Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 02:43 am GMT

PDB ID	:	6TMK
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 Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

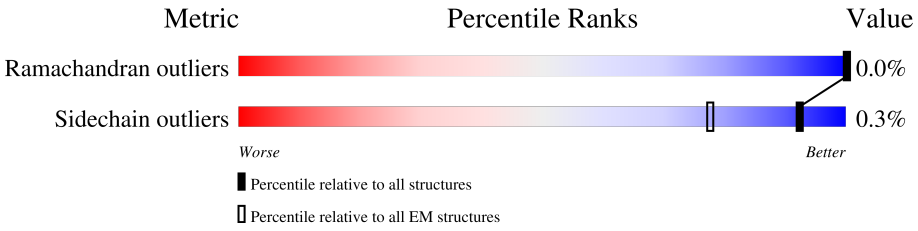
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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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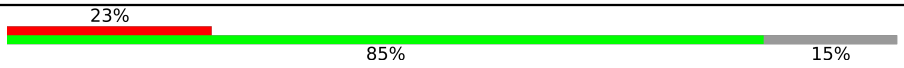
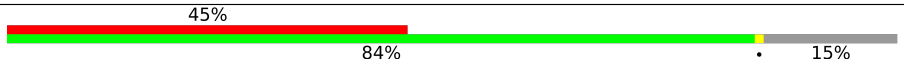
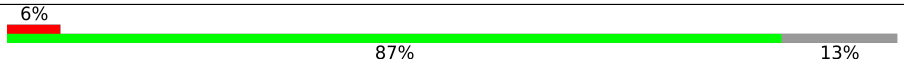
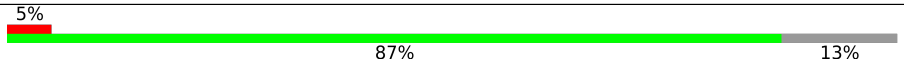
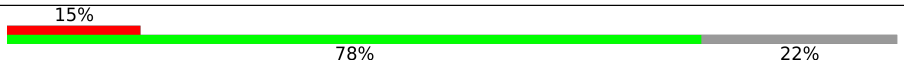
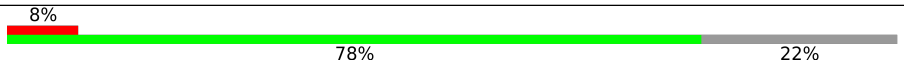
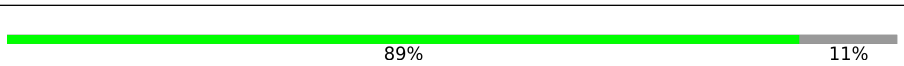
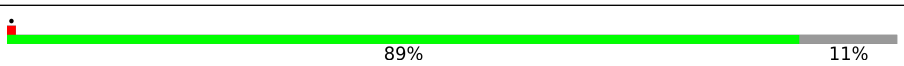
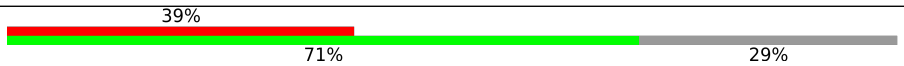
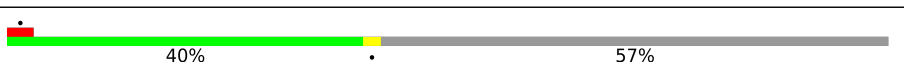
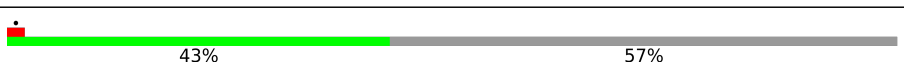
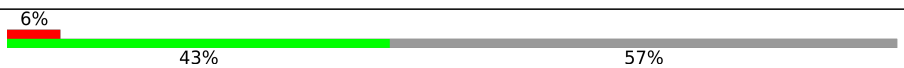
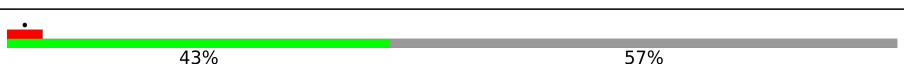
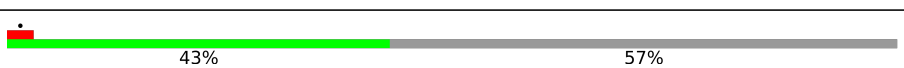
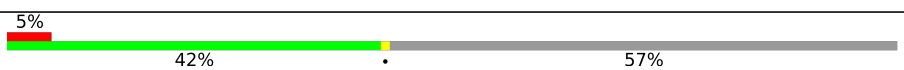
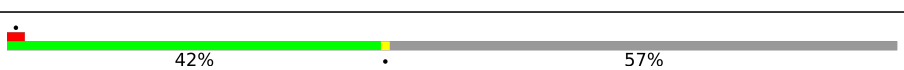
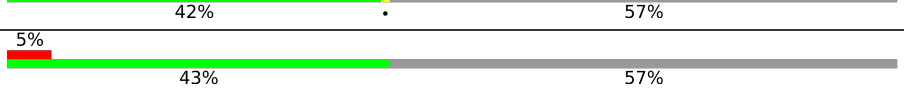
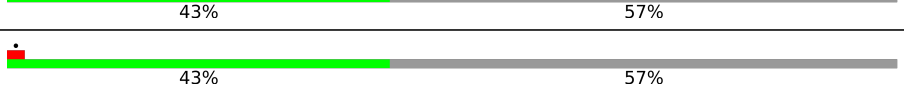
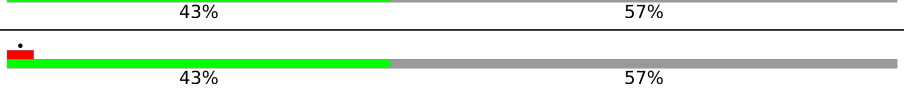
Mol	Chain	Length	Quality of chain
27	D2	560	
27	F1	560	
27	F2	560	
28	g1	314	
28	g2	314	
29	d1	183	
29	d2	183	
30	e1	73	
30	e2	73	
31	G1	252	
31	G2	252	
32	H1	166	
32	H2	166	
32	I1	166	
32	I2	166	
32	J1	166	
32	J2	166	
32	K1	166	
32	K2	166	
32	L1	166	
32	L2	166	
32	M1	166	
32	M2	166	
32	N1	166	
32	N2	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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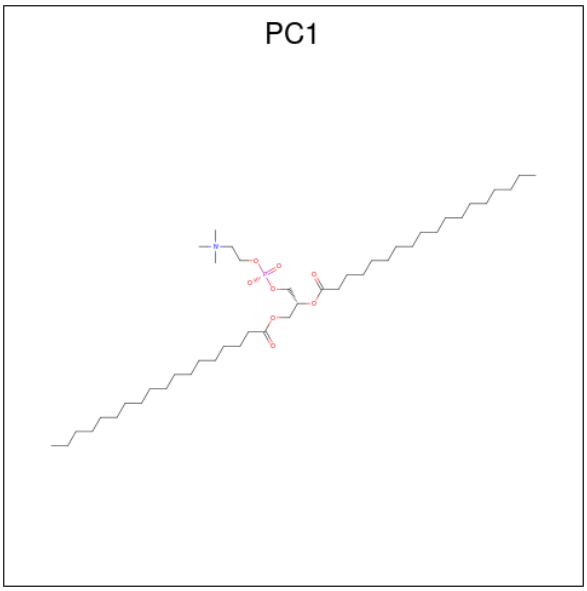
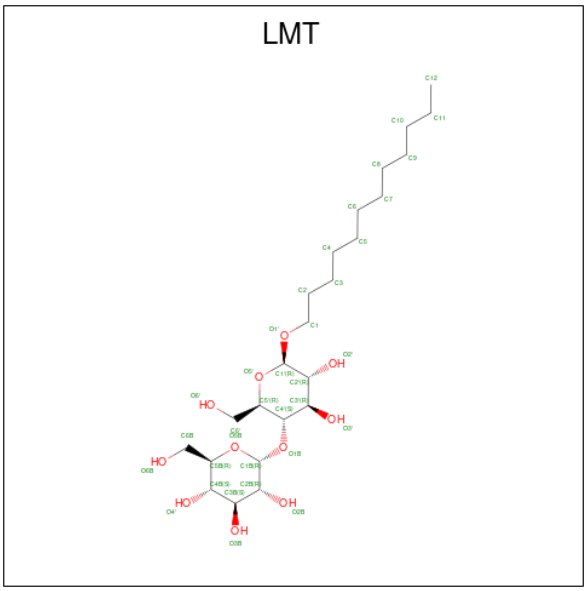
Mol	Chain	Residues	Atoms						AltConf	Trace
32	P1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	Q1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		

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



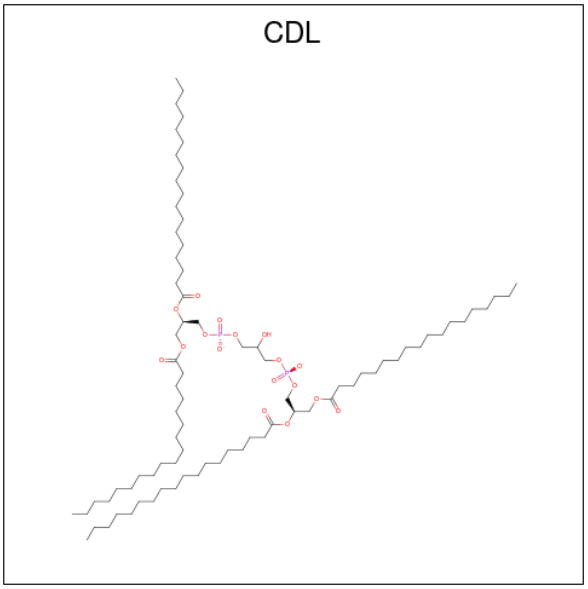
Mol	Chain	Residues	Atoms						AltConf
33	o	1	Total	C	H	N	O	P	0
			284	88	176	2	16	2	
33	o	1	Total	C	H	N	O	P	0
			284	88	176	2	16	2	
33	v	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
33	O	1	Total	C	H	N	O	P	0
			284	88	176	2	16	2	
33	O	1	Total	C	H	N	O	P	0
			284	88	176	2	16	2	
33	V	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

- Molecule 34 is DODECYL-BETA-D-MALTOSIDE (three-letter code: 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
			162	48	92	22	
34	c	1	Total	C	H	O	0
			162	48	92	22	
34	d	1	Total	C	H	O	0
			162	48	92	22	
34	d	1	Total	C	H	O	0
			162	48	92	22	
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
			162	48	92	22	
34	C	1	Total	C	H	O	0
			162	48	92	22	
34	D	1	Total	C	H	O	0
			162	48	92	22	
34	D	1	Total	C	H	O	0
			162	48	92	22	

- Molecule 35 is CARDIOLIPIN (three-letter code: 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
			512	162	312	34	4	
35	b	1	Total	C	H	O	P	0
			512	162	312	34	4	
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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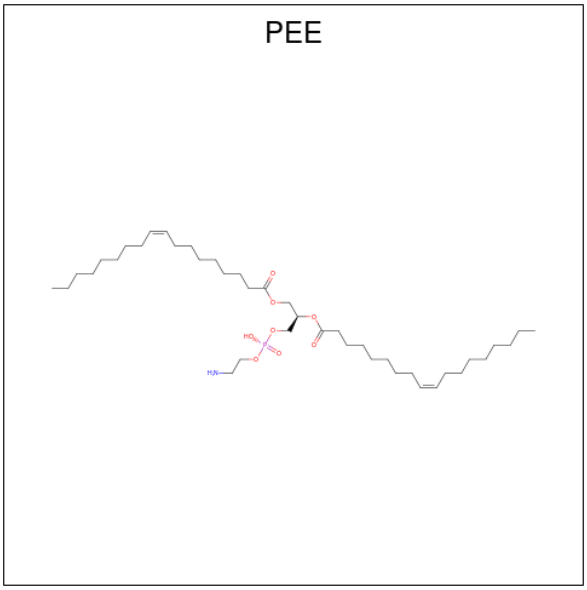
Mol	Chain	Residues	Atoms					AltConf
35	E	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	B	1	Total	C	H	O	P	0
			512	162	312	34	4	
35	B	1	Total	C	H	O	P	0
			512	162	312	34	4	
35	V	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	C	1	Total	C	H	O	P	0
			256	81	156	17	2	
35	D	1	Total	C	H	O	P	0
			256	81	156	17	2	

- Molecule 36 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: 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
			266	82	164	2	16	2	
36	j	1	Total	C	H	N	O	P	0
			266	82	164	2	16	2	
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
			266	82	164	2	16	2	
36	J	1	Total	C	H	N	O	P	0
			266	82	164	2	16	2	

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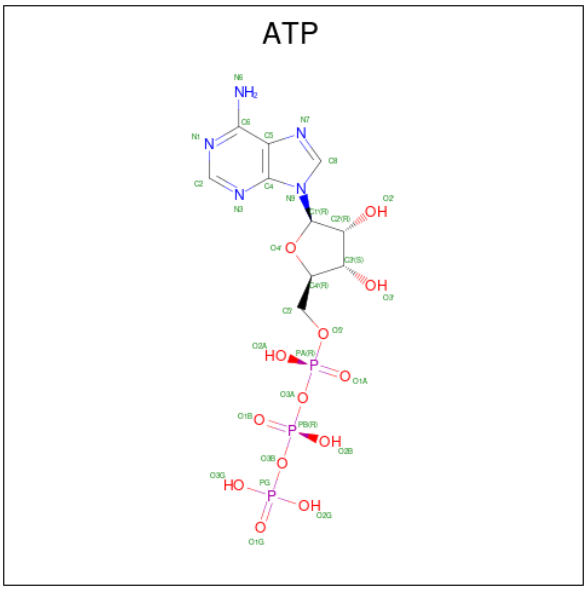
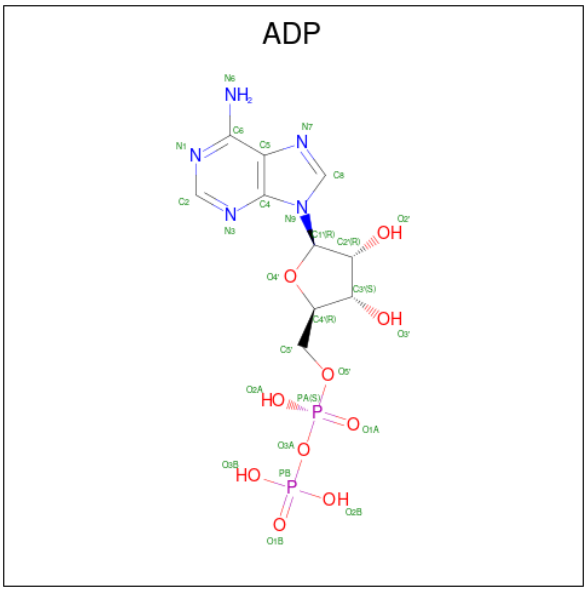
Mol	Chain	Residues	Atoms						AltConf
36	C	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

- Molecule 37 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: 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 (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



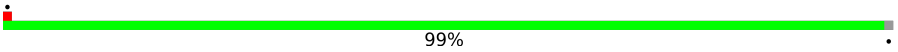
Mol	Chain	Residues	Atoms						AltConf
38	B2	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
38	D2	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	
38	B1	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	
38	D1	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	

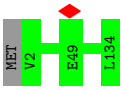
3 Residue-property plots (i)

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

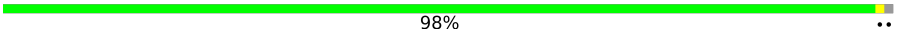
Chain q:

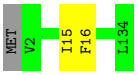




• Molecule 1: ATPTG11

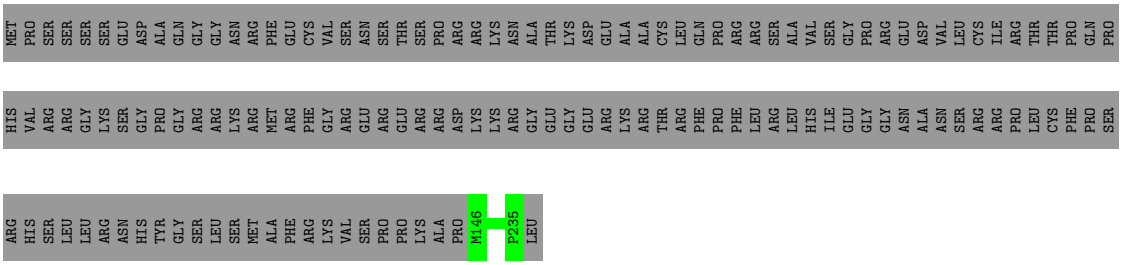
Chain Q:





