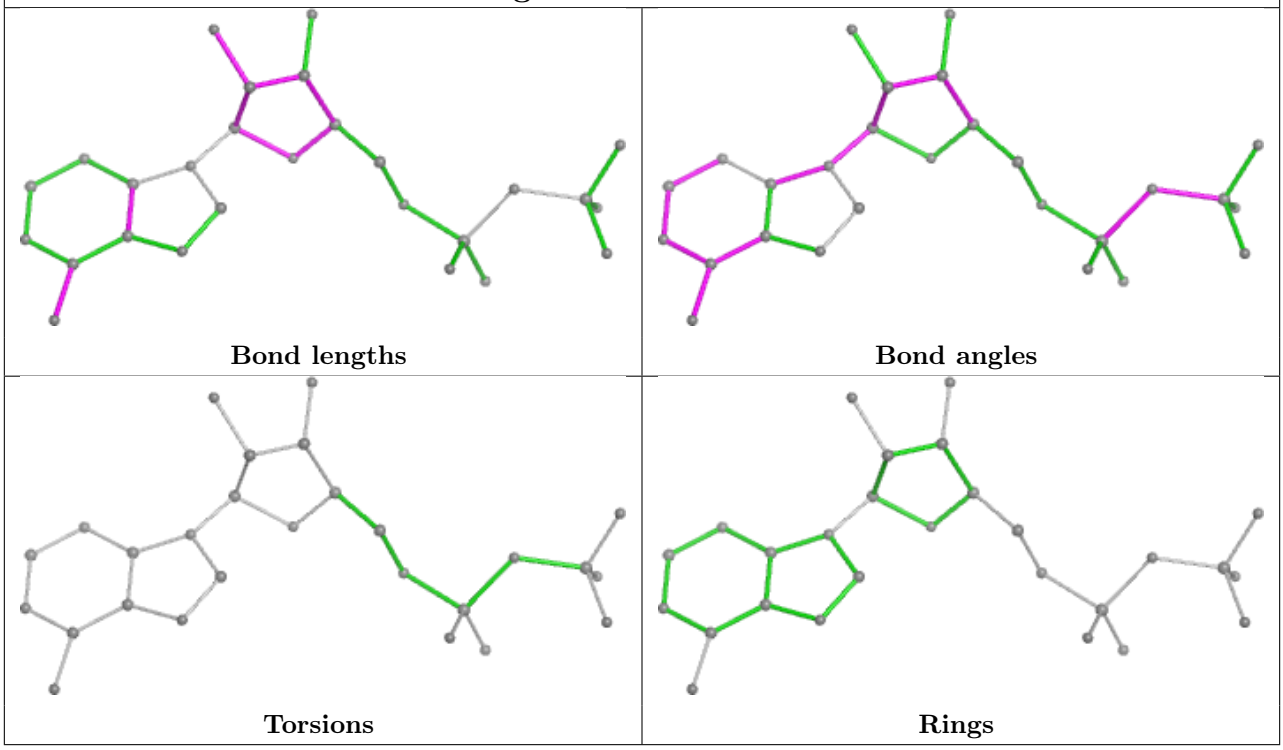


Rings

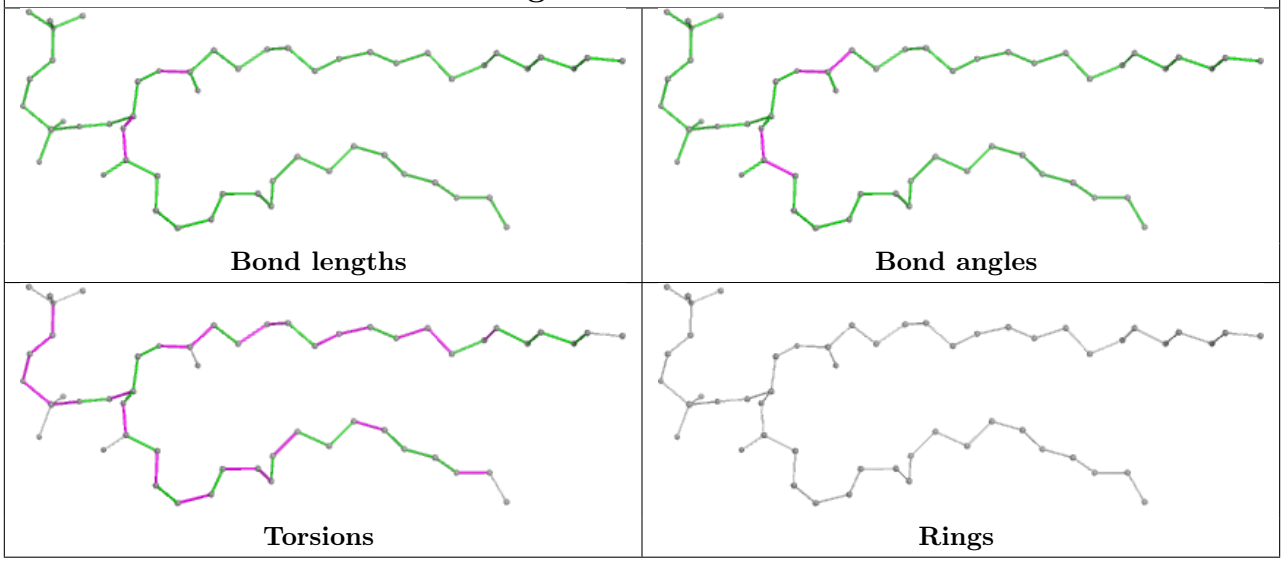
Ligand ATP C1 601



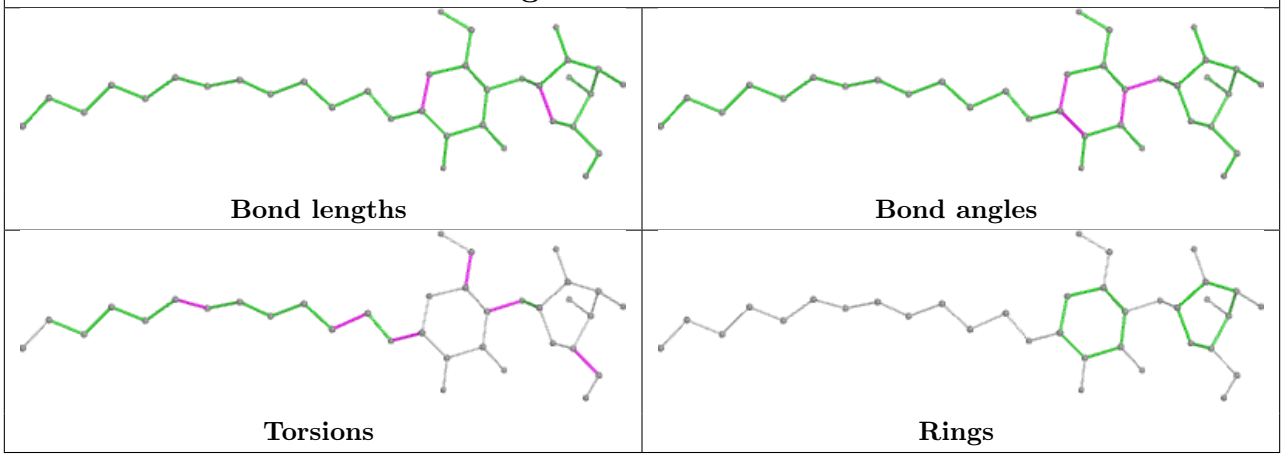
Ligand ADP D1 601



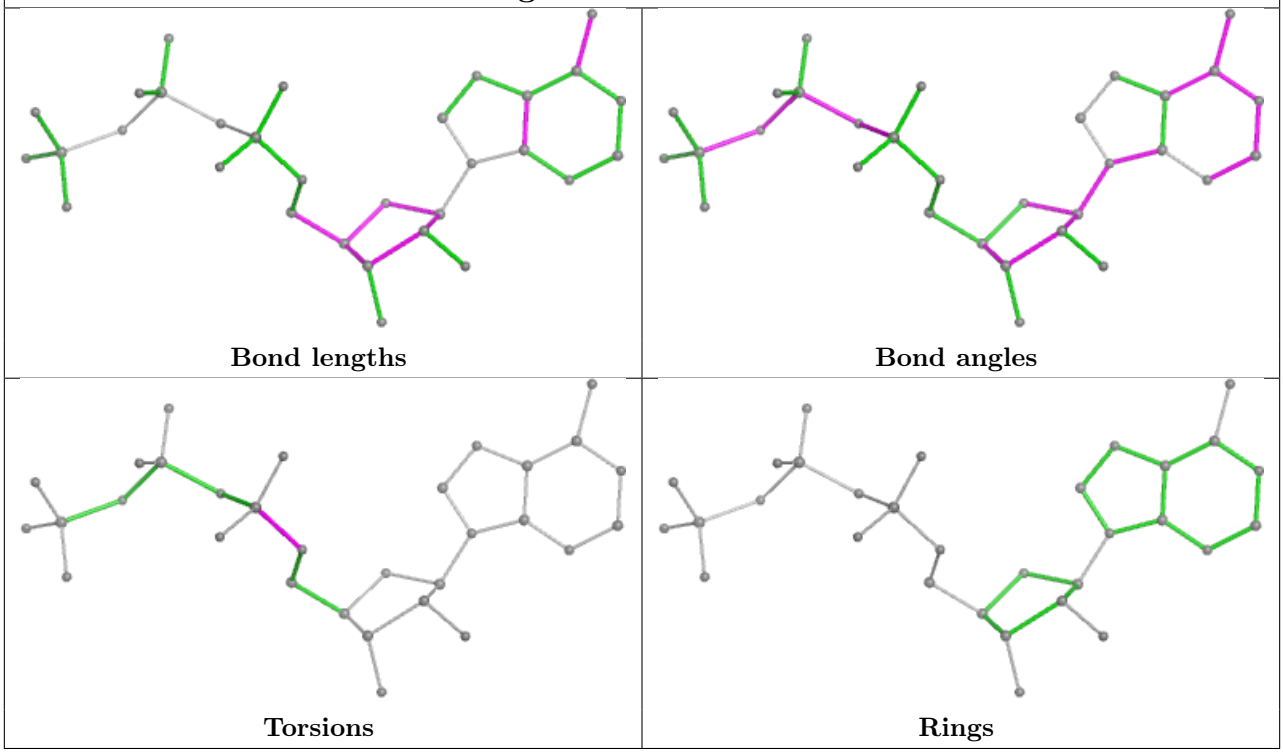
Ligand PC1 V 201



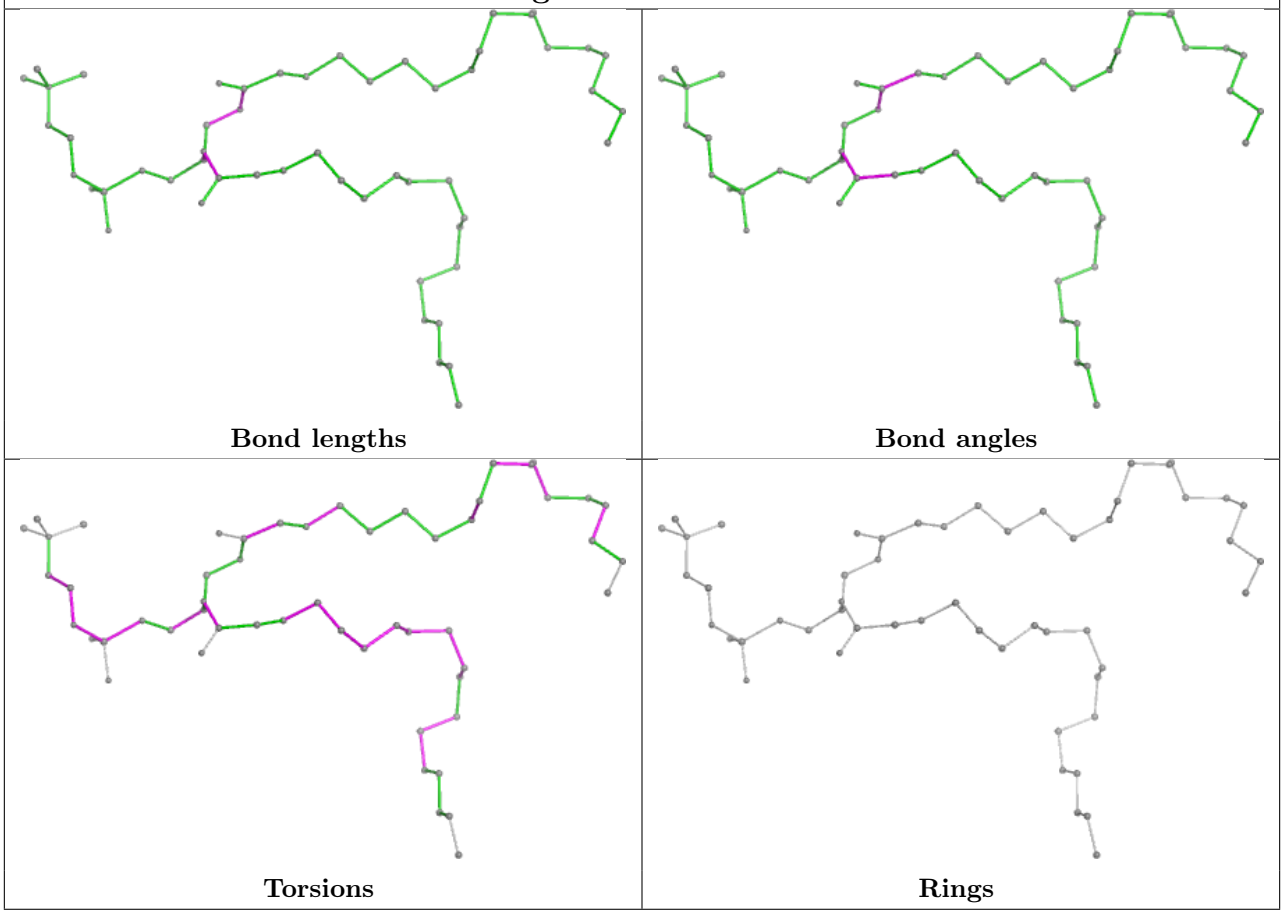
Ligand LMT H 301



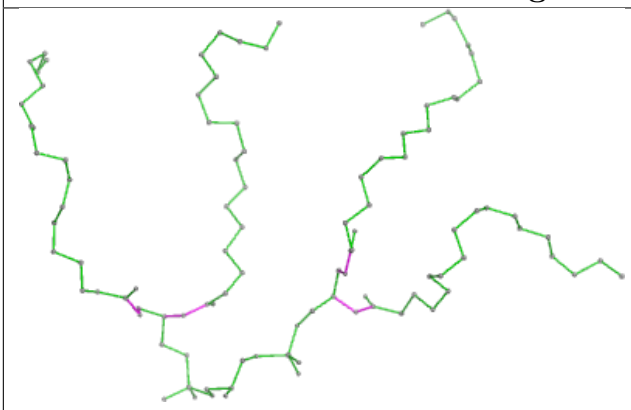
Ligand ATP E2 601



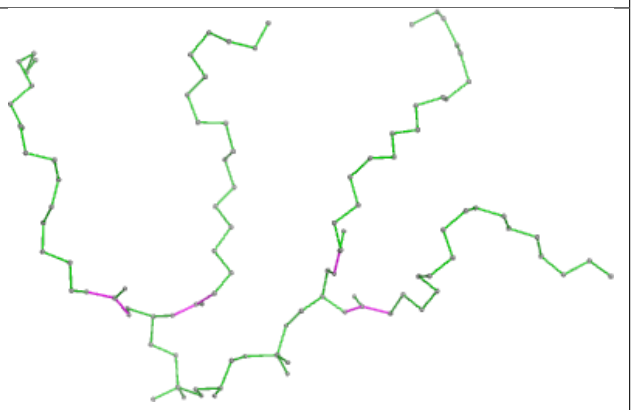
Ligand PC1 o 204



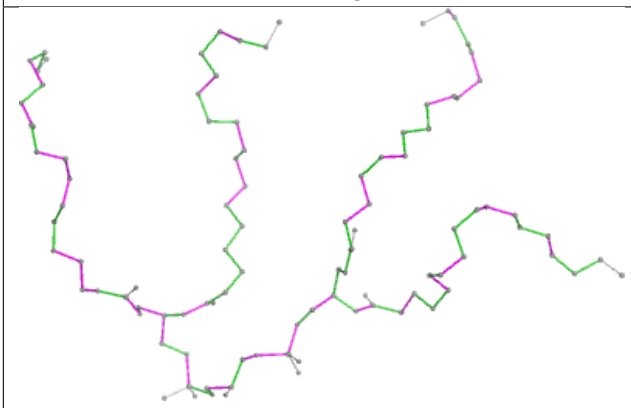
Ligand CDL e 401



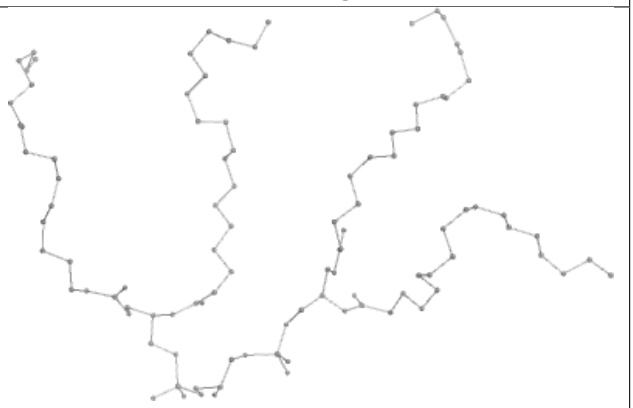
Bond lengths



Bond angles

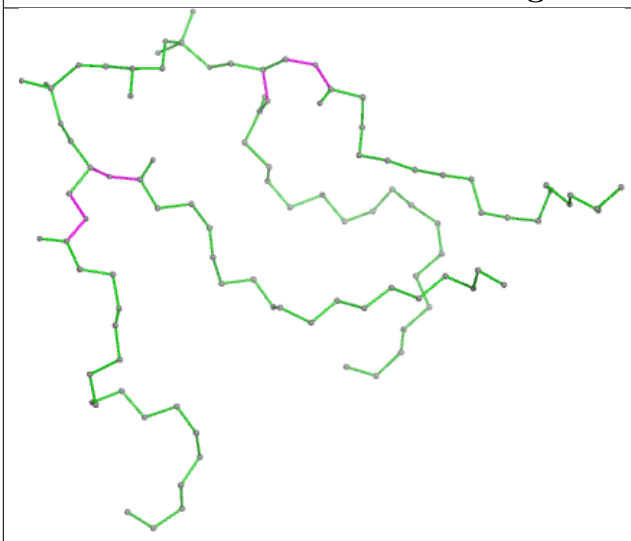


Torsions

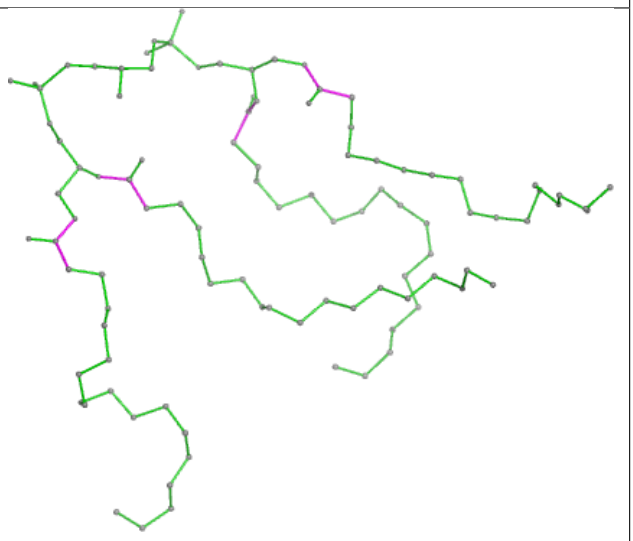


Rings

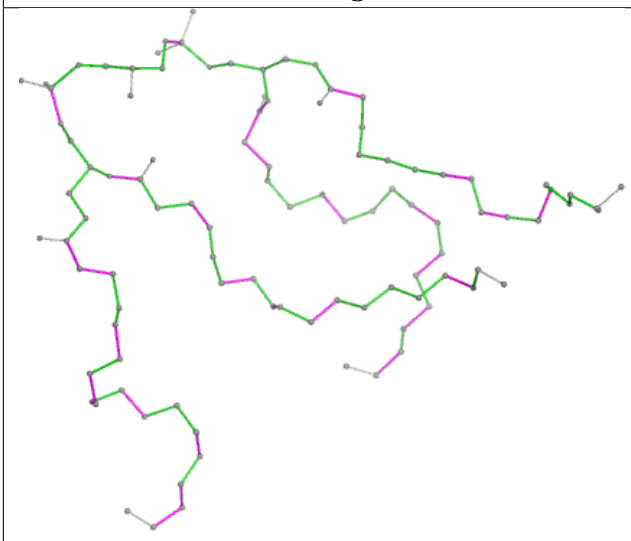
Ligand CDL u 201