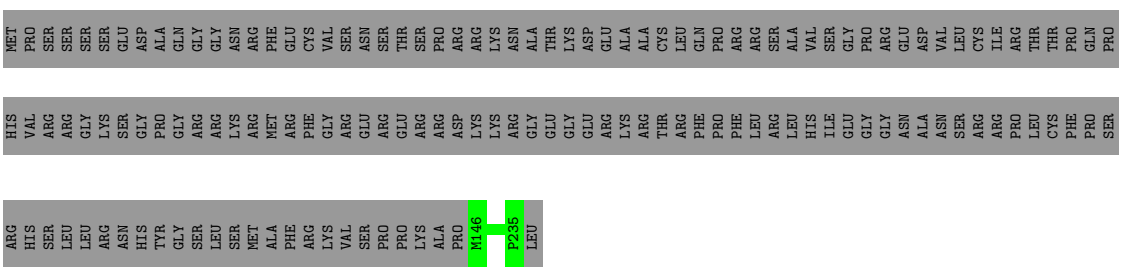
• Molecule 2: ATPTG7

Chain i:



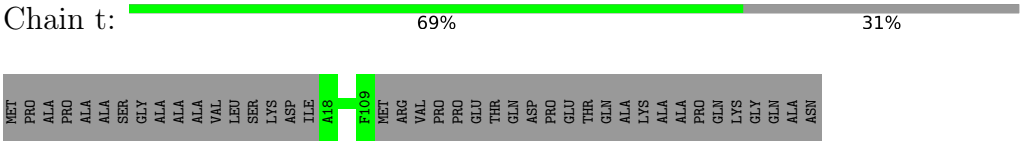
• Molecule 2: ATPTG7

Chain I:



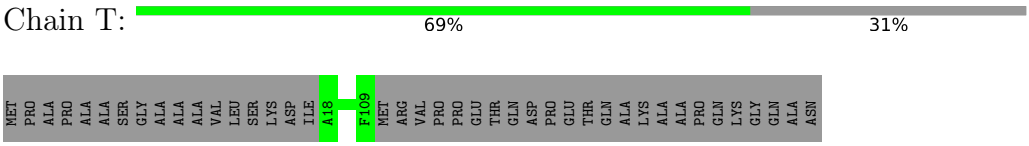
• Molecule 3: ATPTG14

Chain t:



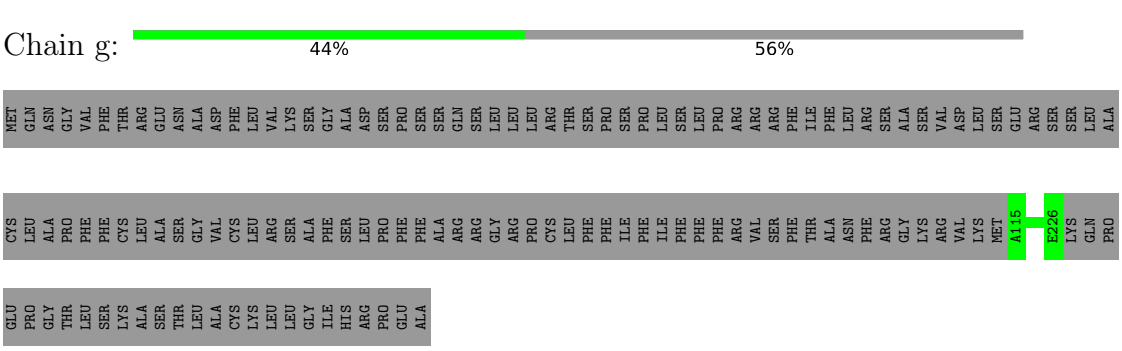
• Molecule 3: ATPTG14

Chain T:



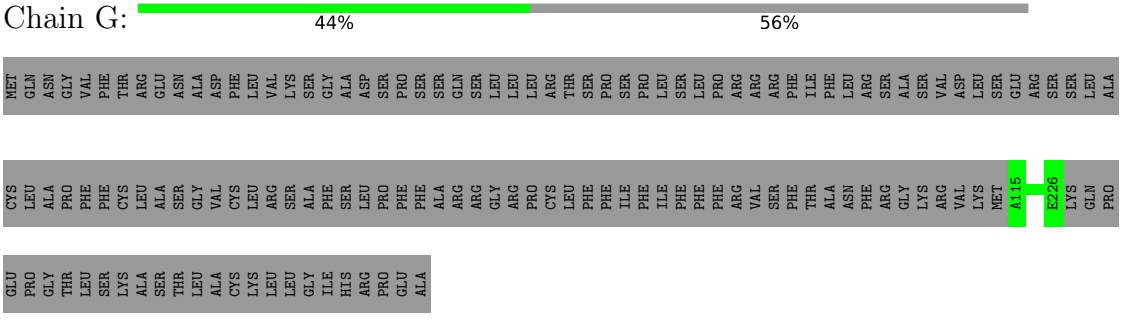
• Molecule 4: ATPTG5

Chain g:



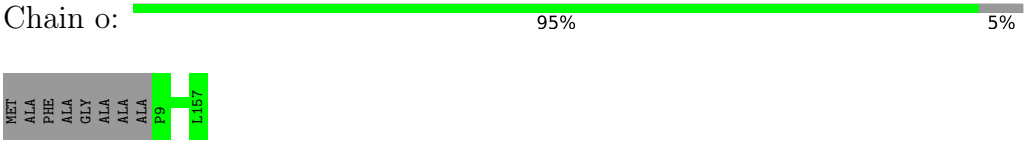
• Molecule 4: ATPTG5

Chain G:



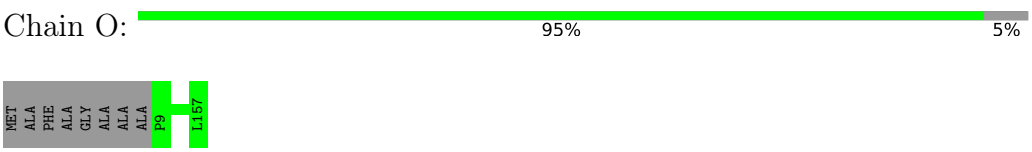
• Molecule 5: subunit k

Chain o:



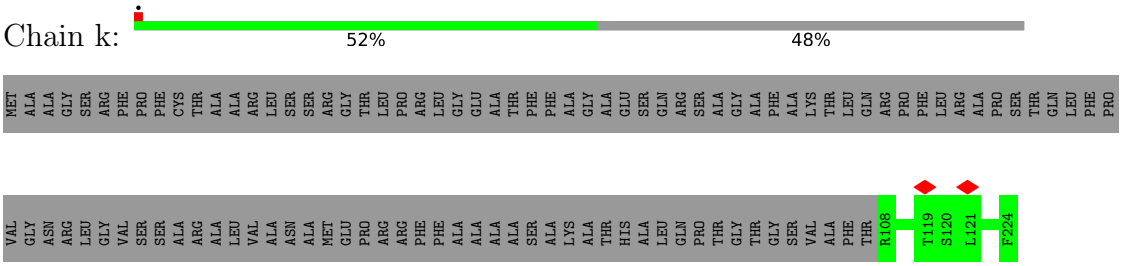
• Molecule 5: subunit k

Chain O:



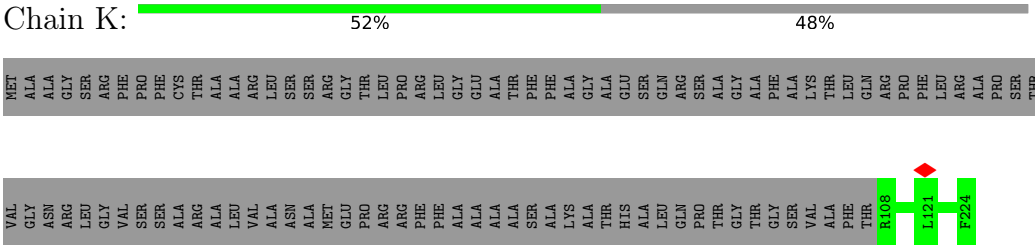
• Molecule 6: subunit a

Chain k:



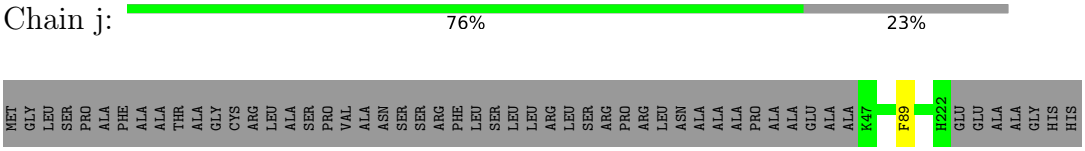
• Molecule 6: subunit a

Chain K:



• Molecule 7: subunit i/j

Chain j:

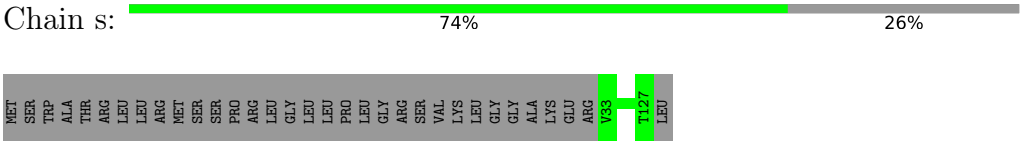


• Molecule 7: subunit i/j

Chain J:

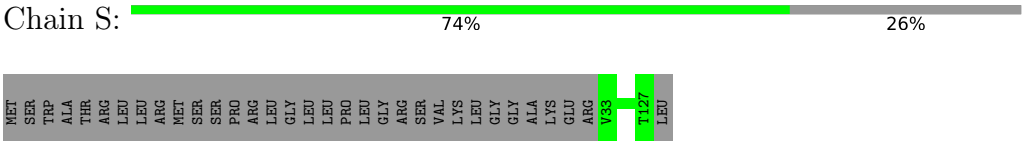
• Molecule 8: ATPTG13

Chain s:



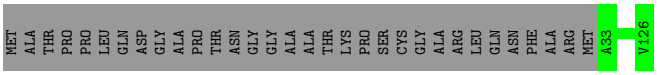
• Molecule 8: ATPTG13

Chain S:



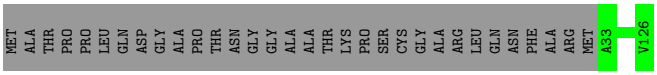
• Molecule 9: ATPTG15

Chain u:



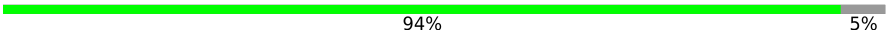
• Molecule 9: ATPTG15

Chain U:



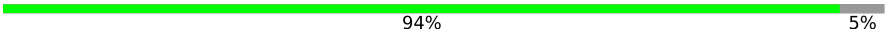
• Molecule 10: ATPTG6

Chain h:



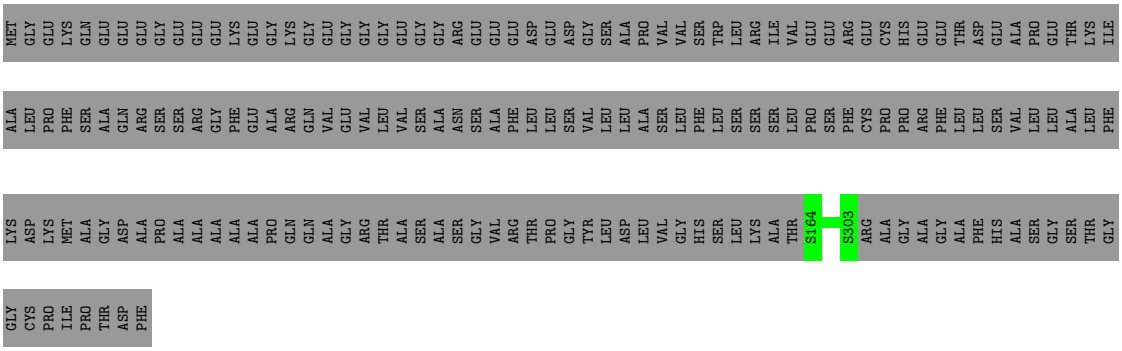
• Molecule 10: ATPTG6

Chain H:



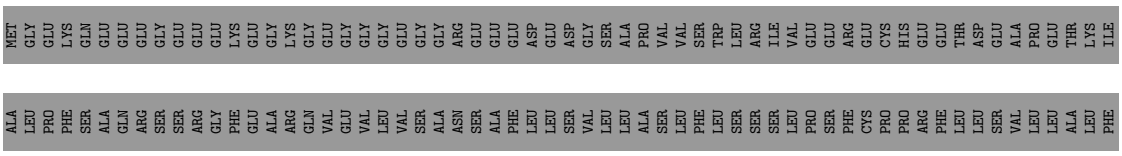
• Molecule 11: ATPTG3

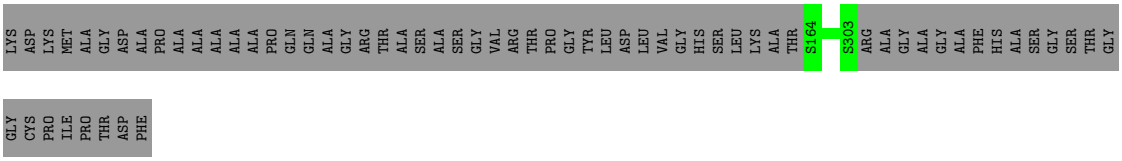
Chain e:



• Molecule 11: ATPTG3

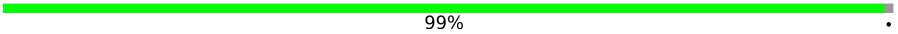
Chain E:





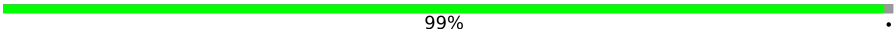
• Molecule 12: ATPTG17

Chain x:



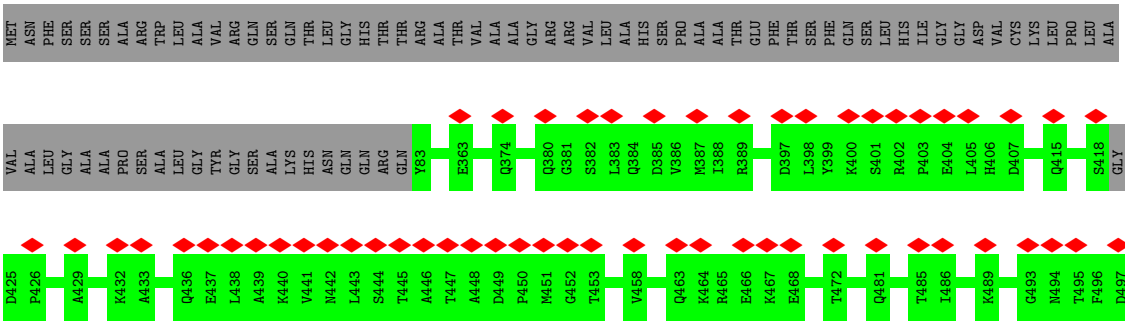
• Molecule 12: ATPTG17

Chain X:



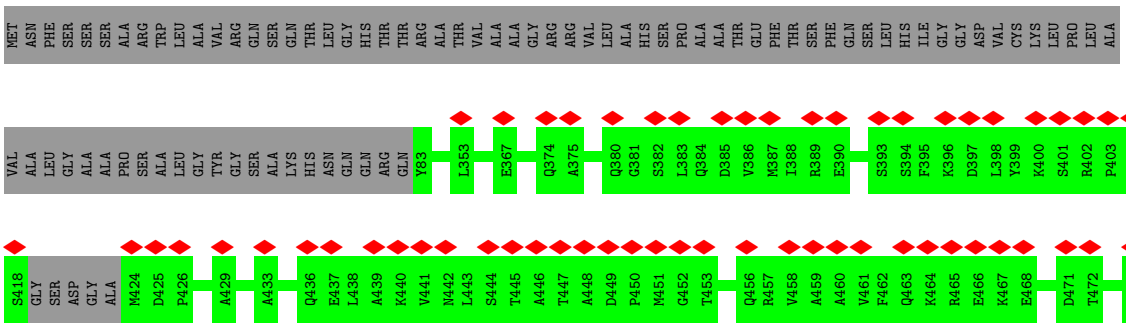
• Molecule 13: subunit b

Chain b:

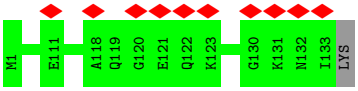


• Molecule 13: subunit b

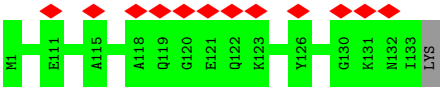
Chain B:



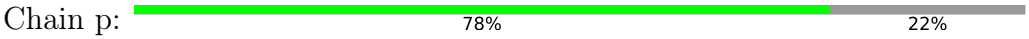
• Molecule 14: ATPTG12

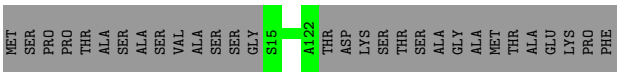


• Molecule 14: ATPTG12

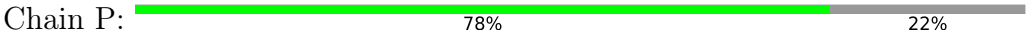


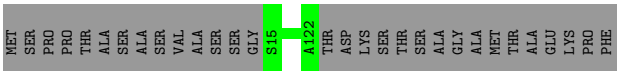
• Molecule 15: ATPTG10





• Molecule 15: ATPTG10





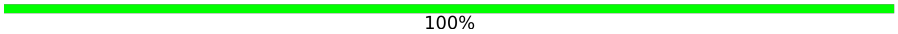
• Molecule 16: subunit f

• Molecule 16: subunit f

• Molecule 17: ATPTG8

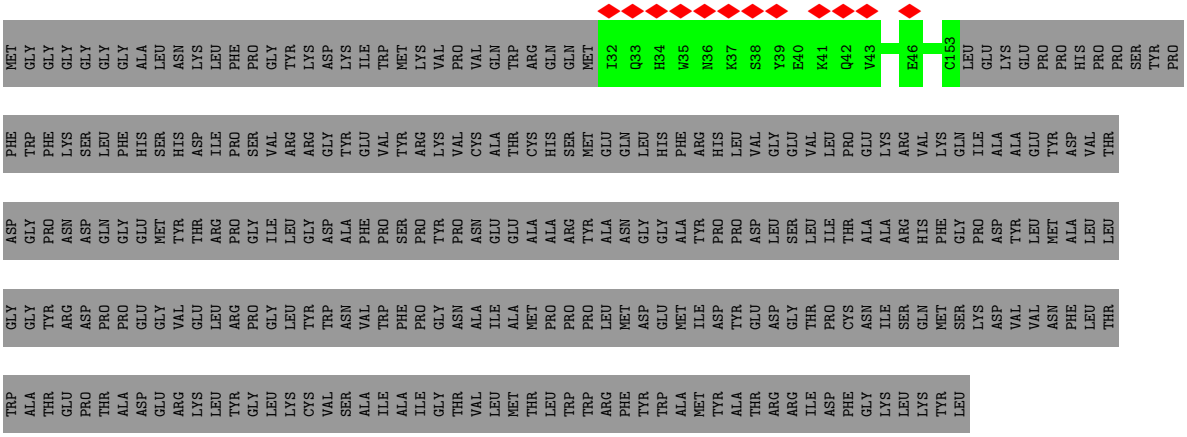
• Molecule 17: ATPTG8

Chain L:



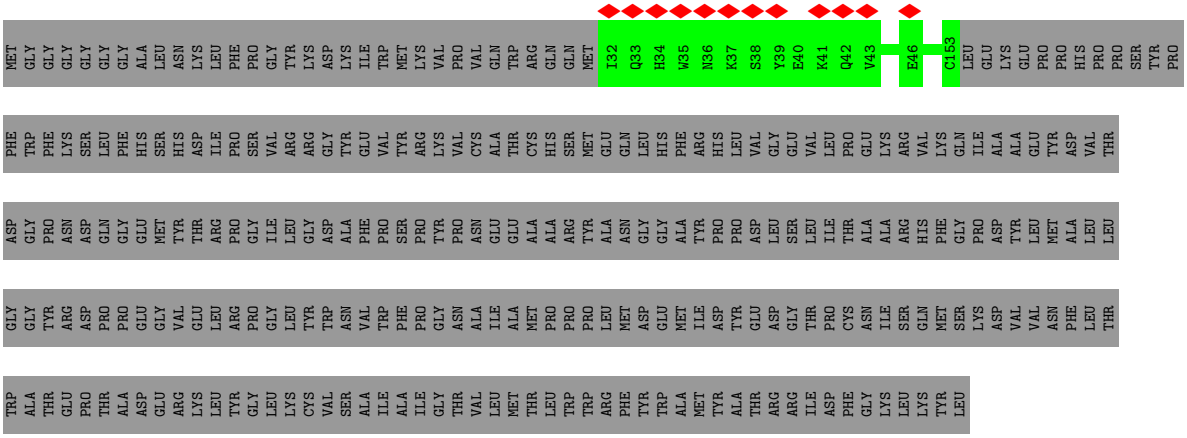
• Molecule 18: ATPTG1

Chain c:



• Molecule 18: ATPTG1

Chain C:



• Molecule 19: ATPTG2

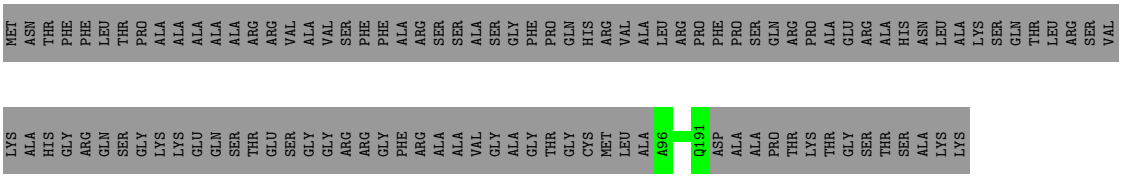
Chain d:

• Molecule 19: ATPTG2

Chain D:

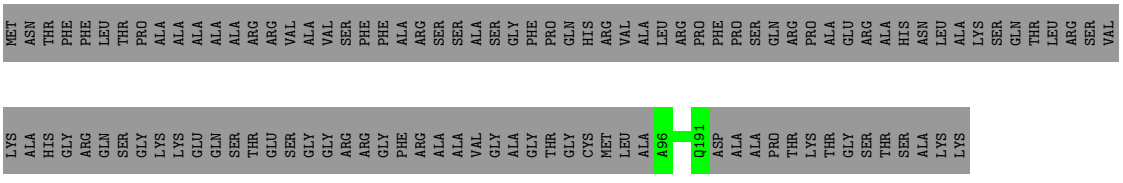
• Molecule 20: subunit 8

Chain m:



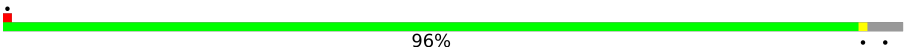
• Molecule 20: subunit 8

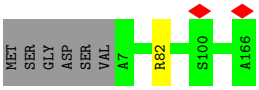
Chain M:



• Molecule 21: ATPTG9

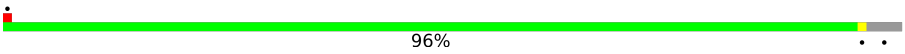
Chain n:

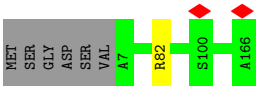




• Molecule 21: ATPTG9

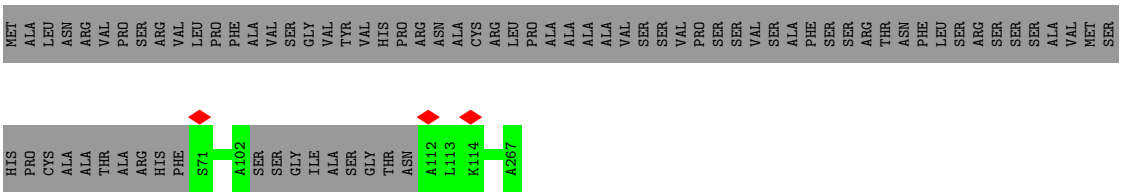
Chain N:





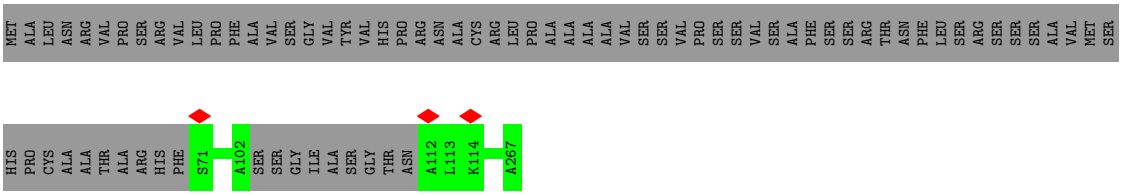
• Molecule 22: ATPTG4

Chain f:



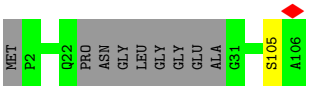
• Molecule 22: ATPTG4

Chain F:



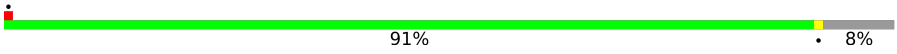
• Molecule 23: ATPTG16

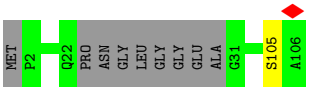
Chain w:



• Molecule 23: ATPTG16

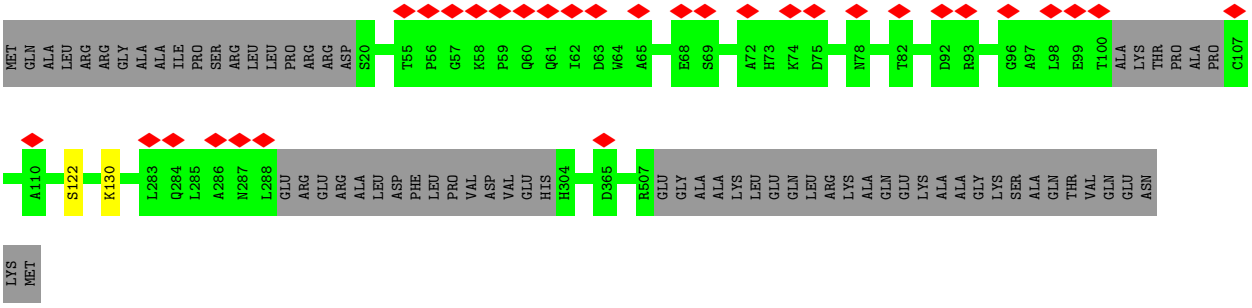
Chain W:





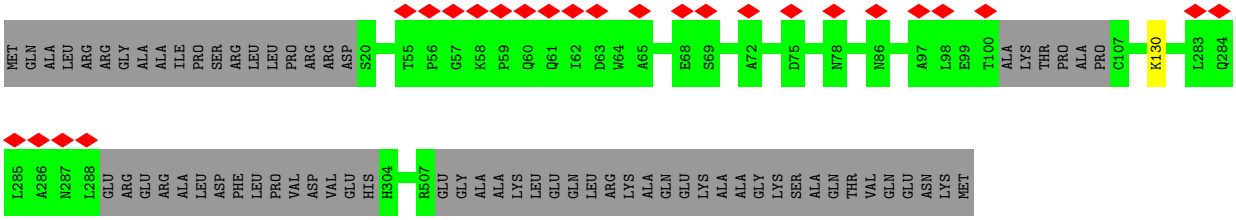
• Molecule 24: subunit d

Chain a:



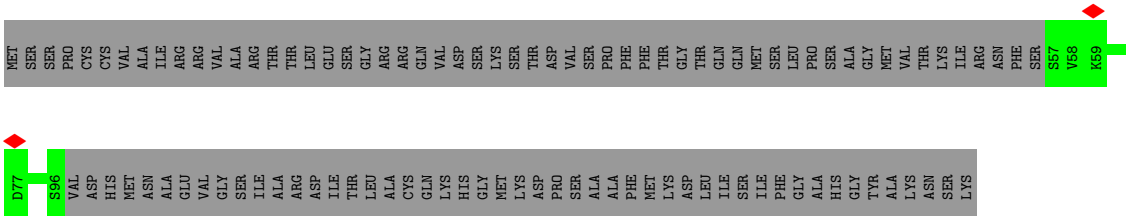
• Molecule 24: subunit d

Chain A:



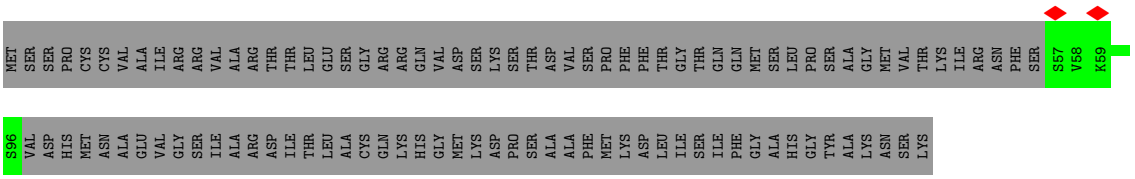
• Molecule 25: Inhibitor of F1

Chain i2:



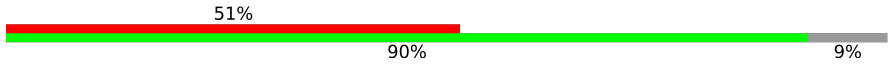
• Molecule 25: Inhibitor of F1

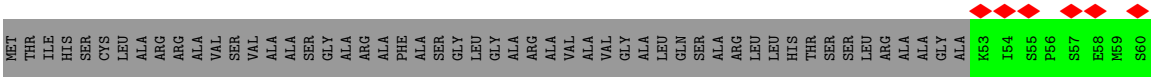
Chain i1:

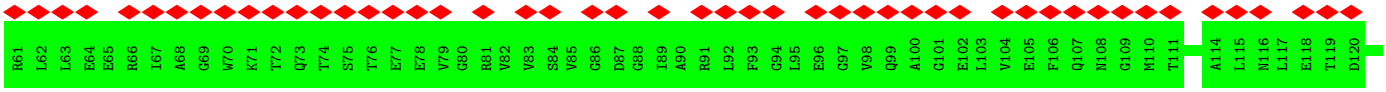


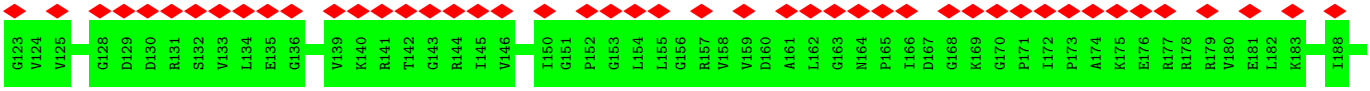
• Molecule 26: ATP synthase subunit alpha,subunit alpha

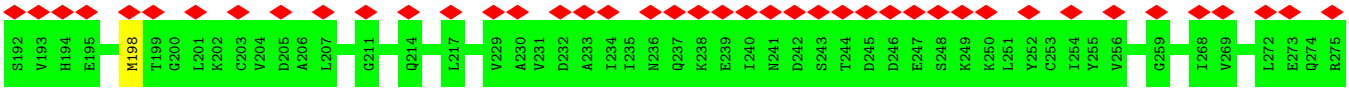
Chain A2:

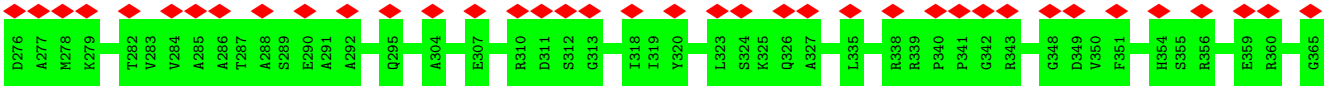


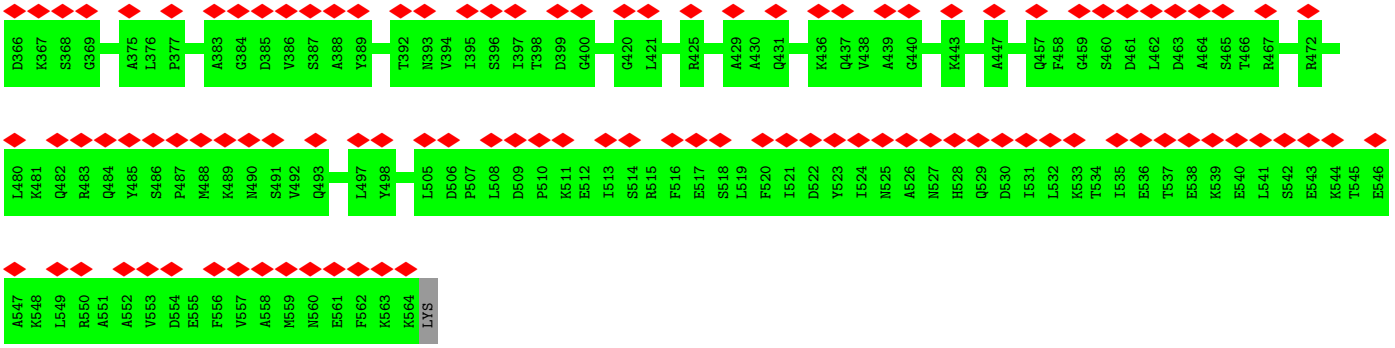






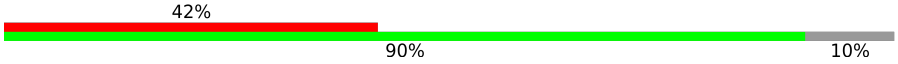


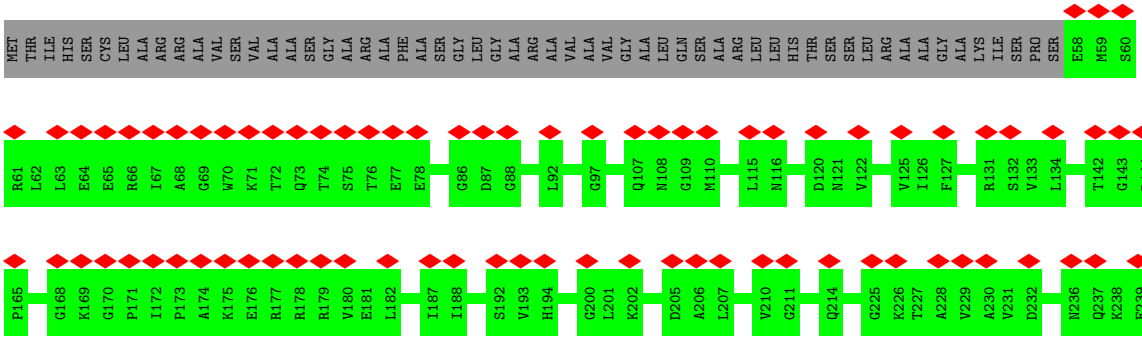




• Molecule 26: ATP synthase subunit alpha,subunit alpha

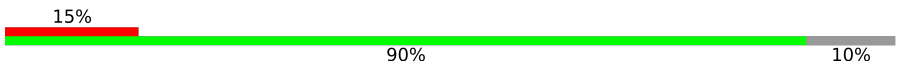
Chain E2:

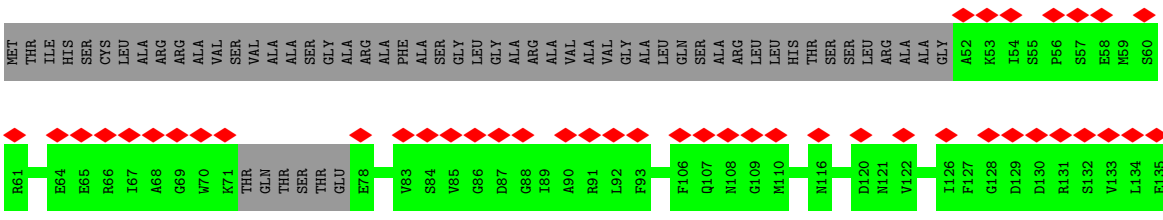


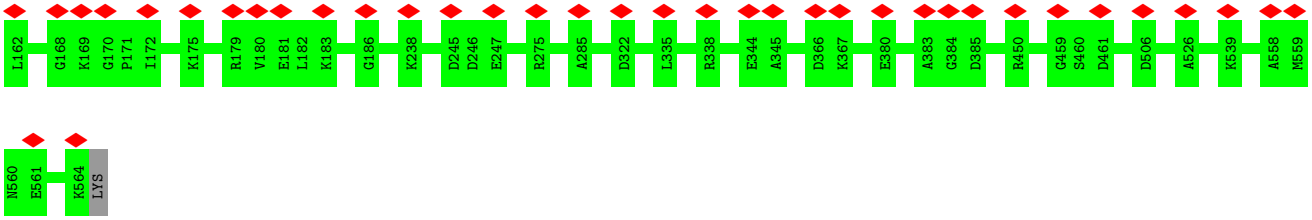


• Molecule 26: ATP synthase subunit alpha,subunit alpha

Chain C2:

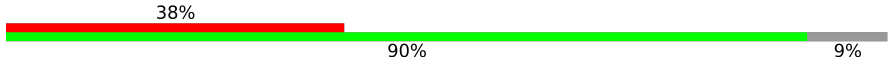


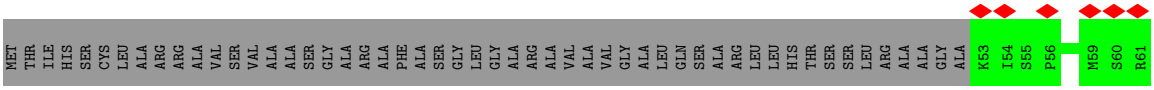


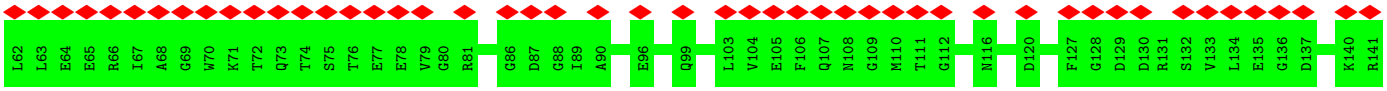


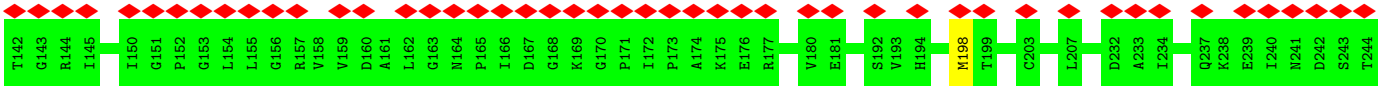
• Molecule 26: ATP synthase subunit alpha,subunit alpha

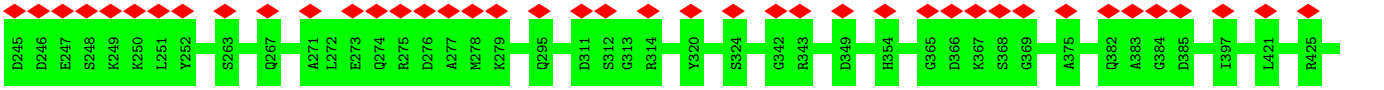
Chain A1:

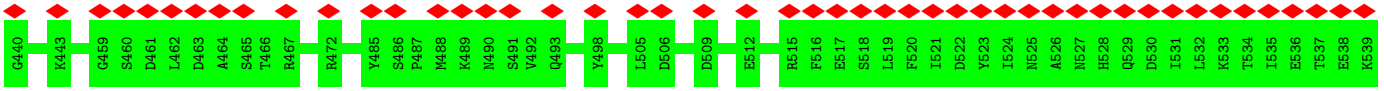


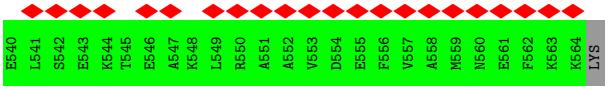






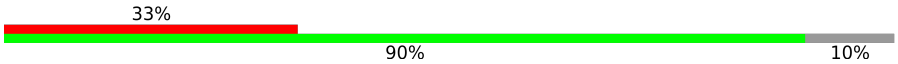


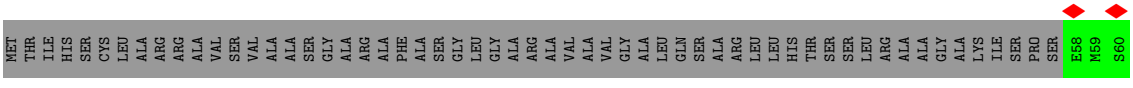


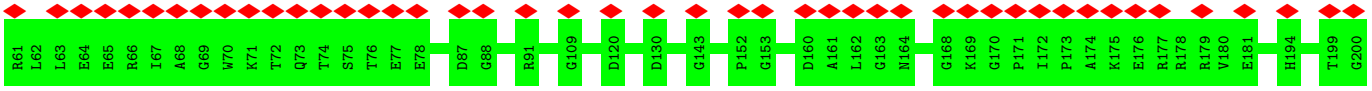


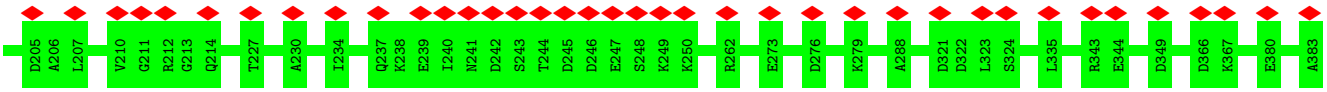
• Molecule 26: ATP synthase subunit alpha,subunit alpha

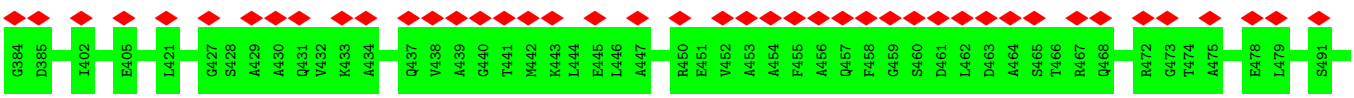
Chain E1:

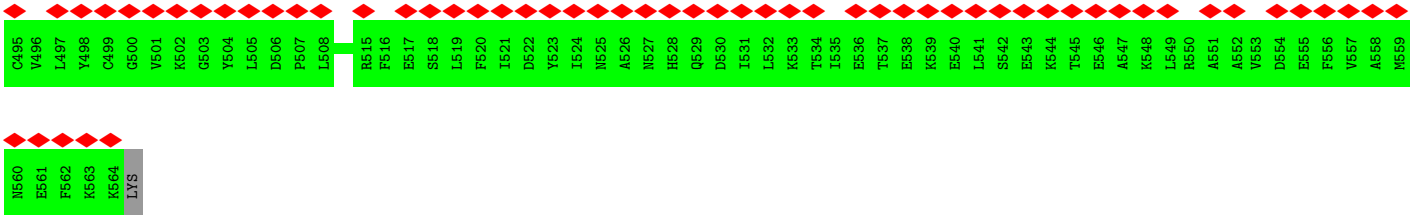






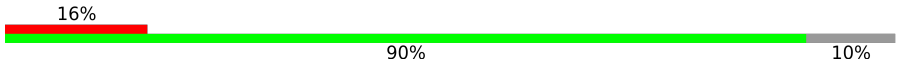


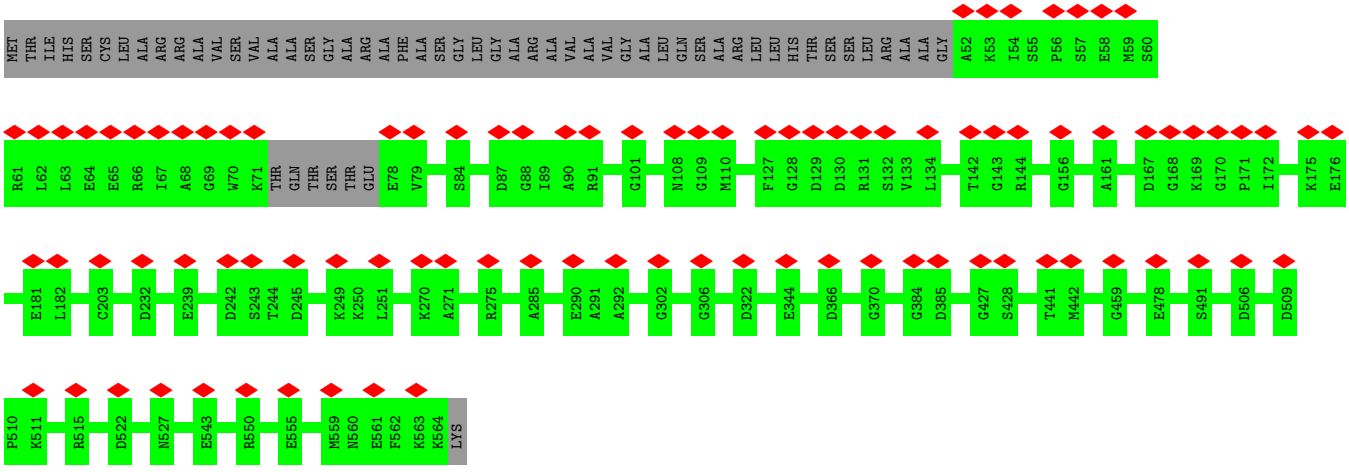




• Molecule 26: ATP synthase subunit alpha,subunit alpha

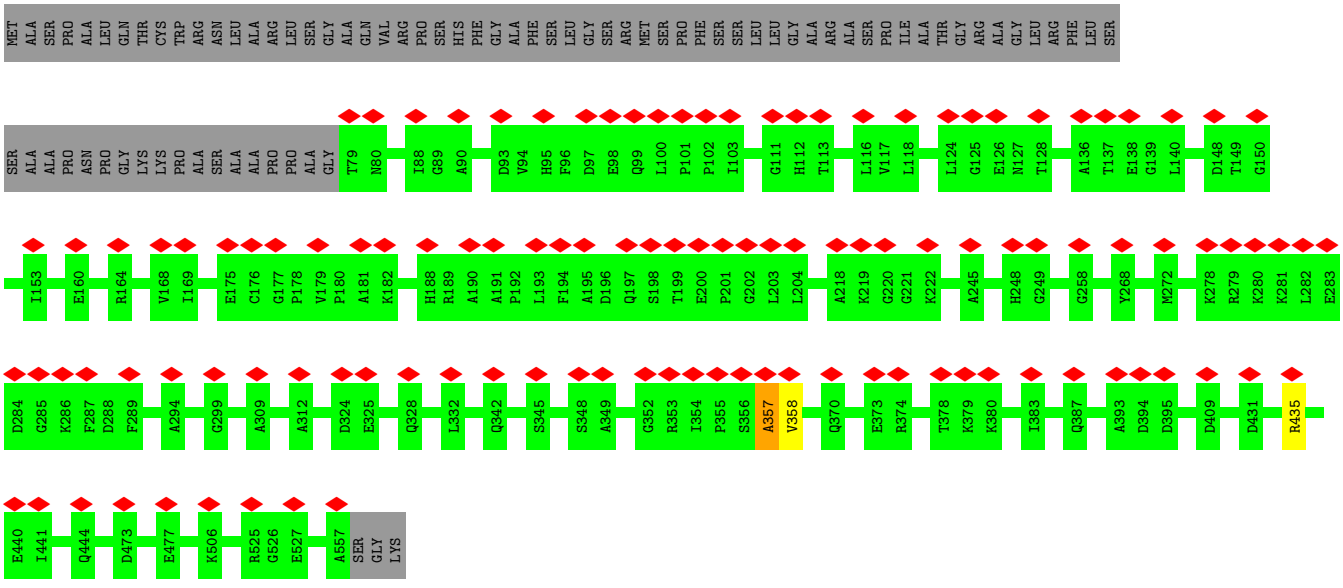
Chain C1:





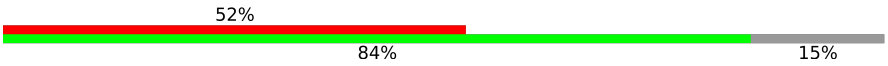
• Molecule 27: ATP synthase subunit beta