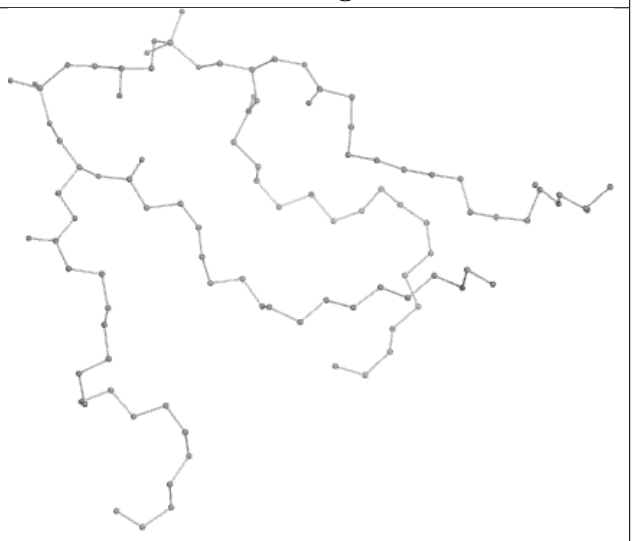
Bond lengths



Bond angles

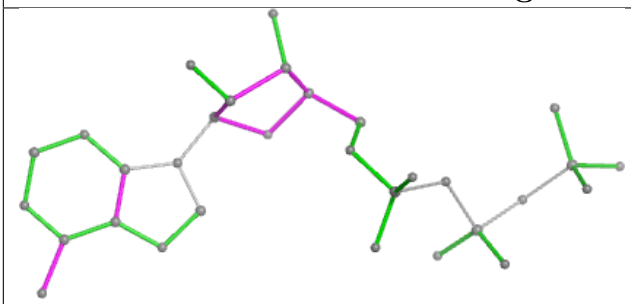


Torsions

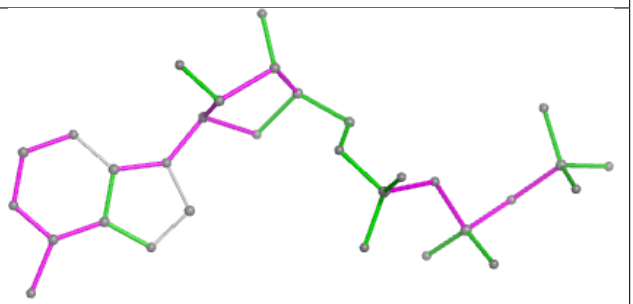


Rings

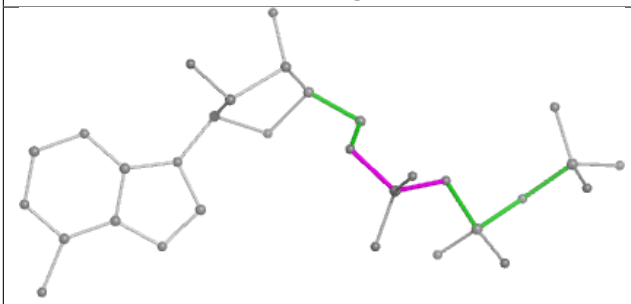
Ligand ATP C2 601



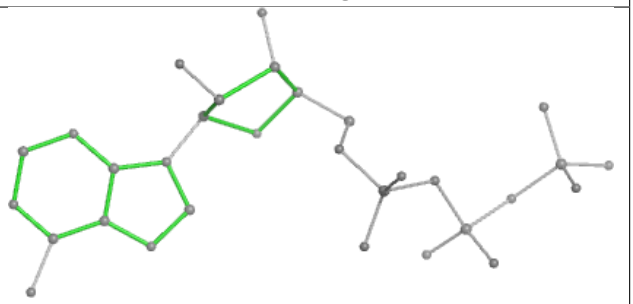
Bond lengths



Bond angles

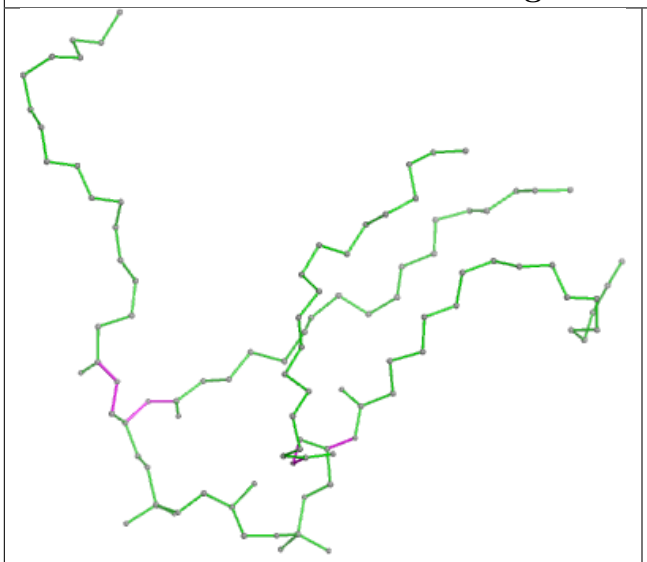


Torsions

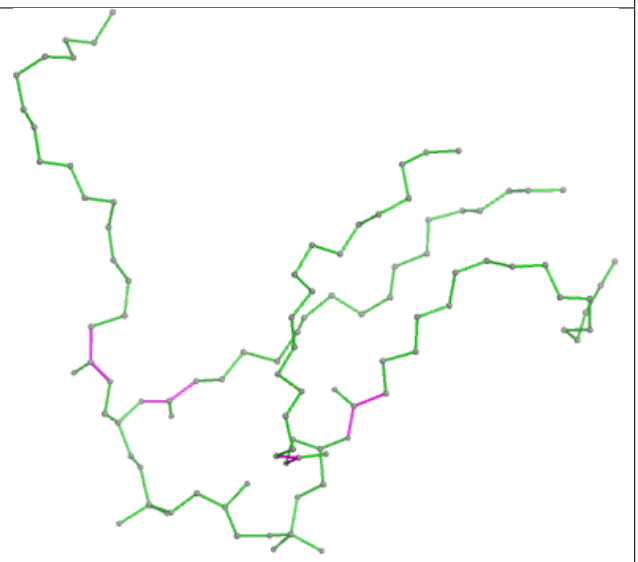


Rings

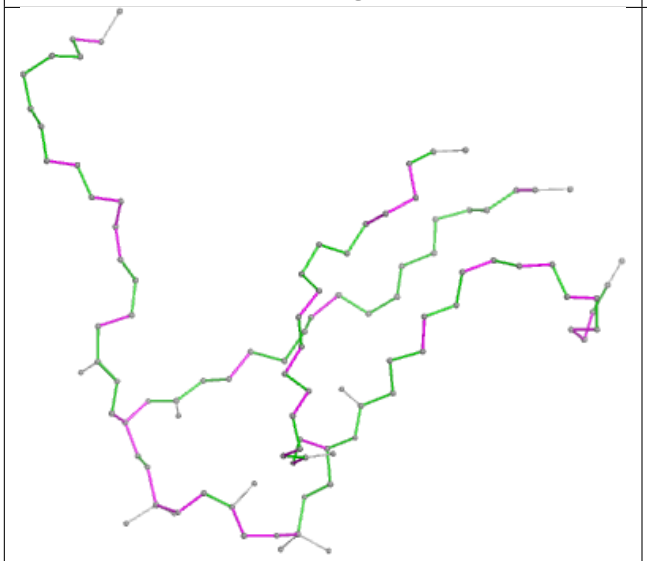
Ligand CDL V 202



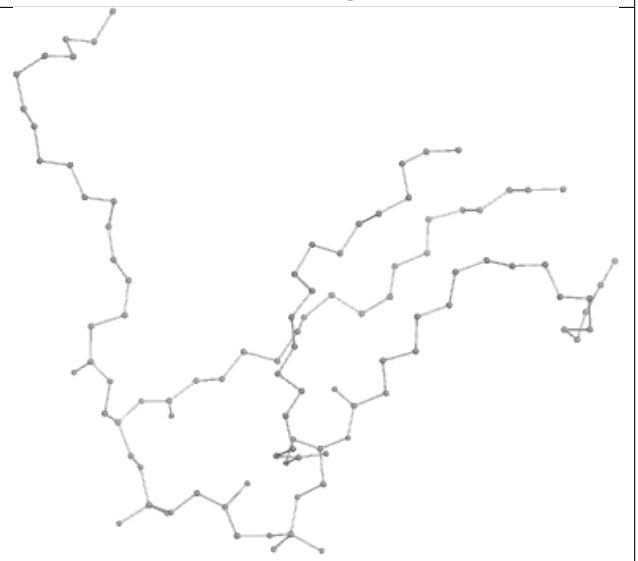
Bond lengths



Bond angles

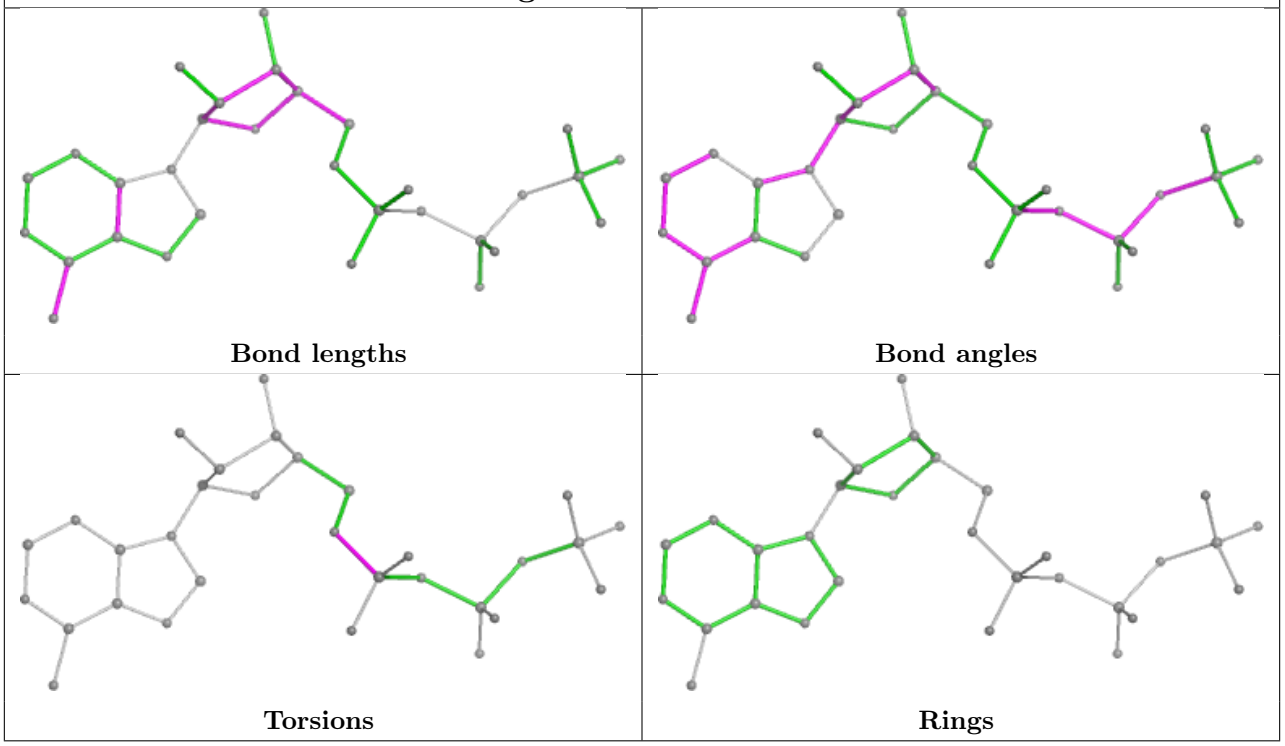


Torsions

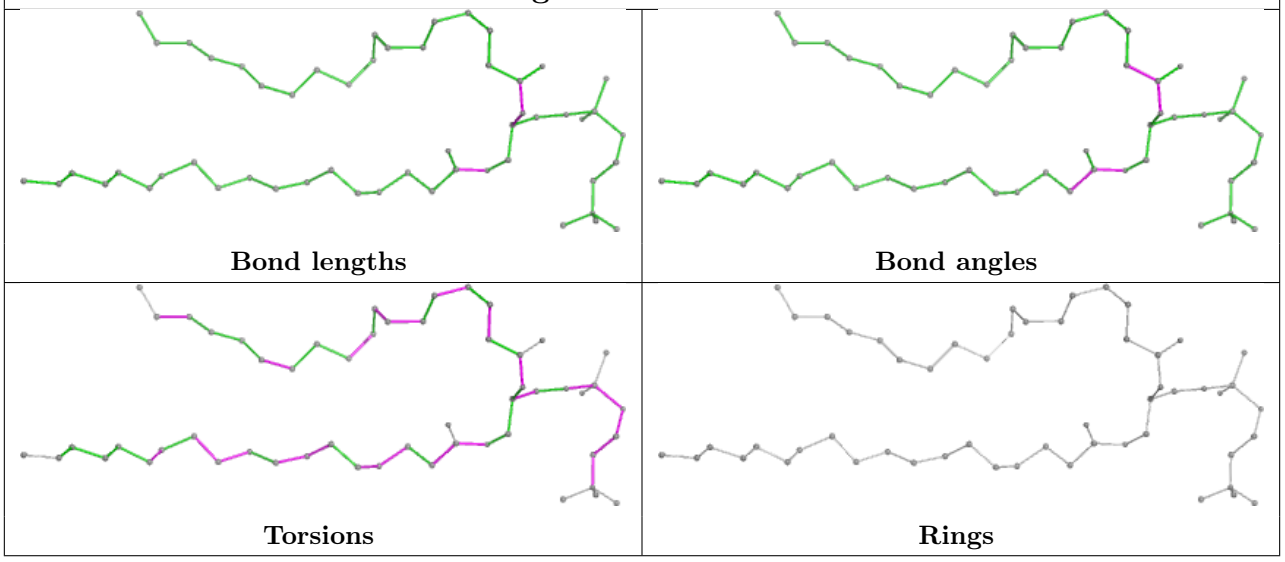


Rings

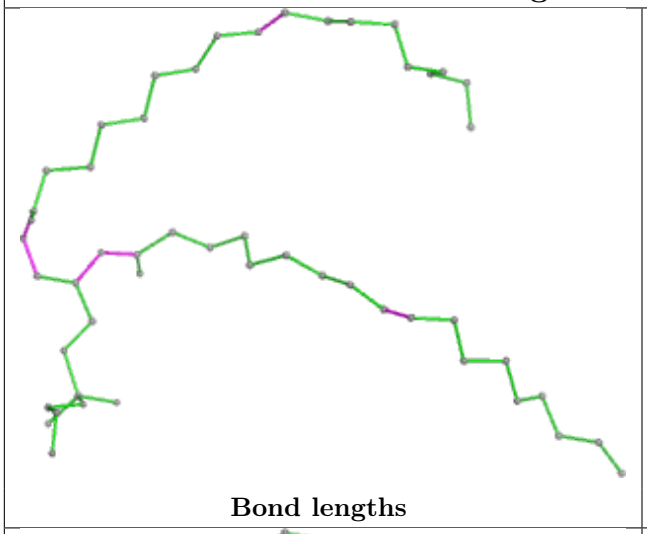
Ligand ATP E1 601



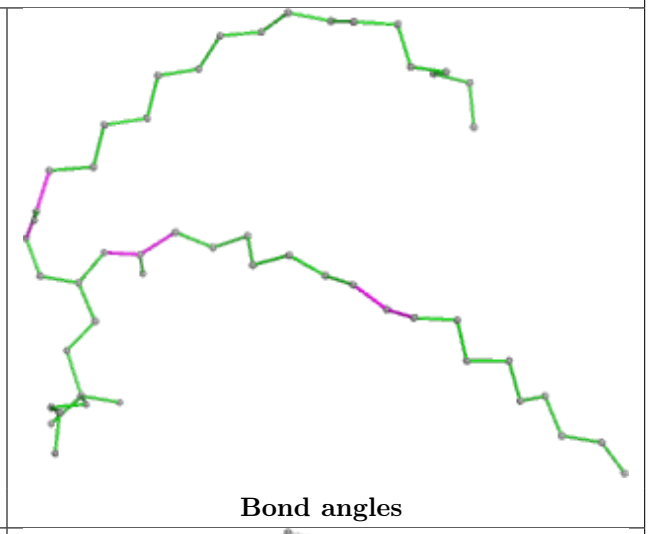