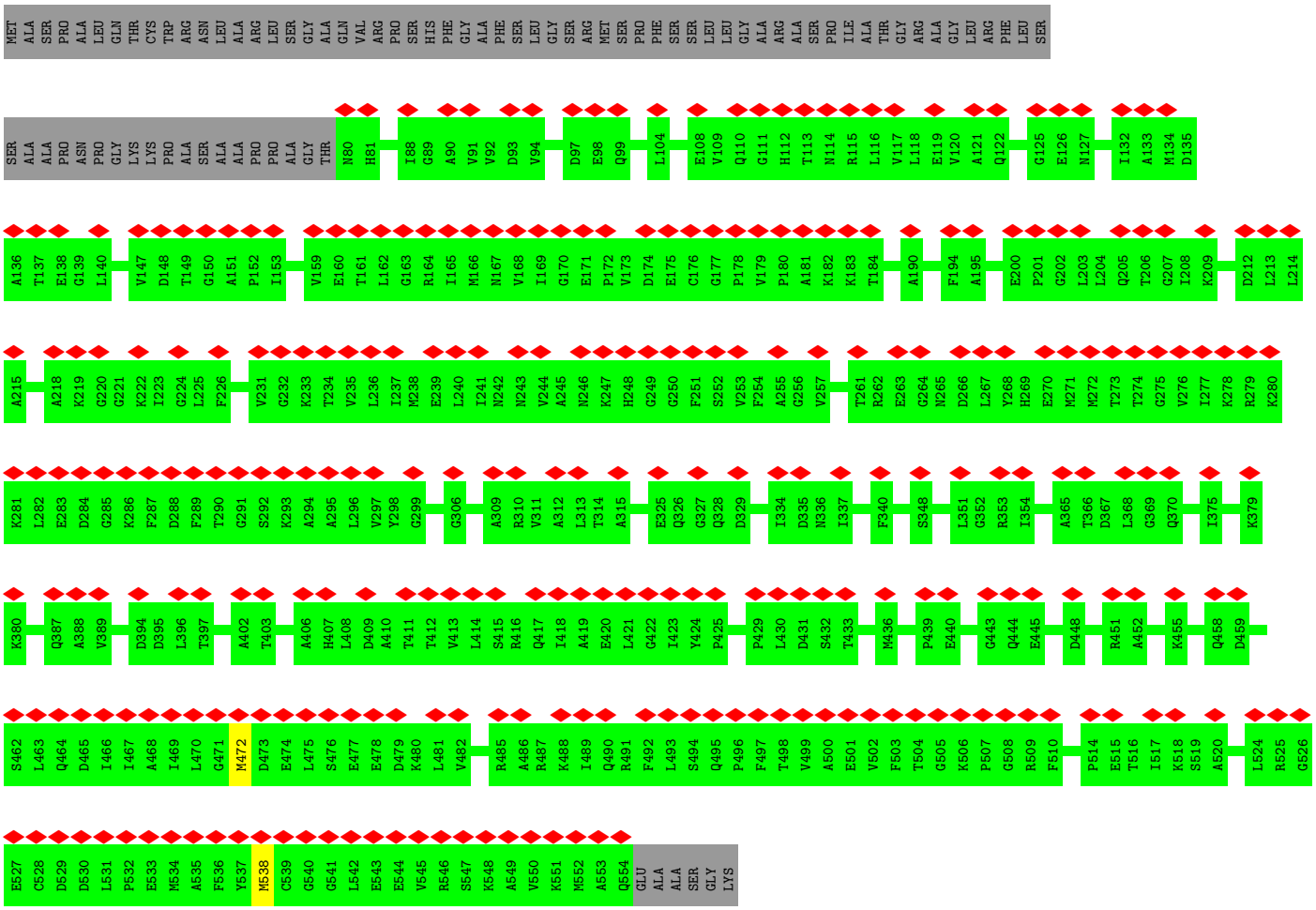
Chain B2:



• Molecule 27: ATP synthase subunit beta

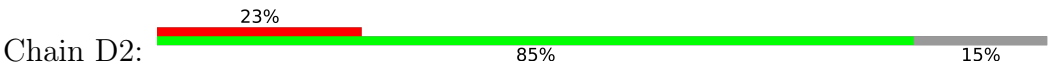
Chain F2:

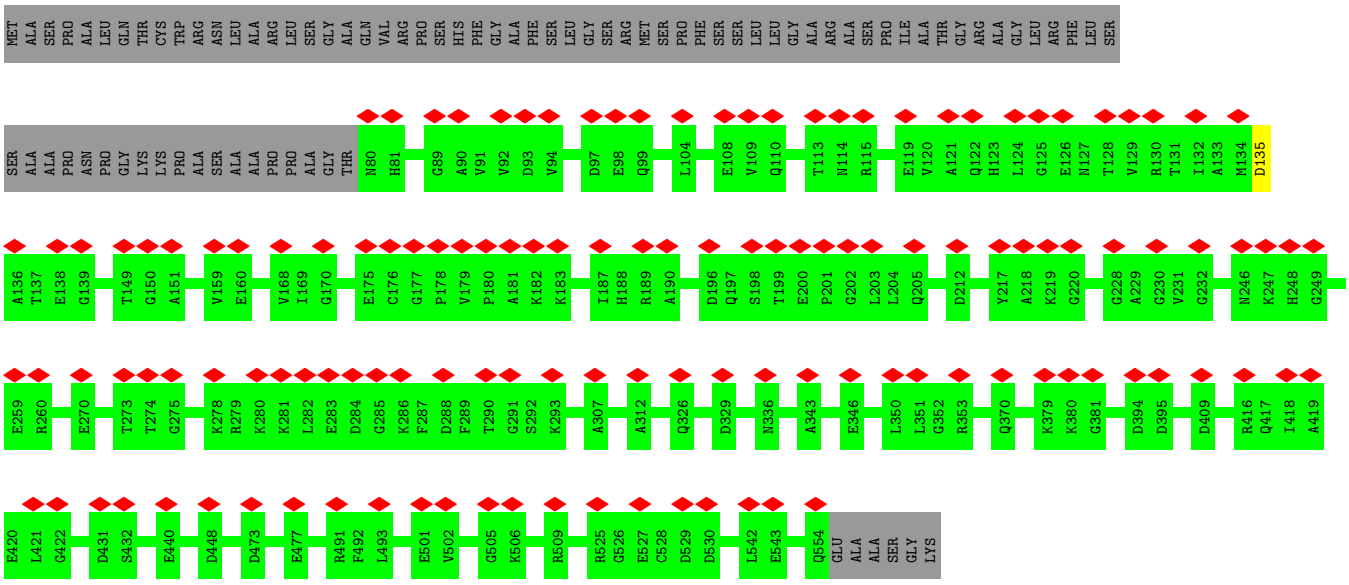




• Molecule 27: ATP synthase subunit beta

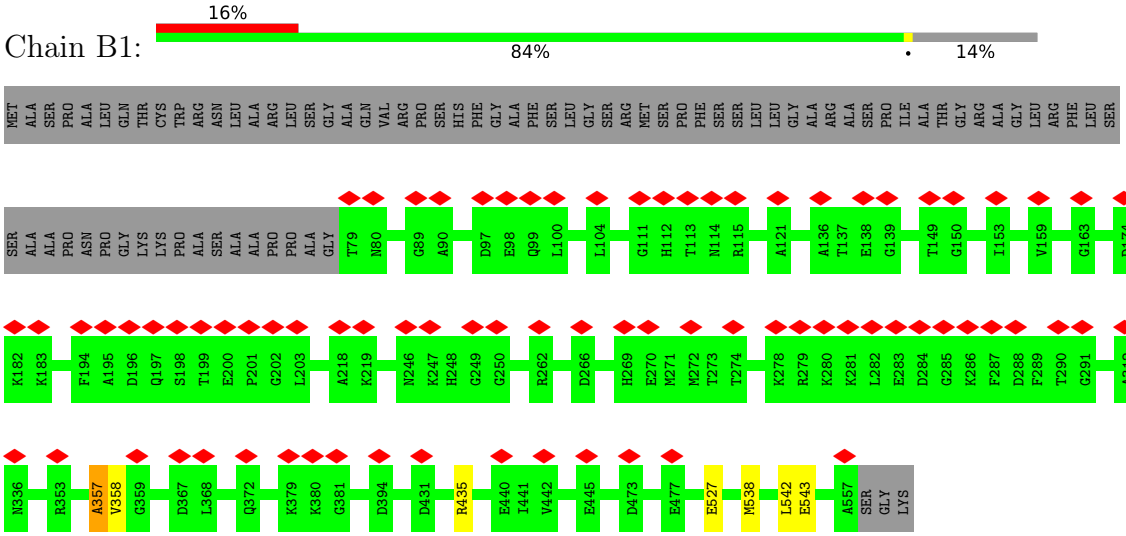
Chain D2:





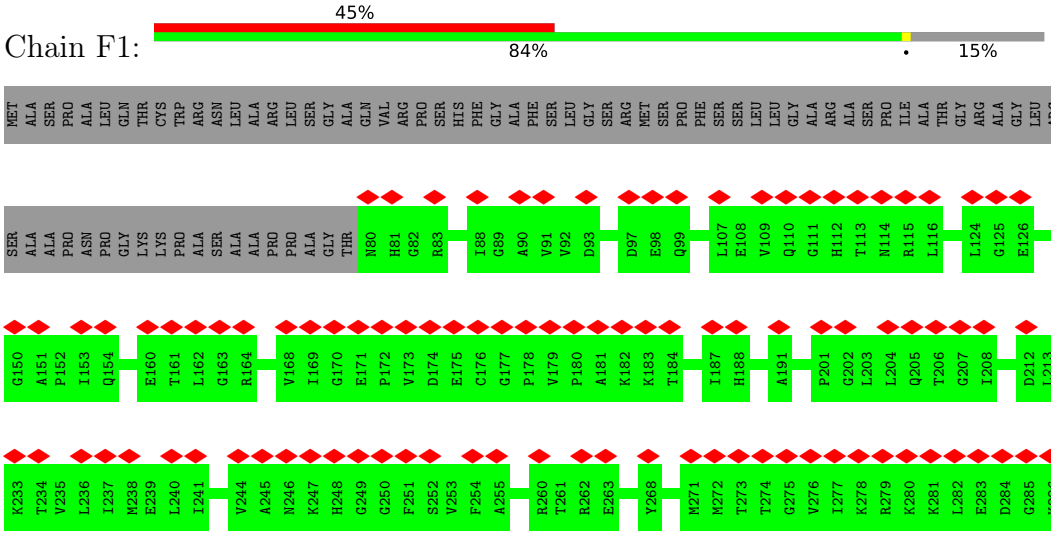
• Molecule 27: ATP synthase subunit beta

Chain B1:



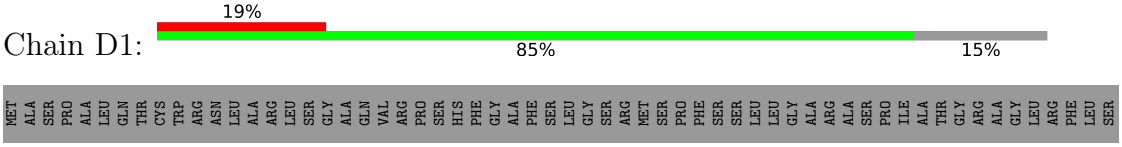
• Molecule 27: ATP synthase subunit beta

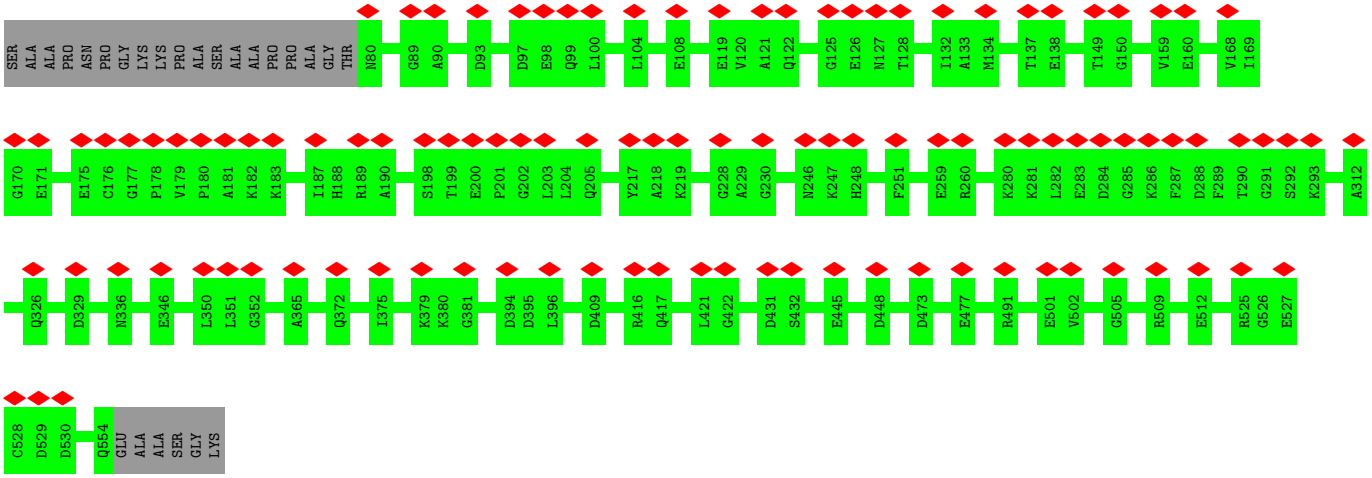
Chain F1:



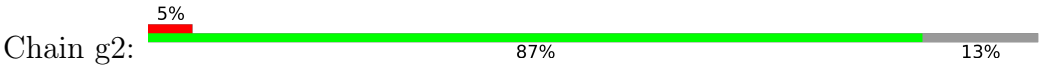
• Molecule 27: ATP synthase subunit beta

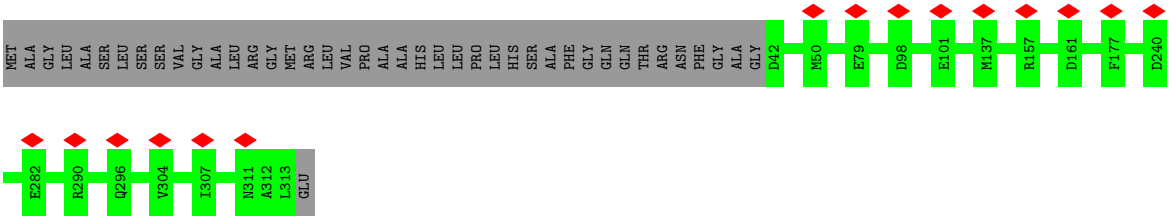
Chain D1:



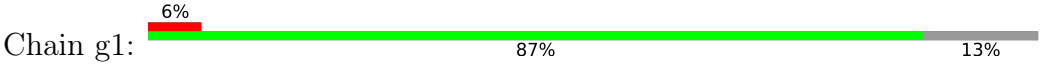


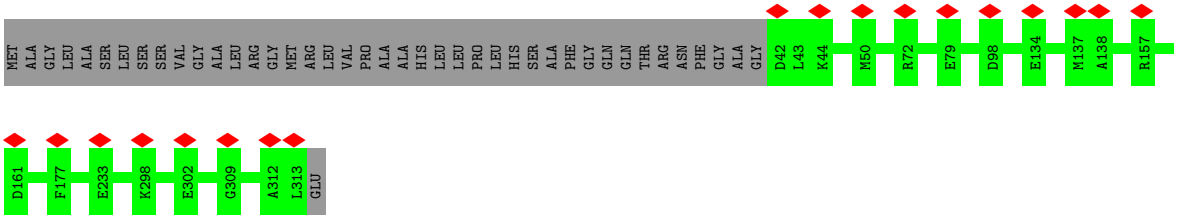
• Molecule 28: ATP synthase subunit gamma



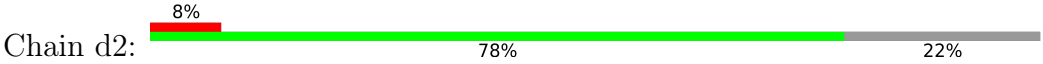


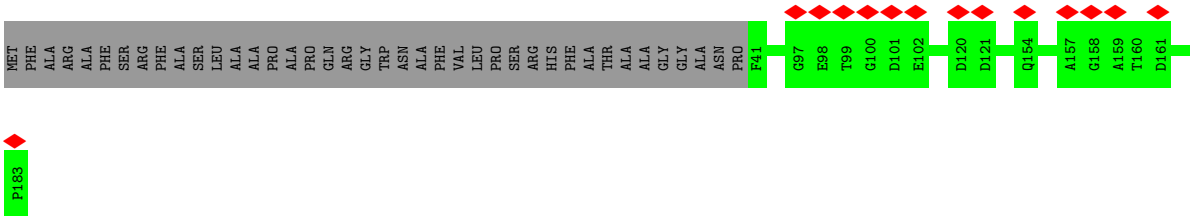
• Molecule 28: ATP synthase subunit gamma





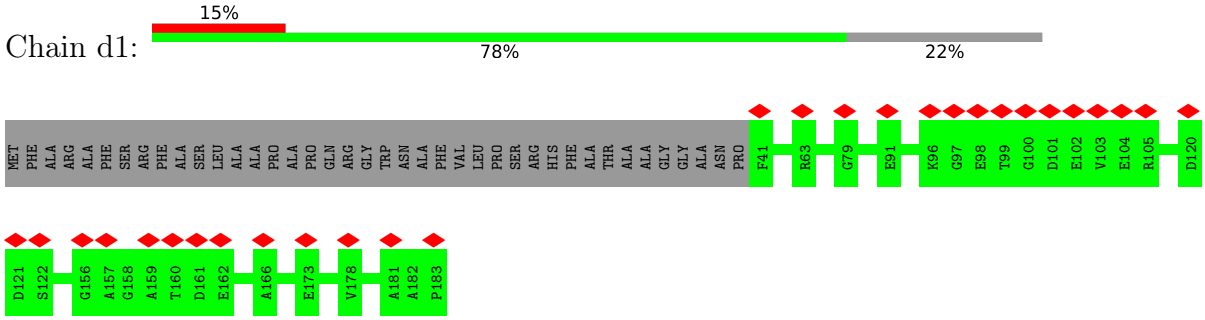
• Molecule 29: ATP synthase subunit delta