Ligand PC1 v 201



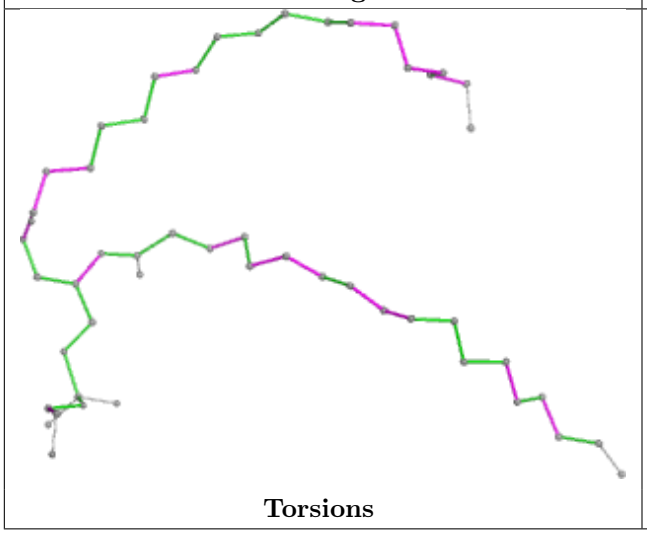
Ligand PEE J 302



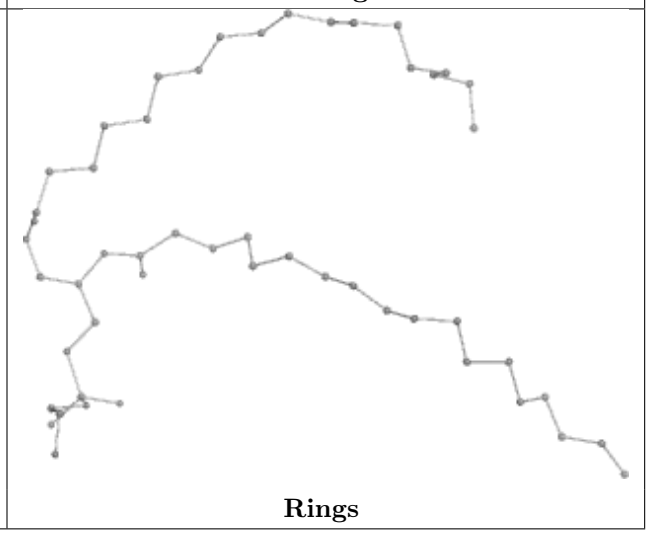
Bond lengths



Bond angles

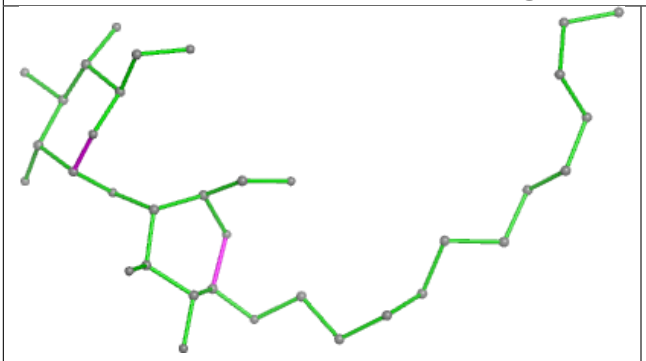


Torsions

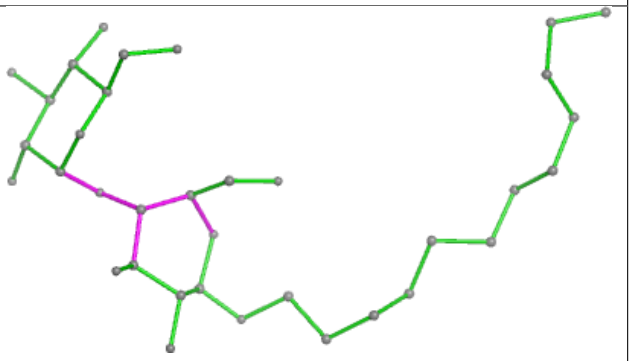


Rings

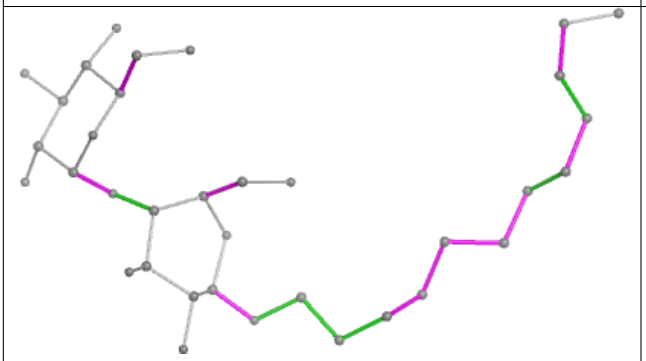
Ligand LMT X 101



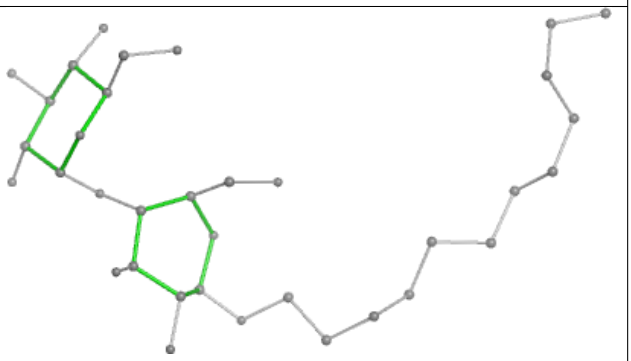
Bond lengths



Bond angles

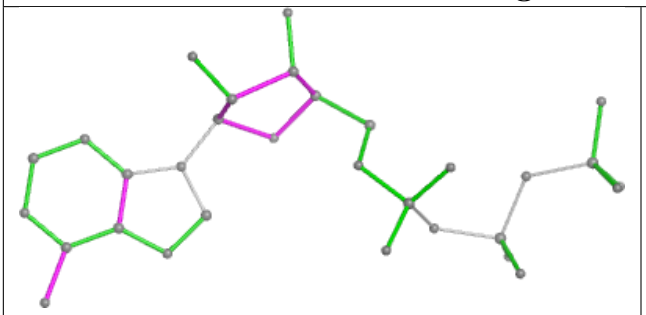


Torsions

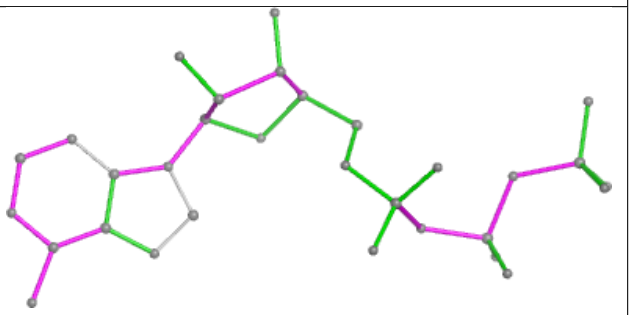


Rings

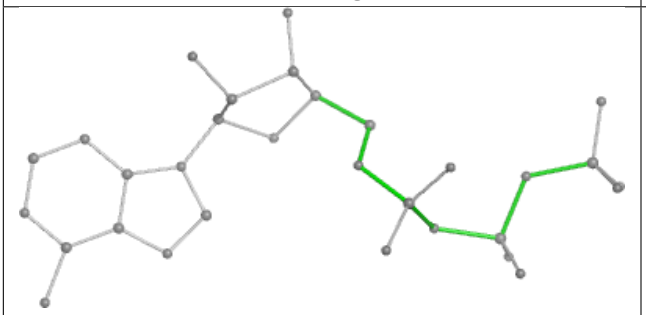
Ligand ATP A2 601



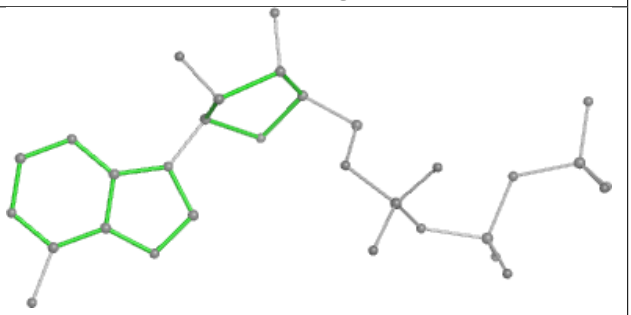
Bond lengths



Bond angles

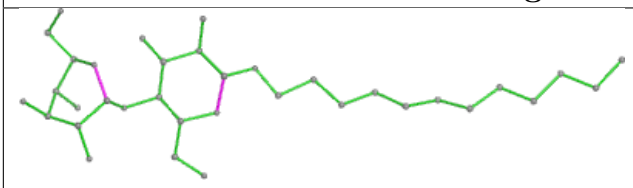


Torsions

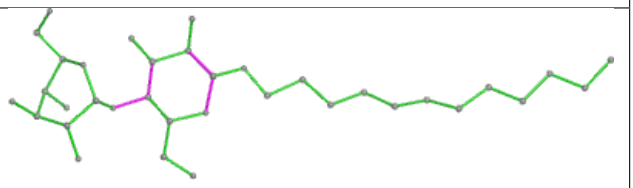


Rings

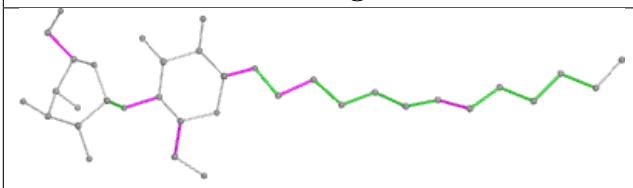
Ligand LMT h 301



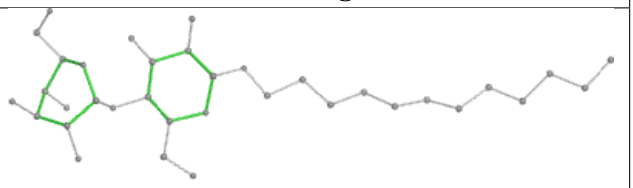
Bond lengths



Bond angles

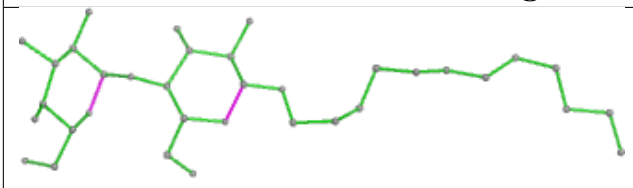


Torsions

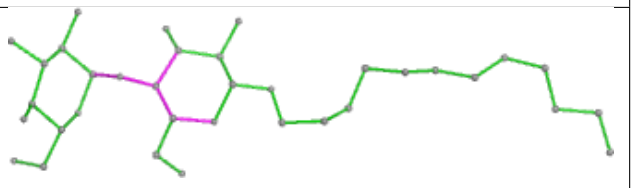


Rings

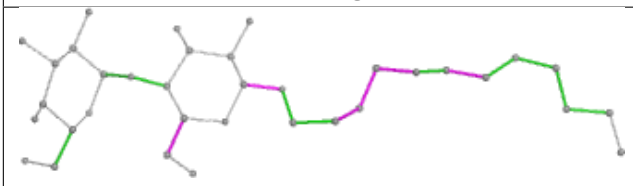
Ligand LMT C 404



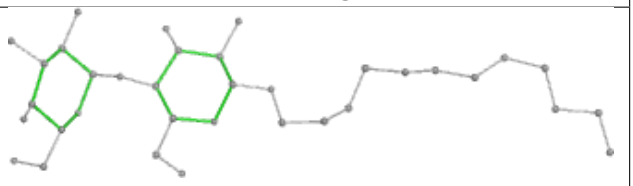
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

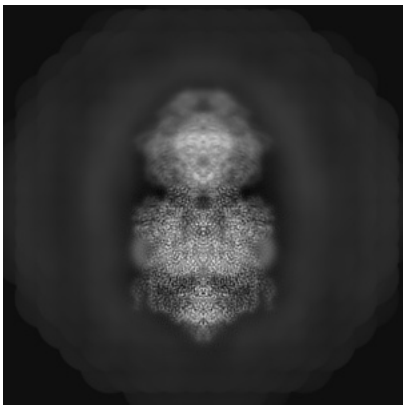
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10524. These allow visual inspection of the internal detail of the map and identification of artifacts.

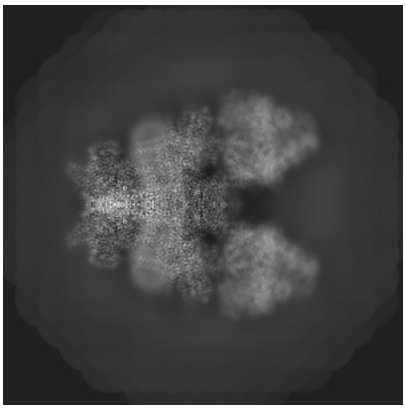
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

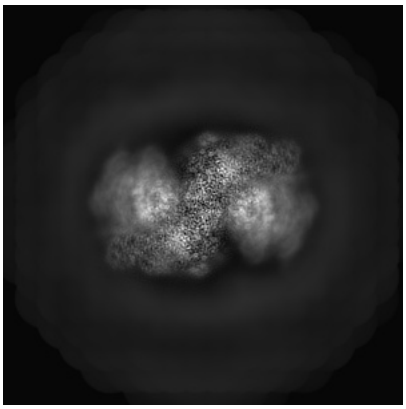
6.1.1 Primary map