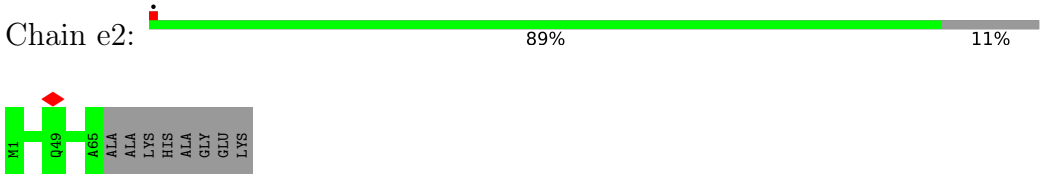
• Molecule 29: ATP synthase subunit delta

Chain d1:



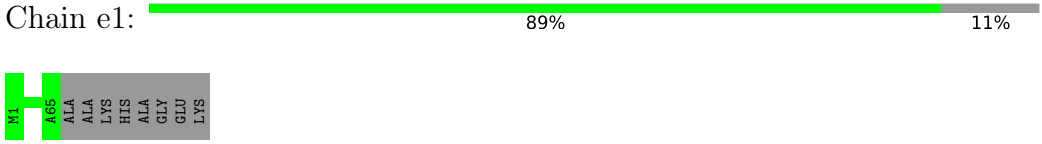
• Molecule 30: ATP synthase subunit epsilon

Chain e2:



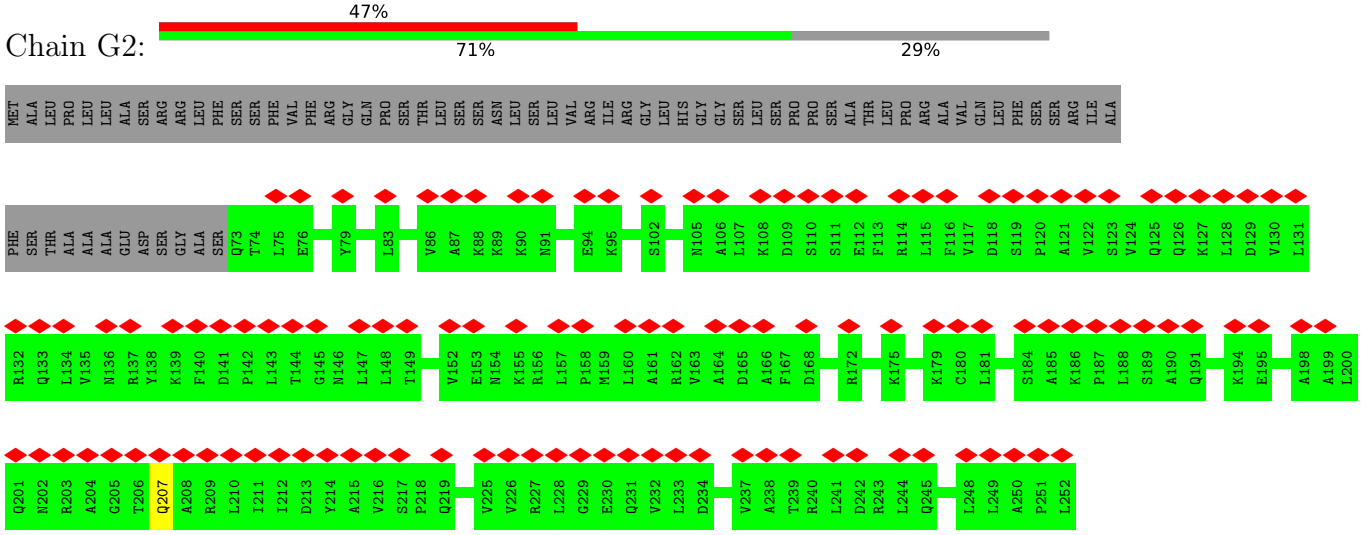
• Molecule 30: ATP synthase subunit epsilon

Chain e1:



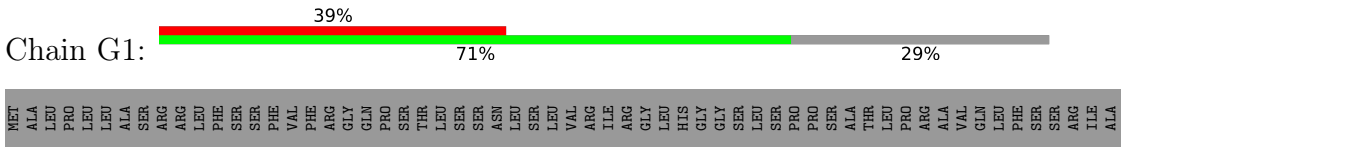
• Molecule 31: Oligomycin sensitivity conferring protein (OSCP)

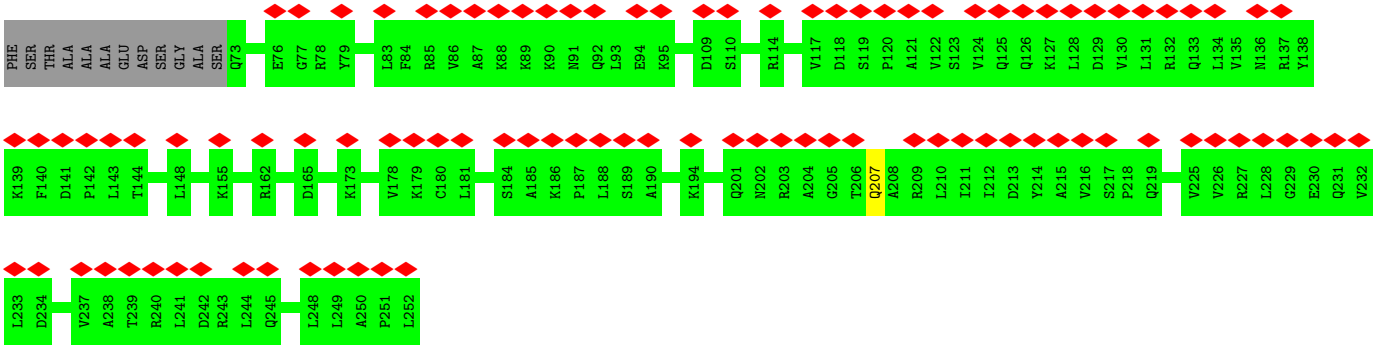
Chain G2:



• Molecule 31: Oligomycin sensitivity conferring protein (OSCP)

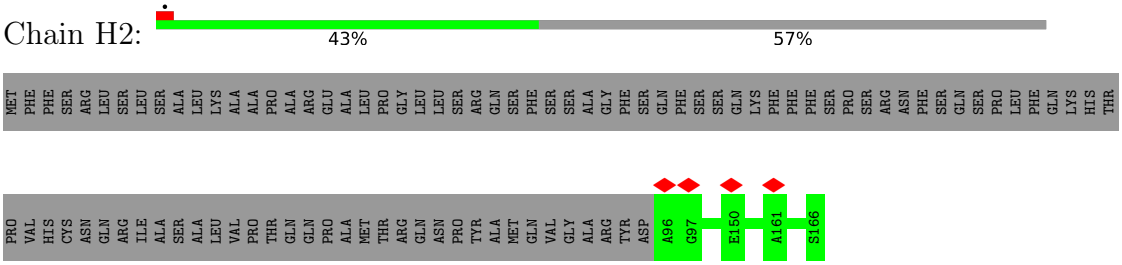
Chain G1:





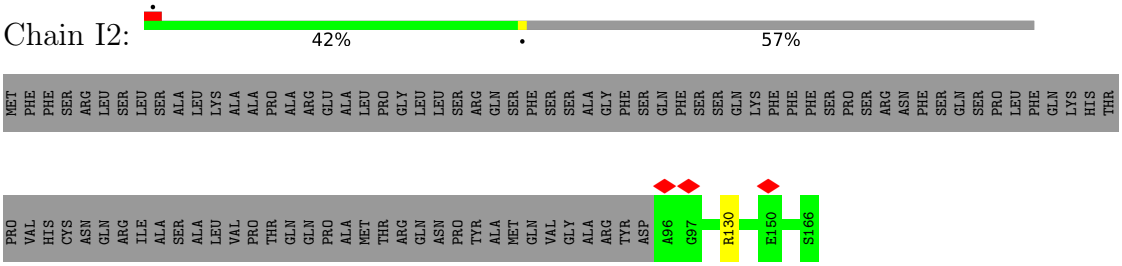
• Molecule 32: subunit c

Chain H2:



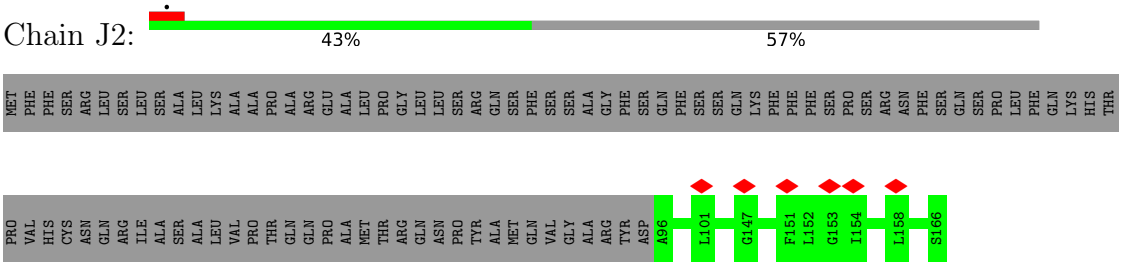
• Molecule 32: subunit c

Chain I2:



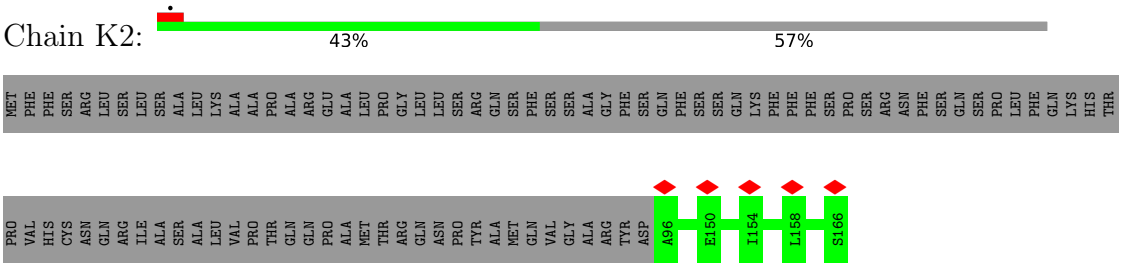
• Molecule 32: subunit c

Chain J2:



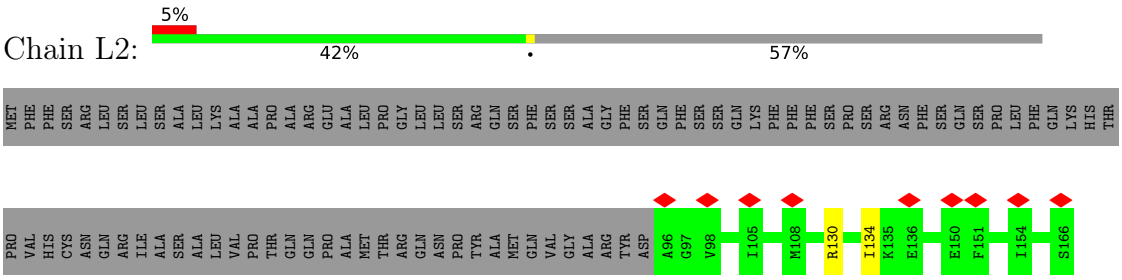
• Molecule 32: subunit c

Chain K2:



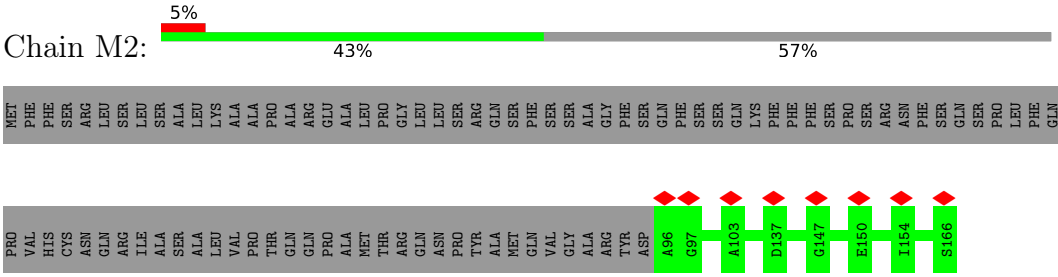
• Molecule 32: subunit c

Chain L2:



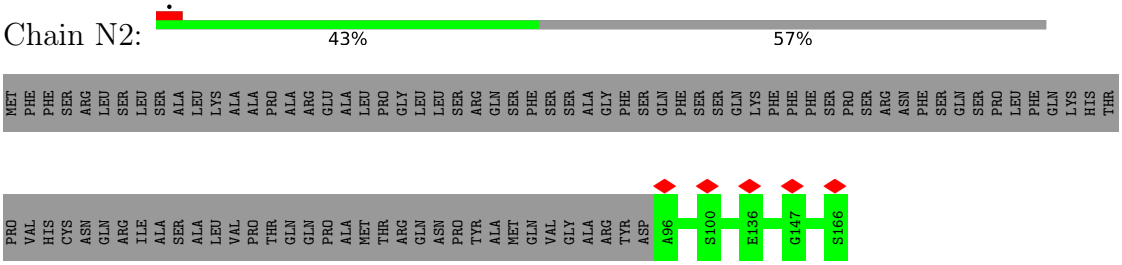
• Molecule 32: subunit c

Chain M2:



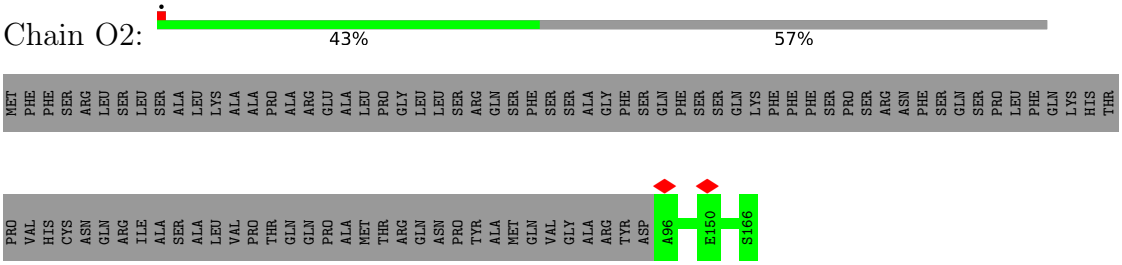
• Molecule 32: subunit c

Chain N2:



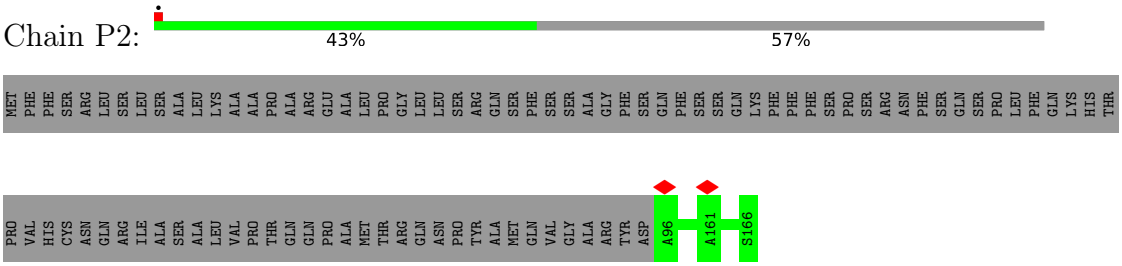
• Molecule 32: subunit c

Chain O2:



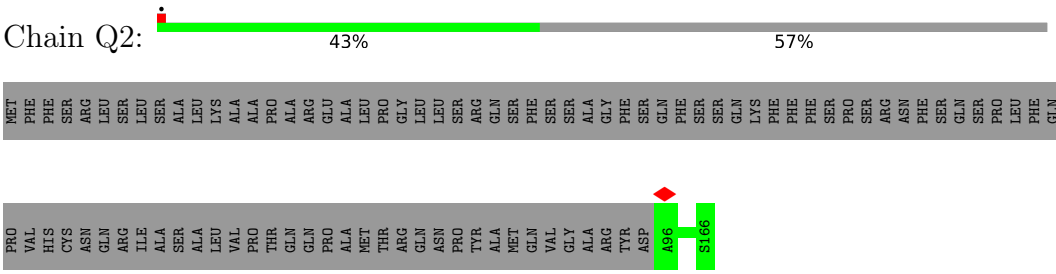
• Molecule 32: subunit c

Chain P2:



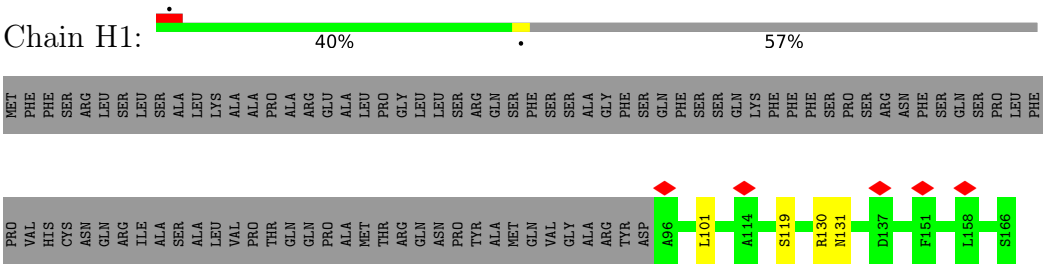
• Molecule 32: subunit c

Chain Q2:



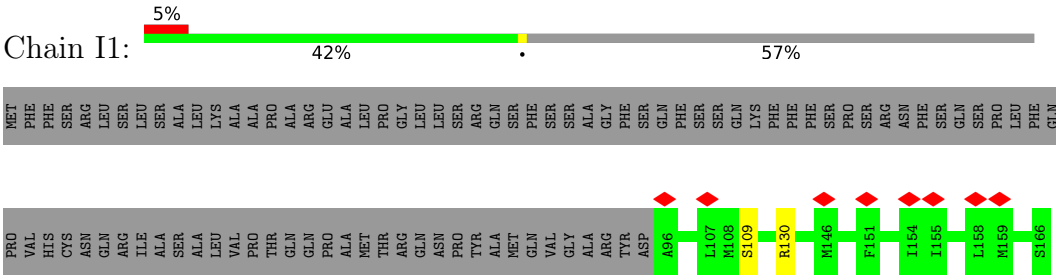
• Molecule 32: subunit c

Chain H1:



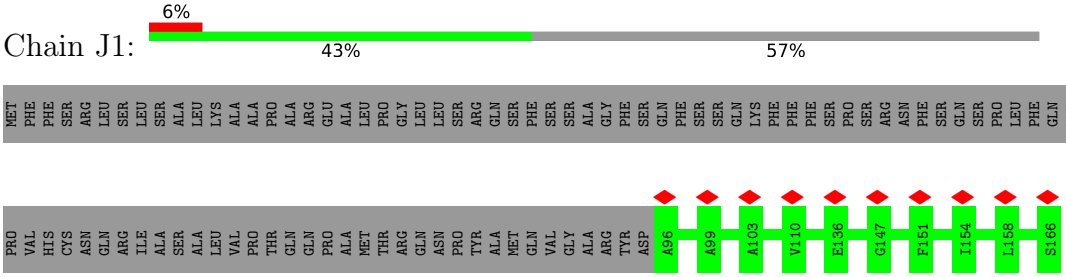
• Molecule 32: subunit c

Chain I1:



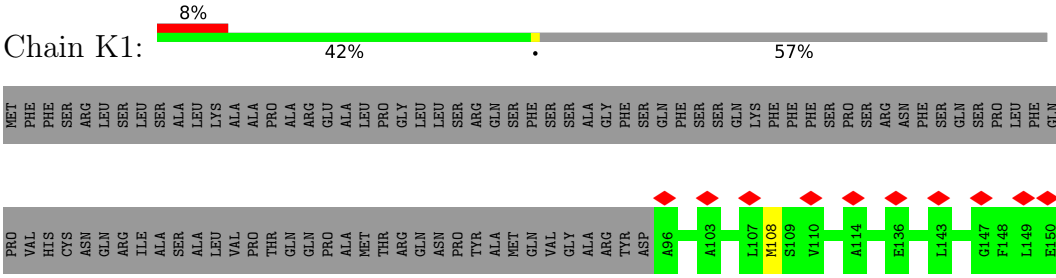
• Molecule 32: subunit c

Chain J1:



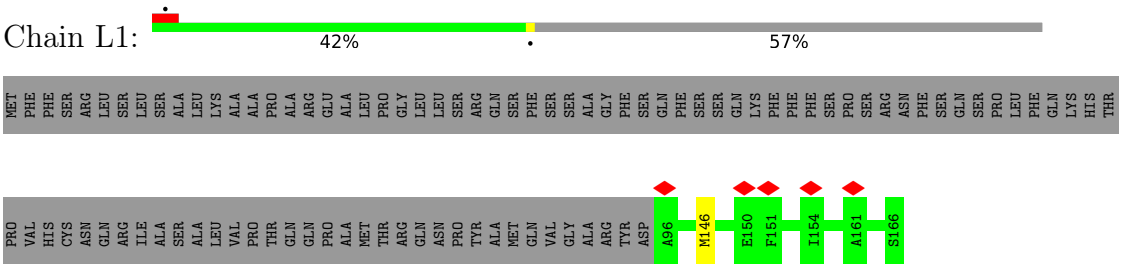
• Molecule 32: subunit c

Chain K1:



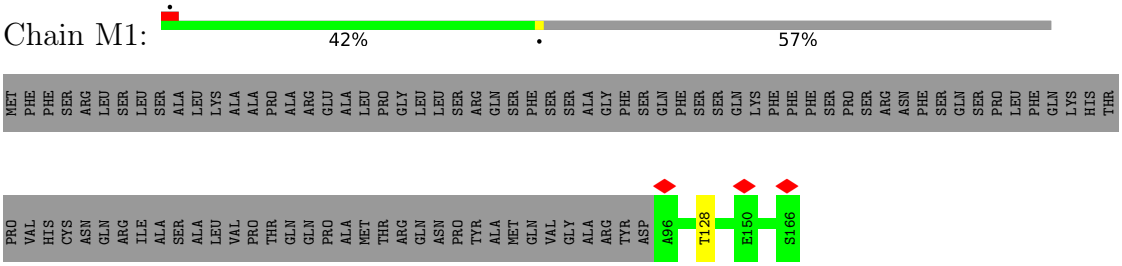
• Molecule 32: subunit c

Chain L1:



• Molecule 32: subunit c

Chain M1:

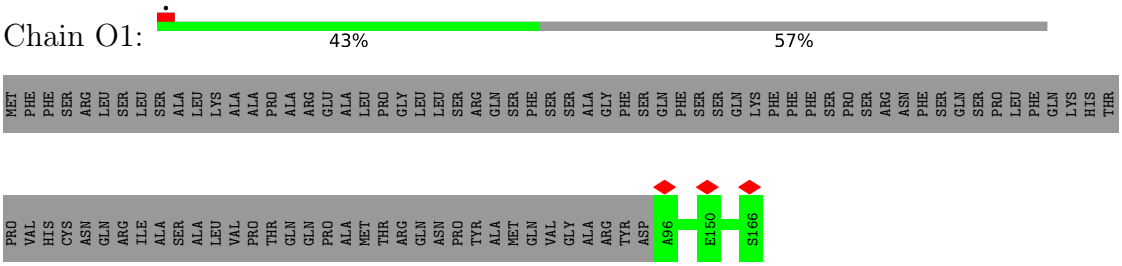


• Molecule 32: subunit c

Chain N1:

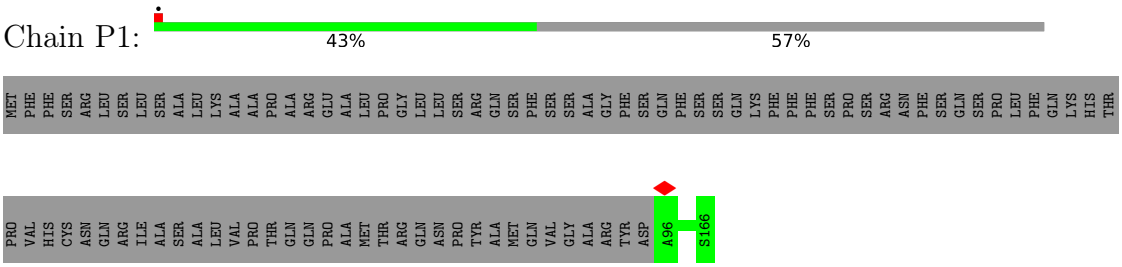
• Molecule 32: subunit c

Chain O1:



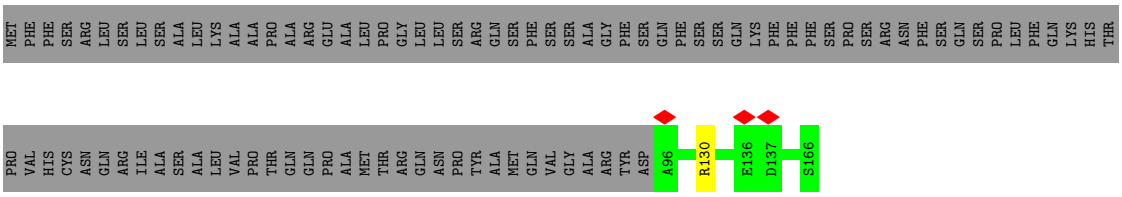
• Molecule 32: subunit c

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, CDL, ADP, ATP, LMT, PEE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	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

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	A1	198	MET	Peptide
26	A2	198	MET	Peptide
27	B1	357	ALA	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	K	115/224 (51%)	112 (97%)	3 (3%)	0	100	100
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	n	158/166 (95%)	156 (99%)	2 (1%)	0	100	100
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%)	34	66
27	B2	477/560 (85%)	454 (95%)	21 (4%)	2 (0%)	34	66
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	I1	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
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%)	60 86
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%)	88 96
10	h	197/204 (97%)	196 (100%)	1 (0%)	88 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%)	93 98
13	b	428/491 (87%)	427 (100%)	1 (0%)	93 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%)	88	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%)	84	95
21	n	138/144 (96%)	137 (99%)	1 (1%)	84	95
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%)	71	91
23	w	84/89 (94%)	83 (99%)	1 (1%)	71	91
24	A	392/447 (88%)	391 (100%)	1 (0%)	92	98
24	a	392/447 (88%)	390 (100%)	2 (0%)	88	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%)	65	87
27	B2	390/447 (87%)	389 (100%)	1 (0%)	92	98
27	D1	388/447 (87%)	388 (100%)	0	100	100
27	D2	388/447 (87%)	387 (100%)	1 (0%)	92	98
27	F1	388/447 (87%)	383 (99%)	5 (1%)	69	90
27	F2	388/447 (87%)	386 (100%)	2 (0%)	88	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%)	86	96
31	G2	154/212 (73%)	153 (99%)	1 (1%)	86	96
32	H1	52/133 (39%)	48 (92%)	4 (8%)	13	35
32	H2	52/133 (39%)	52 (100%)	0	100	100
32	I1	52/133 (39%)	50 (96%)	2 (4%)	33	67
32	I2	52/133 (39%)	51 (98%)	1 (2%)	57	84
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%)	57	84
32	K2	52/133 (39%)	52 (100%)	0	100	100
32	L1	52/133 (39%)	51 (98%)	1 (2%)	57	84
32	L2	52/133 (39%)	50 (96%)	2 (4%)	33	67
32	M1	52/133 (39%)	51 (98%)	1 (2%)	57	84
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%)	57	84
32	Q2	52/133 (39%)	52 (100%)	0	100	100
All	All	13790/18698 (74%)	13746 (100%)	44 (0%)	92	98

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	h	117	ARG

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Mol	Chain	Res	Type
13	b	507	ARG
19	d	42	LYS
21	n	82	ARG
23	w	105	SER
24	a	122	SER
24	a	130	LYS
1	Q	15	ILE
1	Q	16	PHE
10	H	117	ARG
13	B	507	ARG
21	N	82	ARG
23	W	105	SER
24	A	130	LYS
27	B2	435	ARG
27	F2	472	MET
27	F2	538	MET
27	D2	135	ASP
31	G2	207	GLN
32	I2	130	ARG
32	L2	130	ARG
32	L2	134	ILE
27	B1	335	ASP
27	B1	435	ARG
27	B1	527	GLU
27	B1	538	MET
27	B1	542	LEU
27	B1	543	GLU
27	F1	528	CYS
27	F1	536	PHE
27	F1	537	TYR
27	F1	538	MET
27	F1	542	LEU
31	G1	207	GLN
32	H1	101	LEU
32	H1	119	SER
32	H1	130	ARG
32	H1	131	ASN
32	I1	109	SER
32	I1	130	ARG
32	K1	108	MET
32	L1	146	MET
32	M1	128	THR

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Mol	Chain	Res	Type
32	Q1	130	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
2	i	202	GLN
10	h	67	ASN
13	b	517	ASN
24	a	321	GLN
2	I	206	HIS
10	H	67	ASN
24	A	321	GLN
26	E2	527	ASN
27	B2	80	ASN
27	B2	86	GLN
27	B2	99	GLN
27	F2	80	ASN
27	D2	86	GLN
27	D2	269	HIS
32	N2	115	GLN
26	E1	527	ASN
26	C1	490	ASN
27	B1	80	ASN
27	B1	99	GLN
27	D1	269	HIS
29	d1	172	GLN
32	L1	115	GLN
32	N1	115	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides 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	$\#\|Z\| > 2$
35	CDL	h	302	-	99,99,99	0.87	6 (6%)	105,111,111	0.98	4 (3%)
35	CDL	c	401	-	99,99,99	0.88	6 (6%)	105,111,111	0.91	4 (3%)
34	LMT	H	301	-	36,36,36	1.13	2 (5%)	47,47,47	1.03	2 (4%)
34	LMT	d	401	-	36,36,36	1.15	2 (5%)	47,47,47	0.90	1 (2%)
34	LMT	C	404	-	36,36,36	1.11	2 (5%)	47,47,47	1.14	3 (6%)
37	ATP	C1	601	-	26,33,33	4.78	9 (34%)	31,52,52	2.52	9 (29%)
35	CDL	e	401	-	99,99,99	0.88	8 (8%)	105,111,111	1.01	4 (3%)
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	1.01	4 (3%)
35	CDL	B	602	-	99,99,99	0.88	8 (8%)	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%)
37	ATP	E1	601	-	26,33,33	4.81	8 (30%)	31,52,52	2.49	8 (25%)
33	PC1	O	201	-	53,53,53	0.96	3 (5%)	59,61,61	1.05	3 (5%)
37	ATP	A2	601	-	26,33,33	4.80	7 (26%)	31,52,52	2.49	8 (25%)
37	ATP	C2	601	-	26,33,33	4.82	8 (30%)	31,52,52	2.47	8 (25%)
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%)
34	LMT	C	402	-	36,36,36	1.10	2 (5%)	47,47,47	1.00	1 (2%)
35	CDL	V	202	-	99,99,99	0.88	7 (7%)	105,111,111	0.97	4 (3%)
33	PC1	V	201	-	53,53,53	0.99	3 (5%)	59,61,61	0.98	2 (3%)
33	PC1	v	201	-	53,53,53	0.99	3 (5%)	59,61,61	0.99	2 (3%)
35	CDL	v	202	-	99,99,99	0.88	7 (7%)	105,111,111	0.98	4 (3%)
34	LMT	d	403	-	36,36,36	1.12	2 (5%)	47,47,47	0.85	1 (2%)
34	LMT	O	202	-	36,36,36	1.12	2 (5%)	47,47,47	0.94	1 (2%)
36	PEE	J	302	-	50,50,50	1.14	6 (12%)	53,55,55	1.15	3 (5%)
35	CDL	B	601	-	99,99,99	0.87	7 (7%)	105,111,111	1.00	3 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	PC1	o	201	-	53,53,53	0.96	4 (7%)	59,61,61	1.04	3 (5%)
35	CDL	d	402	-	99,99,99	0.88	8 (8%)	105,111,111	1.02	3 (2%)
36	PEE	c	403	-	50,50,50	1.15	5 (10%)	53,55,55	1.01	2 (3%)
34	LMT	D	403	-	36,36,36	1.11	2 (5%)	47,47,47	0.89	1 (2%)
34	LMT	h	301	-	36,36,36	1.13	2 (5%)	47,47,47	1.03	2 (4%)
35	CDL	C	401	-	99,99,99	0.88	6 (6%)	105,111,111	0.85	3 (2%)
38	ADP	B1	601	-	24,29,29	3.67	9 (37%)	29,45,45	3.44	6 (20%)
35	CDL	b	601	-	99,99,99	0.87	8 (8%)	105,111,111	1.00	4 (3%)
34	LMT	x	101	-	36,36,36	1.16	2 (5%)	47,47,47	1.03	3 (6%)
38	ADP	D2	601	-	24,29,29	3.68	9 (37%)	29,45,45	3.46	6 (20%)
38	ADP	D1	601	-	24,29,29	3.69	8 (33%)	29,45,45	3.58	7 (24%)
33	PC1	o	204	5	53,53,53	0.96	4 (7%)	59,61,61	1.04	2 (3%)
35	CDL	b	602	-	99,99,99	0.88	8 (8%)	105,111,111	0.98	4 (3%)
35	CDL	U	201	-	99,99,99	0.88	7 (7%)	105,111,111	1.00	4 (3%)
34	LMT	c	404	-	36,36,36	1.11	2 (5%)	47,47,47	1.07	2 (4%)
37	ATP	E2	601	-	26,33,33	4.80	8 (30%)	31,52,52	2.47	9 (29%)
34	LMT	D	401	-	36,36,36	1.15	2 (5%)	47,47,47	0.86	1 (2%)
36	PEE	j	301	-	50,50,50	1.12	6 (12%)	53,55,55	1.08	3 (5%)
35	CDL	D	402	-	99,99,99	0.88	8 (8%)	105,111,111	1.02	3 (2%)
38	ADP	B2	601	-	24,29,29	3.67	9 (37%)	29,45,45	3.70	8 (27%)
37	ATP	A1	601	-	26,33,33	4.81	7 (26%)	31,52,52	2.43	8 (25%)
34	LMT	c	402	-	36,36,36	1.10	2 (5%)	47,47,47	1.01	1 (2%)
35	CDL	H	302	-	99,99,99	0.87	7 (7%)	105,111,111	0.98	4 (3%)
34	LMT	o	202	-	36,36,36	1.12	2 (5%)	47,47,47	0.91	1 (2%)
35	CDL	O	203	-	99,99,99	0.88	7 (7%)	105,111,111	1.00	5 (4%)
35	CDL	o	203	-	99,99,99	0.88	7 (7%)	105,111,111	1.00	5 (4%)
36	PEE	J	301	-	50,50,50	1.12	6 (12%)	53,55,55	1.07	3 (5%)
36	PEE	j	302	-	50,50,50	1.14	6 (12%)	53,55,55	1.08	3 (5%)