X

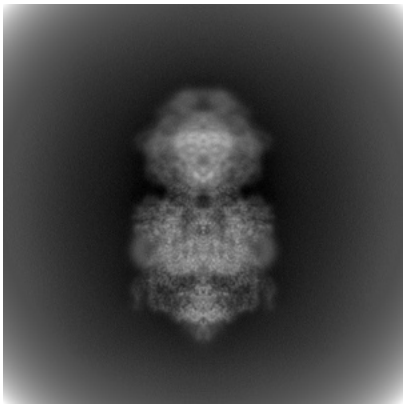


Y

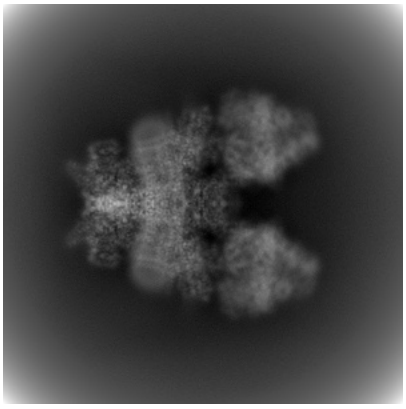


Z

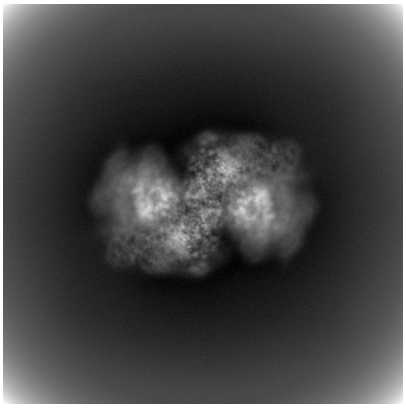
6.1.2 Raw map



X



Y

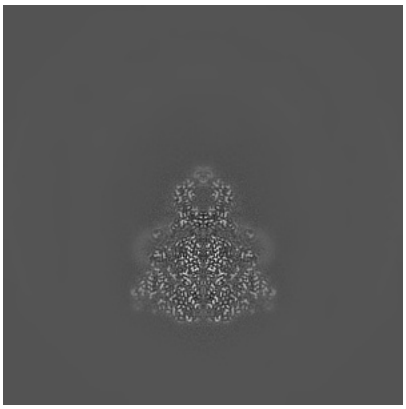


Z

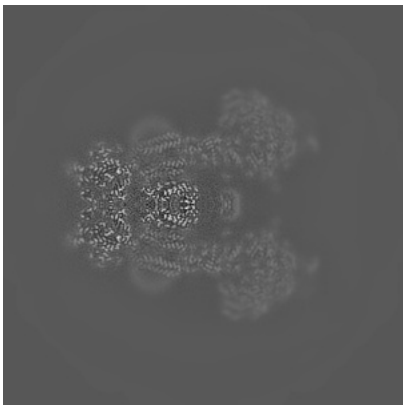
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

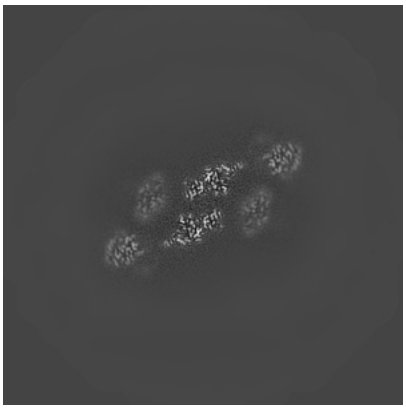
6.2.1 Primary map



X Index: 280

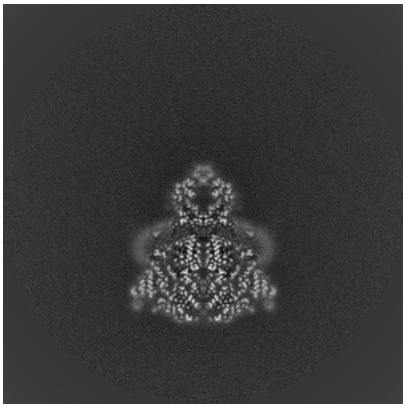


Y Index: 280

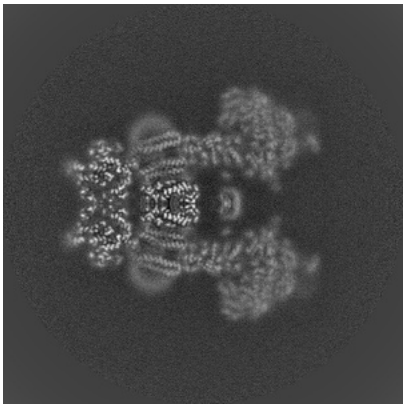


Z Index: 280

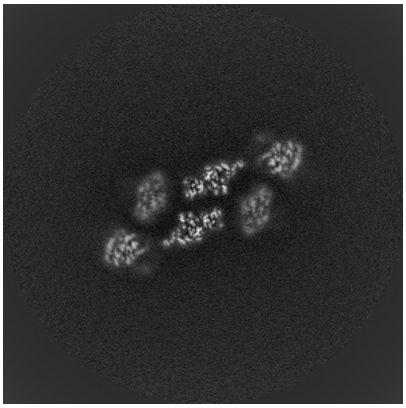
6.2.2 Raw map



X Index: 280



Y Index: 280

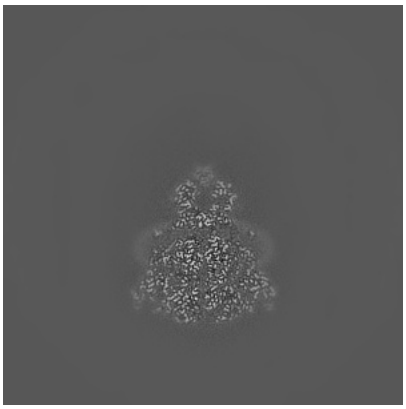


Z Index: 280

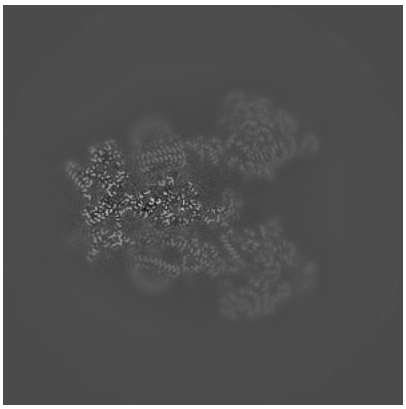
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

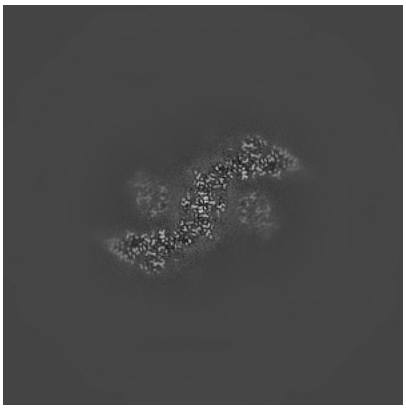
6.3.1 Primary map



X Index: 282

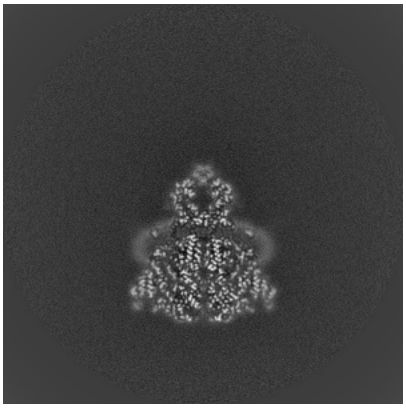


Y Index: 289

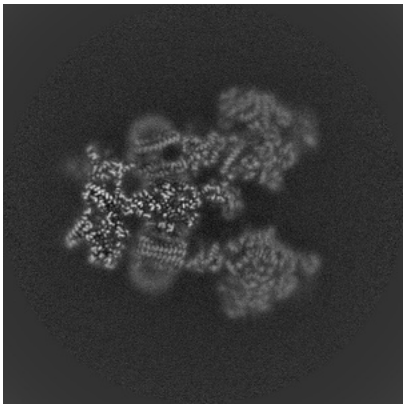


Z Index: 253

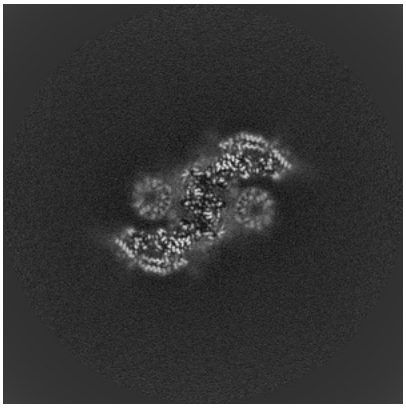
6.3.2 Raw map



X Index: 279



Y Index: 271

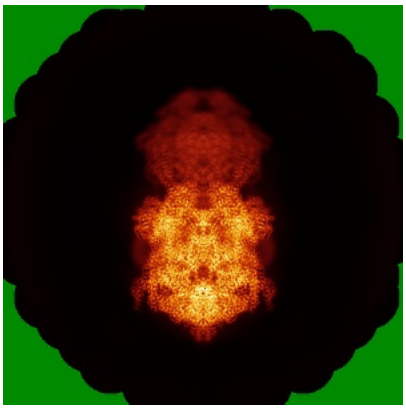


Z Index: 248

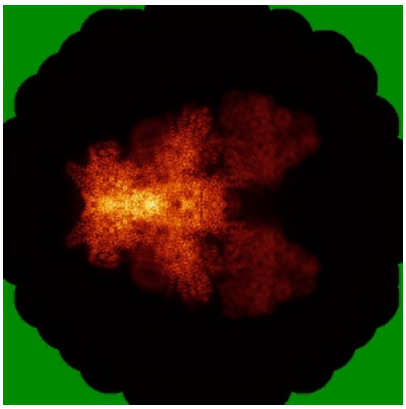
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

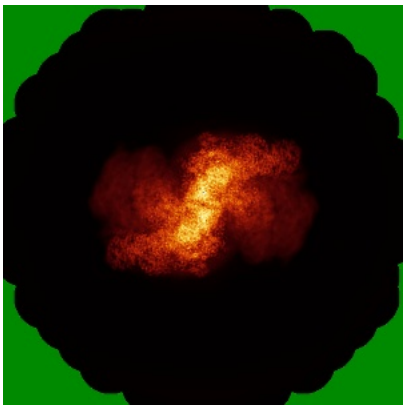
6.4.1 Primary map



X

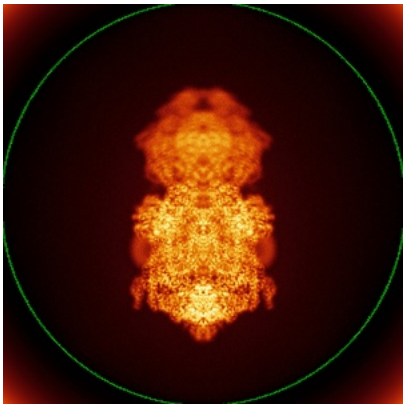


Y

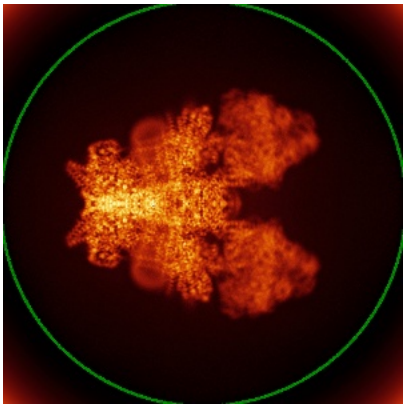


Z

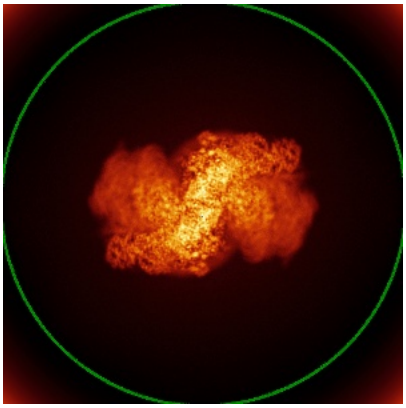
6.4.2 Raw map



X



Y

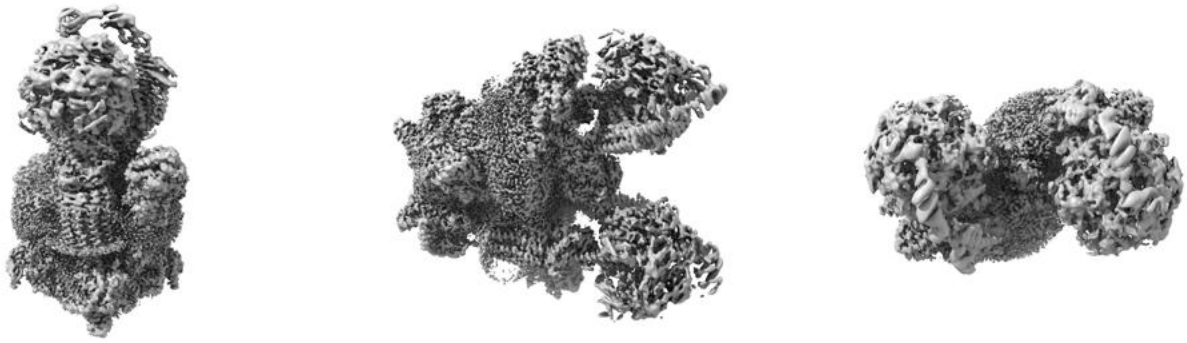


Z

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 0.024. 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.

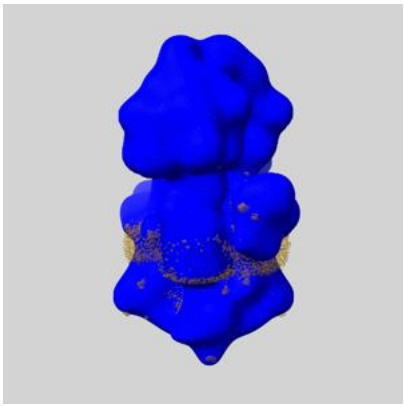
6.6 Mask visualisation (i)

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

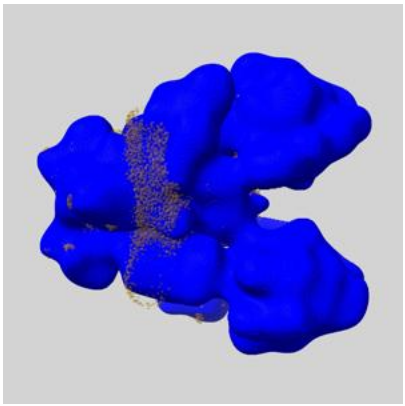
A mask typically either:

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

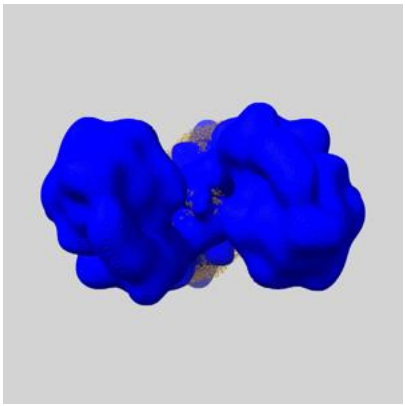
6.6.1 emd_10524_msk_1.map (i)



X



Y

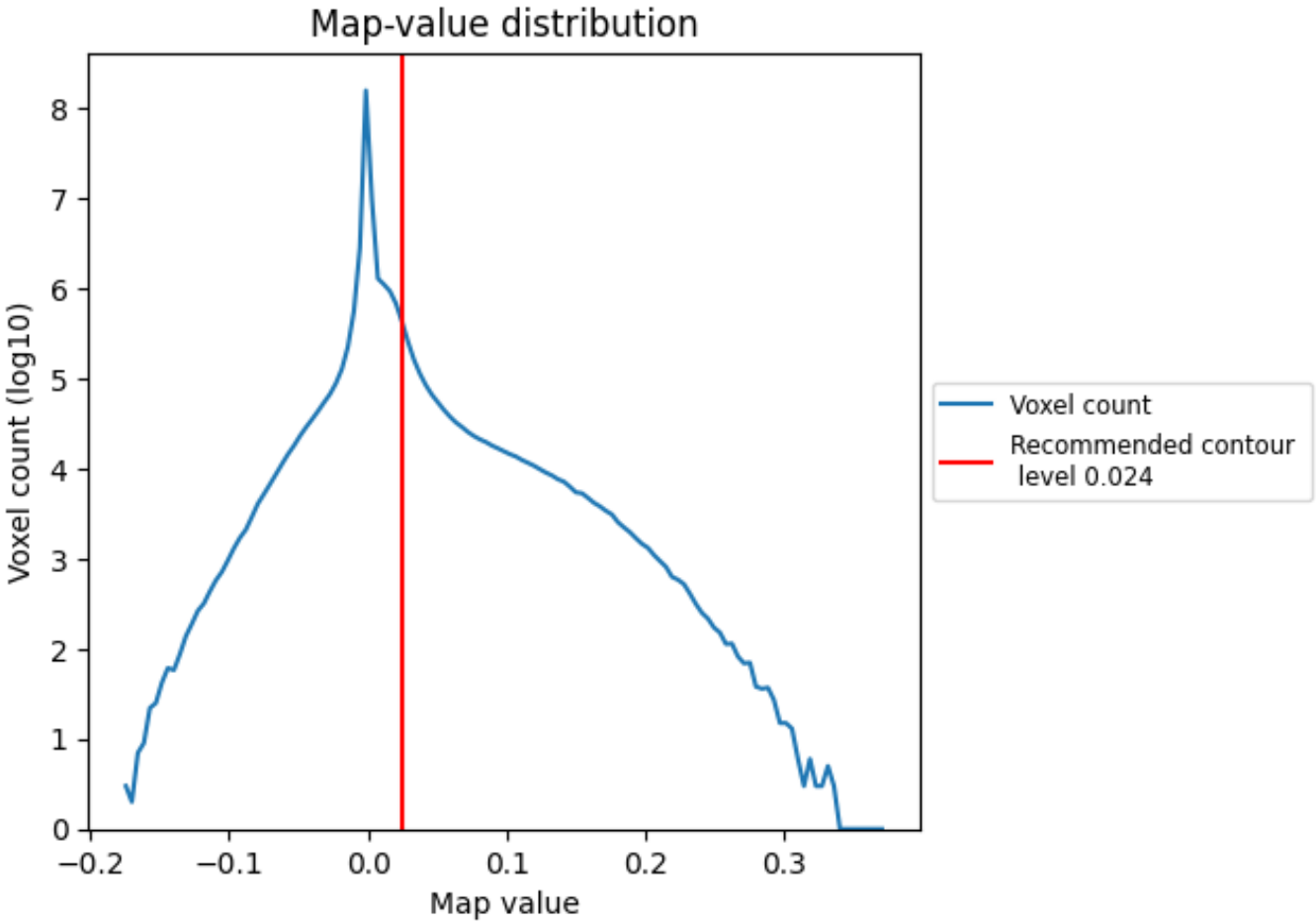


Z

7 Map analysis

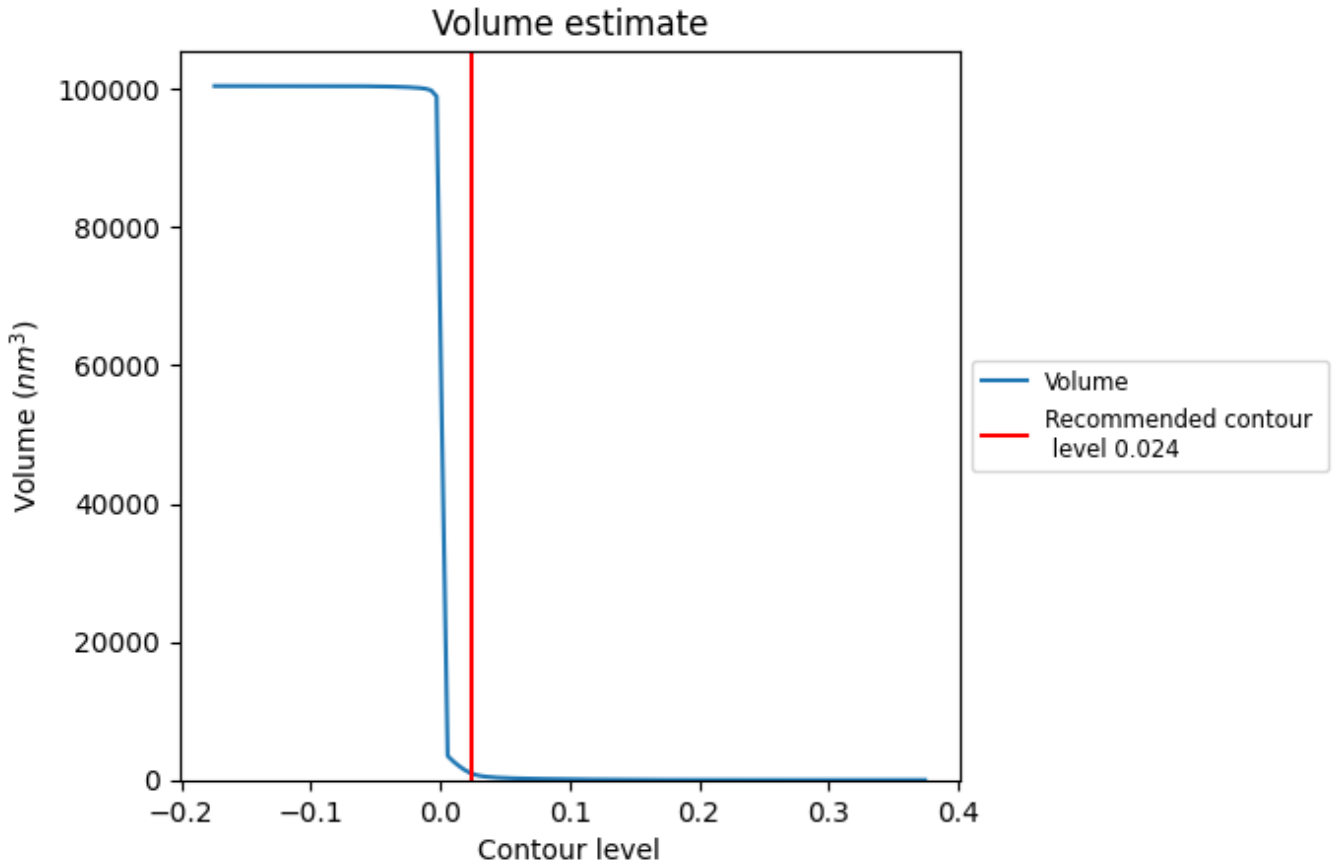
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

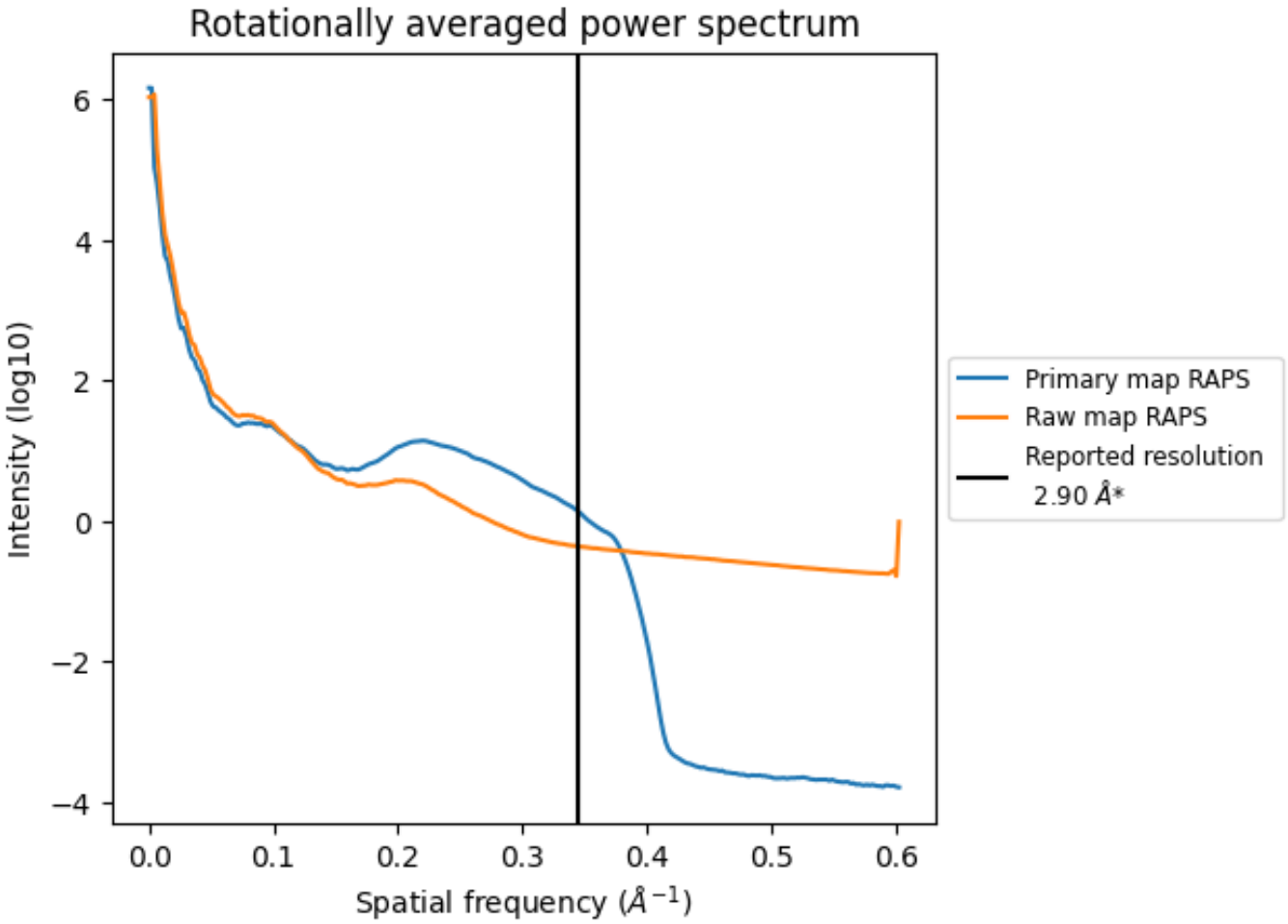
7.2 Volume estimate (i)



The volume at the recommended contour level is 964 nm^3; this corresponds to an approximate mass of 871 kDa.

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

7.3 Rotationally averaged power spectrum (i)

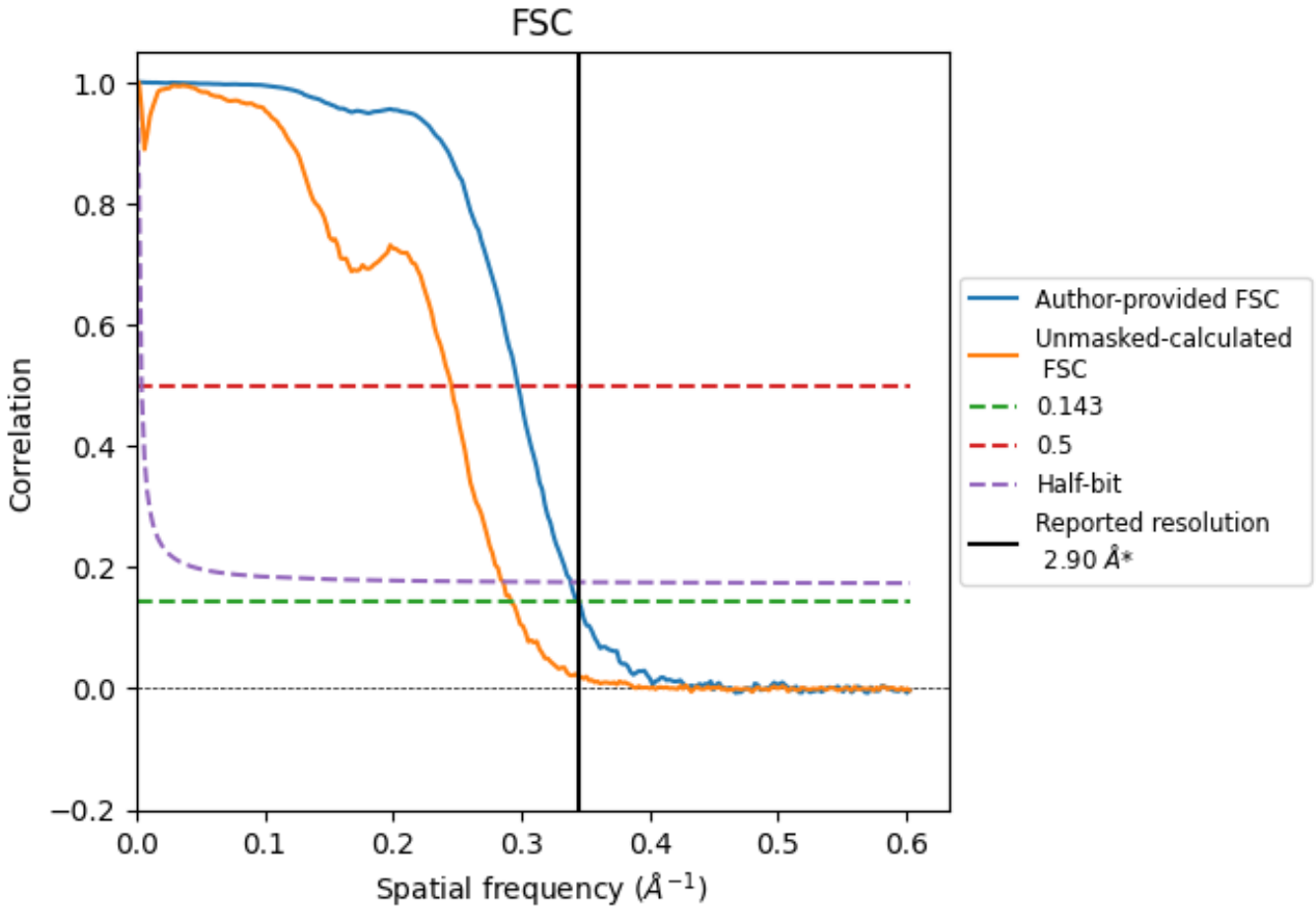


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

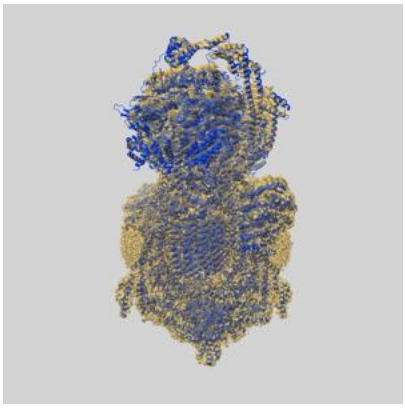
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.36	2.96
Unmasked-calculated*	3.42	4.07	3.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 2.9 by more than 10 %

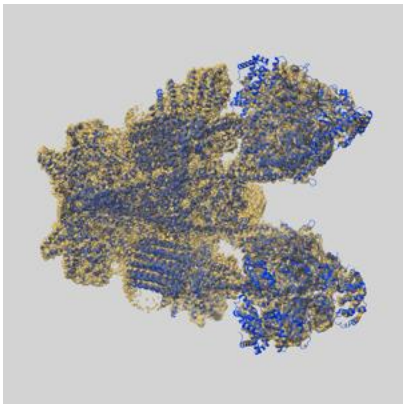
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10524 and PDB model 6TMK. Per-residue inclusion information can be found in section 3 on page 22.

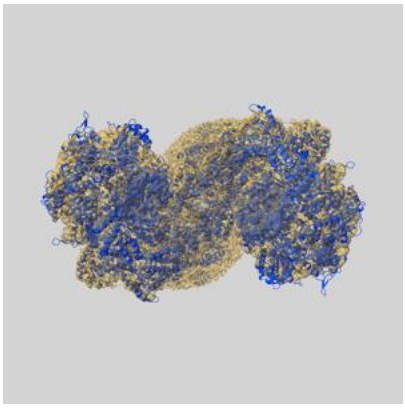
9.1 Map-model overlay



X



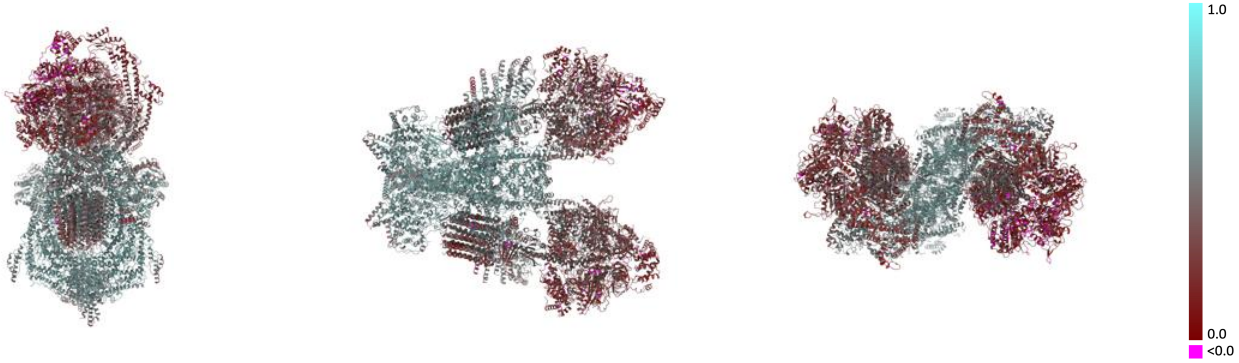
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.024 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.

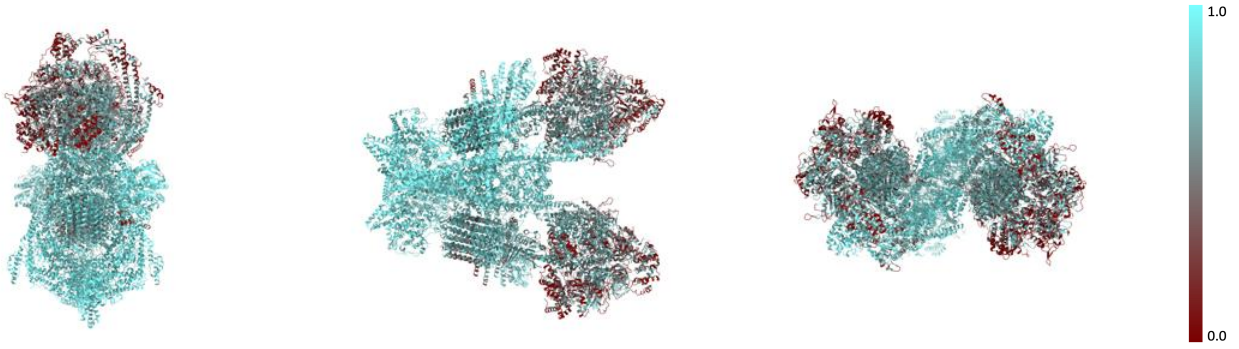
9.2 Q-score mapped to coordinate model



X Y Z

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

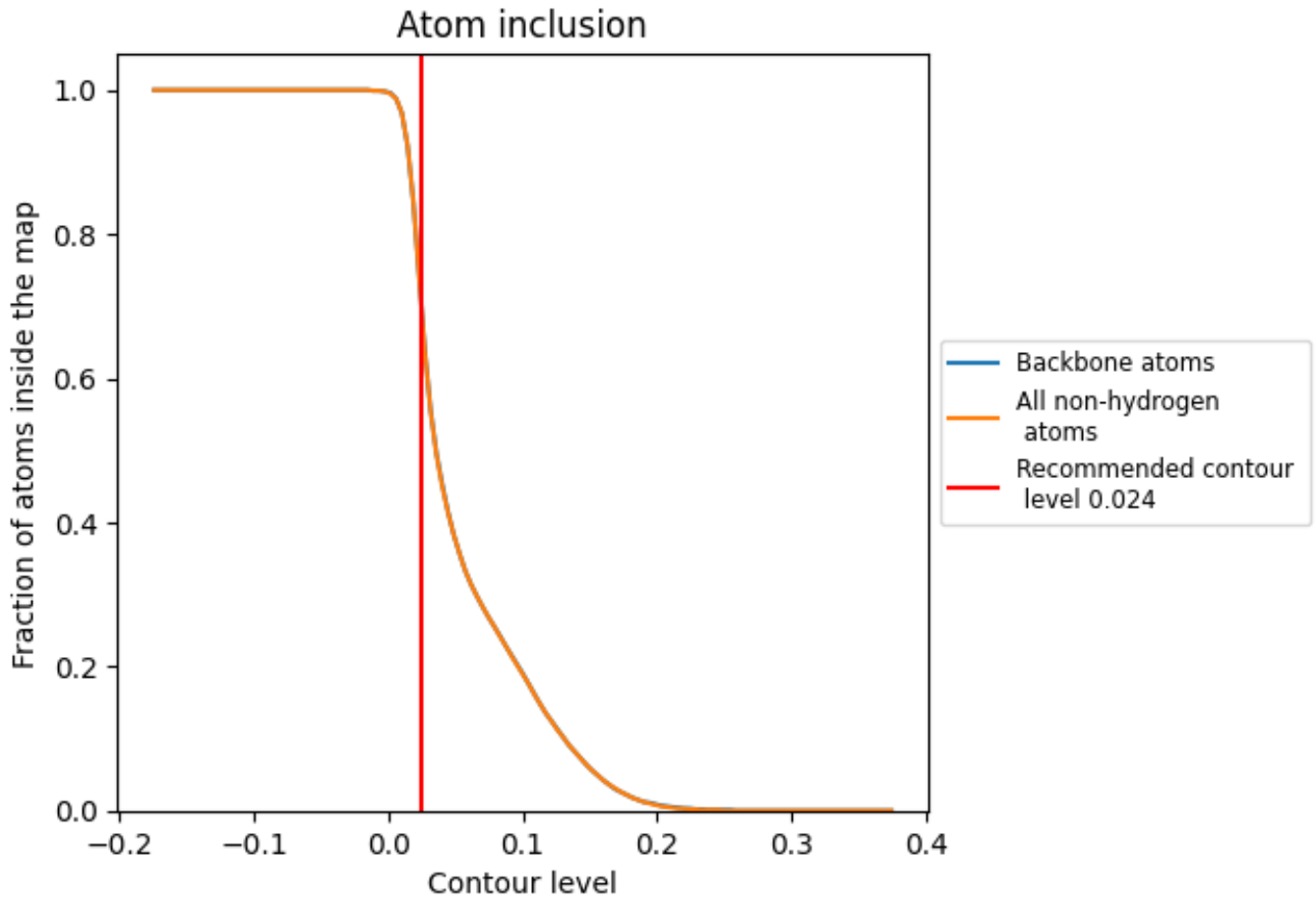
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.024).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 72% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7150	0.4280
A	0.8470	0.4810
A1	0.4340	0.2970
A2	0.3700	0.1910
B	0.7260	0.4360
B1	0.6200	0.3500
B2	0.5910	0.2850
C	0.8440	0.5420
C1	0.6150	0.3250
C2	0.6100	0.3240
D	0.9320	0.6040
D1	0.5760	0.3110
D2	0.5550	0.2820
E	0.9330	0.6020
E1	0.4690	0.2590
E2	0.4100	0.1970
F	0.9180	0.5630
F1	0.3650	0.2420
F2	0.3170	0.1800
G	0.9400	0.5900
G1	0.3520	0.1840
G2	0.2880	0.1440
H	0.9410	0.6190
H1	0.7040	0.3560
H2	0.7450	0.4120
I	0.9050	0.5370
I1	0.6660	0.3560
I2	0.7120	0.4010
J	0.9650	0.6490
J1	0.6560	0.3200
J2	0.7140	0.3860
K	0.8900	0.5740
K1	0.6900	0.3410
K2	0.7200	0.3920
L	0.9450	0.5990

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Chain	Atom inclusion	Q-score
L1	0.7120	0.3660
L2	0.6760	0.3680
M	0.9560	0.6260
M1	0.7520	0.4060
M2	0.6840	0.3570
N	0.9060	0.5500
N1	0.7500	0.4400
N2	0.7300	0.4070
O	0.8920	0.5760
O1	0.8070	0.4980
O2	0.7790	0.4730
P	0.9440	0.5960
P1	0.8010	0.4790
P2	0.7890	0.4520
Q	0.8810	0.4970
Q1	0.7870	0.4470
Q2	0.7830	0.4280
R	0.8220	0.4970
S	0.9240	0.5760
T	0.9240	0.5390
U	0.8830	0.5770
V	0.9490	0.6250
W	0.9520	0.6180
X	0.9420	0.6040
a	0.8360	0.4830
b	0.7520	0.4400
c	0.8340	0.5400
d	0.9330	0.6040
d1	0.6060	0.2770
d2	0.7000	0.4080
e	0.9320	0.6020
e1	0.7470	0.4260
e2	0.7600	0.4350
f	0.9200	0.5610
g	0.9380	0.5910
g1	0.7300	0.4080
g2	0.7310	0.4070
h	0.9420	0.6200
i	0.9030	0.5430
i1	0.7200	0.4160
i2	0.7300	0.4320
j	0.9650	0.6470

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Chain	Atom inclusion	Q-score
k	0.8930	0.5730
l	0.9440	0.5980
m	0.9600	0.6270
n	0.9070	0.5510
o	0.8920	0.5740
p	0.9460	0.5960
q	0.8620	0.4970
r	0.8300	0.5060
s	0.9230	0.5760
t	0.9180	0.5370
u	0.8850	0.5790
v	0.9470	0.6240
w	0.9560	0.6180
x	0.9410	0.6020