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
35	CDL	h	302	-	-	45/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	CDL	c	401	-	-	64/110/110/110	-
34	LMT	H	301	-	-	9/21/61/61	0/2/2/2
34	LMT	d	401	-	-	9/21/61/61	0/2/2/2
34	LMT	C	404	-	-	7/21/61/61	0/2/2/2
37	ATP	C1	601	-	-	5/18/38/38	0/3/3/3
35	CDL	e	401	-	-	49/110/110/110	-
33	PC1	O	204	5	-	25/57/57/57	-
35	CDL	u	201	-	-	37/110/110/110	-
35	CDL	B	602	-	-	48/110/110/110	-
35	CDL	E	401	-	-	49/110/110/110	-
37	ATP	E1	601	-	-	3/18/38/38	0/3/3/3
33	PC1	O	201	-	-	22/57/57/57	-
37	ATP	A2	601	-	-	0/18/38/38	0/3/3/3
37	ATP	C2	601	-	-	4/18/38/38	0/3/3/3
36	PEE	C	403	-	-	22/54/54/54	-
34	LMT	X	101	-	-	12/21/61/61	0/2/2/2
34	LMT	C	402	-	-	8/21/61/61	0/2/2/2
35	CDL	V	202	-	-	39/110/110/110	-
33	PC1	V	201	-	-	31/57/57/57	-
33	PC1	v	201	-	-	31/57/57/57	-
35	CDL	v	202	-	-	40/110/110/110	-
34	LMT	d	403	-	-	5/21/61/61	0/2/2/2
34	LMT	O	202	-	-	4/21/61/61	0/2/2/2
36	PEE	J	302	-	-	19/54/54/54	-
35	CDL	B	601	-	-	39/110/110/110	-
33	PC1	o	201	-	-	23/57/57/57	-
35	CDL	d	402	-	-	45/110/110/110	-
36	PEE	c	403	-	-	22/54/54/54	-
34	LMT	D	403	-	-	5/21/61/61	0/2/2/2
34	LMT	h	301	-	-	9/21/61/61	0/2/2/2
35	CDL	C	401	-	-	60/110/110/110	-
38	ADP	B1	601	-	-	4/12/32/32	0/3/3/3
35	CDL	b	601	-	-	39/110/110/110	-
34	LMT	x	101	-	-	12/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	ADP	D2	601	-	-	2/12/32/32	0/3/3/3
38	ADP	D1	601	-	-	0/12/32/32	0/3/3/3
33	PC1	o	204	5	-	25/57/57/57	-
35	CDL	b	602	-	-	50/110/110/110	-
35	CDL	U	201	-	-	38/110/110/110	-
34	LMT	c	404	-	-	7/21/61/61	0/2/2/2
37	ATP	E2	601	-	-	3/18/38/38	0/3/3/3
34	LMT	D	401	-	-	11/21/61/61	0/2/2/2
36	PEE	j	301	-	-	22/54/54/54	-
35	CDL	D	402	-	-	46/110/110/110	-
38	ADP	B2	601	-	-	4/12/32/32	0/3/3/3
37	ATP	A1	601	-	-	0/18/38/38	0/3/3/3
34	LMT	c	402	-	-	8/21/61/61	0/2/2/2
35	CDL	H	302	-	-	45/110/110/110	-
34	LMT	o	202	-	-	4/21/61/61	0/2/2/2
35	CDL	O	203	-	-	40/110/110/110	-
35	CDL	o	203	-	-	40/110/110/110	-
36	PEE	J	301	-	-	22/54/54/54	-
36	PEE	j	302	-	-	20/54/54/54	-

All (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
37	C1	601	ATP	C2'-C1'	-17.28	1.27	1.53
37	E1	601	ATP	O4'-C1'	11.21	1.56	1.41
37	A1	601	ATP	O4'-C1'	11.17	1.56	1.41
37	E2	601	ATP	O4'-C1'	11.16	1.56	1.41
37	C2	601	ATP	O4'-C1'	11.15	1.56	1.41
37	A2	601	ATP	O4'-C1'	11.05	1.56	1.41
37	C1	601	ATP	O4'-C1'	11.00	1.56	1.41
38	B1	601	ADP	C2'-C3'	-10.64	1.24	1.53
38	D2	601	ADP	C2'-C3'	-10.57	1.24	1.53
38	D1	601	ADP	C2'-C3'	-10.51	1.24	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	B2	601	ADP	C2'-C3'	-10.39	1.24	1.53
37	A1	601	ATP	C3'-C4'	-9.35	1.29	1.53
37	E1	601	ATP	C3'-C4'	-9.34	1.29	1.53
37	A2	601	ATP	C3'-C4'	-9.32	1.29	1.53
37	C2	601	ATP	C3'-C4'	-9.31	1.29	1.53
37	E2	601	ATP	C3'-C4'	-9.31	1.29	1.53
37	C1	601	ATP	C3'-C4'	-9.28	1.29	1.53
38	D2	601	ADP	O4'-C1'	7.91	1.52	1.41
38	B1	601	ADP	O4'-C1'	7.83	1.52	1.41
38	D1	601	ADP	O4'-C1'	7.78	1.51	1.41
38	B2	601	ADP	O4'-C1'	7.62	1.51	1.41
38	B2	601	ADP	O4'-C4'	-6.63	1.30	1.45
38	D1	601	ADP	O4'-C4'	-6.29	1.30	1.45
38	B1	601	ADP	O4'-C4'	-6.22	1.31	1.45
38	D2	601	ADP	O4'-C4'	-6.17	1.31	1.45
38	B1	601	ADP	C3'-C4'	5.95	1.68	1.53
38	D2	601	ADP	C3'-C4'	5.92	1.68	1.53
38	D1	601	ADP	C3'-C4'	5.90	1.68	1.53
38	B2	601	ADP	C3'-C4'	5.77	1.67	1.53
38	D1	601	ADP	C2'-C1'	5.04	1.61	1.53
38	B2	601	ADP	C2'-C1'	4.97	1.61	1.53
37	C1	601	ATP	C2'-C3'	4.89	1.66	1.53
37	E2	601	ATP	C2'-C3'	4.83	1.66	1.53
37	A2	601	ATP	C2'-C3'	4.82	1.66	1.53
37	E1	601	ATP	C2'-C3'	4.77	1.66	1.53
37	C2	601	ATP	C2'-C3'	4.74	1.66	1.53
37	C2	601	ATP	O4'-C4'	4.71	1.55	1.45
37	A1	601	ATP	C2'-C3'	4.70	1.66	1.53
37	A1	601	ATP	O4'-C4'	4.67	1.55	1.45
37	E2	601	ATP	O4'-C4'	4.66	1.55	1.45
37	E1	601	ATP	O4'-C4'	4.65	1.55	1.45
38	D2	601	ADP	C2'-C1'	4.65	1.60	1.53
37	A2	601	ATP	O4'-C4'	4.58	1.55	1.45
37	C1	601	ATP	O4'-C4'	4.48	1.55	1.45
38	B1	601	ADP	C2'-C1'	4.45	1.60	1.53
38	D1	601	ADP	O2'-C2'	3.88	1.52	1.43
38	D2	601	ADP	O2'-C2'	3.86	1.52	1.43
38	B2	601	ADP	O2'-C2'	3.84	1.52	1.43
38	B1	601	ADP	O2'-C2'	3.81	1.51	1.43
36	J	302	PEE	C39-C38	3.74	1.53	1.31
36	j	302	PEE	C39-C38	3.74	1.53	1.31
36	C	403	PEE	C19-C18	3.72	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	403	PEE	C39-C38	3.71	1.53	1.31
36	c	403	PEE	C19-C18	3.71	1.53	1.31
36	C	403	PEE	C39-C38	3.70	1.53	1.31
36	J	302	PEE	C19-C18	3.66	1.53	1.31
36	J	301	PEE	C39-C38	3.65	1.53	1.31
36	j	301	PEE	C39-C38	3.65	1.52	1.31
36	j	302	PEE	C19-C18	3.64	1.52	1.31
36	J	301	PEE	C19-C18	3.60	1.52	1.31
36	j	301	PEE	C19-C18	3.58	1.52	1.31
34	D	401	LMT	O5B-C1B	3.47	1.50	1.41
34	d	401	LMT	O5B-C1B	3.47	1.50	1.41
34	x	101	LMT	O5B-C1B	3.44	1.50	1.41
34	X	101	LMT	O5B-C1B	3.44	1.50	1.41
34	o	202	LMT	O5B-C1B	3.42	1.50	1.41
34	O	202	LMT	O5B-C1B	3.41	1.50	1.41
38	B1	601	ADP	C5-C4	-3.37	1.32	1.40
34	h	301	LMT	O5'-C1'	3.35	1.50	1.41
34	H	301	LMT	O5B-C1B	3.35	1.50	1.41
38	D2	601	ADP	C5-C4	-3.34	1.32	1.40
34	H	301	LMT	O5'-C1'	3.33	1.50	1.41
34	h	301	LMT	O5B-C1B	3.32	1.50	1.41
38	B2	601	ADP	C5-C4	-3.32	1.32	1.40
34	d	403	LMT	O5B-C1B	3.29	1.50	1.41
37	E2	601	ATP	C6-N6	3.29	1.46	1.34
37	A2	601	ATP	C6-N6	3.29	1.46	1.34
34	c	402	LMT	O5B-C1B	3.28	1.50	1.41
34	D	403	LMT	O5B-C1B	3.28	1.50	1.41
37	E1	601	ATP	C6-N6	3.28	1.46	1.34
37	C2	601	ATP	C6-N6	3.27	1.46	1.34
38	D1	601	ADP	C5-C4	-3.27	1.32	1.40
34	C	402	LMT	O5B-C1B	3.26	1.50	1.41
34	D	401	LMT	O5'-C1'	3.26	1.50	1.41
34	C	404	LMT	O5B-C1B	3.26	1.50	1.41
37	A1	601	ATP	C6-N6	3.25	1.45	1.34
34	c	404	LMT	O5B-C1B	3.25	1.50	1.41
37	C1	601	ATP	C6-N6	3.25	1.45	1.34
34	d	401	LMT	O5'-C1'	3.23	1.50	1.41
34	X	101	LMT	O5'-C1'	3.22	1.50	1.41
34	x	101	LMT	O5'-C1'	3.22	1.50	1.41
38	D1	601	ADP	C6-N6	3.15	1.45	1.34
38	D2	601	ADP	C6-N6	3.15	1.45	1.34
38	B1	601	ADP	C6-N6	3.11	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	B2	601	ADP	C6-N6	3.11	1.45	1.34
34	d	403	LMT	O5'-C1'	3.06	1.49	1.41
34	D	403	LMT	O5'-C1'	3.03	1.49	1.41
34	O	202	LMT	O5'-C1'	3.01	1.49	1.41
34	C	404	LMT	O5'-C1'	3.00	1.49	1.41
34	C	402	LMT	O5'-C1'	3.00	1.49	1.41
34	c	404	LMT	O5'-C1'	2.98	1.49	1.41
34	c	402	LMT	O5'-C1'	2.97	1.49	1.41
34	o	202	LMT	O5'-C1'	2.96	1.49	1.41
33	O	201	PC1	O21-C2	-2.91	1.39	1.46
33	o	201	PC1	O21-C2	-2.89	1.39	1.46
35	O	203	CDL	OA6-CA4	-2.83	1.39	1.46
35	o	203	CDL	OA6-CA4	-2.79	1.39	1.46
35	E	401	CDL	OA6-CA4	-2.79	1.39	1.46
35	e	401	CDL	OA6-CA4	-2.77	1.39	1.46
35	u	201	CDL	OA6-CA4	-2.77	1.39	1.46
35	U	201	CDL	OA6-CA4	-2.75	1.39	1.46
35	C	401	CDL	OB6-CB4	-2.74	1.39	1.46
35	V	202	CDL	OB6-CB4	-2.74	1.39	1.46
36	c	403	PEE	O2-C2	-2.74	1.39	1.46
35	U	201	CDL	OB6-CB4	-2.73	1.39	1.46
35	v	202	CDL	OB6-CB4	-2.73	1.39	1.46
35	b	601	CDL	OB6-CB4	-2.72	1.39	1.46
36	C	403	PEE	O2-C2	-2.72	1.39	1.46
35	h	302	CDL	OA6-CA4	-2.71	1.39	1.46
35	H	302	CDL	OA6-CA4	-2.70	1.39	1.46
35	u	201	CDL	OB6-CB4	-2.69	1.39	1.46
35	B	601	CDL	OB6-CB4	-2.69	1.39	1.46
35	B	601	CDL	OA6-CA4	-2.64	1.40	1.46
35	H	302	CDL	OB6-CB4	-2.63	1.40	1.46
35	b	601	CDL	OA6-CA4	-2.63	1.40	1.46
35	h	302	CDL	OB6-CB4	-2.63	1.40	1.46
37	E1	601	ATP	C5-C4	-2.62	1.34	1.40
35	c	401	CDL	OB6-CB4	-2.62	1.40	1.46
37	C1	601	ATP	C5-C4	-2.62	1.34	1.40
35	D	402	CDL	OB6-CB4	-2.62	1.40	1.46
35	d	402	CDL	OB6-CB4	-2.62	1.40	1.46
37	C2	601	ATP	C5-C4	-2.61	1.34	1.40
37	E2	601	ATP	C5-C4	-2.61	1.34	1.40
37	A2	601	ATP	C5-C4	-2.61	1.34	1.40
37	A1	601	ATP	C5-C4	-2.61	1.34	1.40
35	C	401	CDL	OA8-CA7	2.60	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	B	602	CDL	OB6-CB4	-2.59	1.40	1.46
35	V	202	CDL	OA6-CA4	-2.59	1.40	1.46
35	v	202	CDL	OA6-CA4	-2.58	1.40	1.46
35	o	203	CDL	OB6-CB4	-2.58	1.40	1.46
35	b	602	CDL	OB6-CB4	-2.57	1.40	1.46
35	c	401	CDL	OA8-CA7	2.57	1.40	1.33
35	E	401	CDL	OB8-CB7	2.56	1.40	1.33
35	O	203	CDL	OB6-CB4	-2.56	1.40	1.46
36	j	301	PEE	O2-C2	-2.56	1.40	1.46
36	j	302	PEE	O2-C2	-2.56	1.40	1.46
36	J	302	PEE	O2-C2	-2.54	1.40	1.46
35	e	401	CDL	OB8-CB7	2.54	1.40	1.33
36	J	301	PEE	O2-C2	-2.54	1.40	1.46
35	C	401	CDL	OA6-CA4	-2.53	1.40	1.46
35	c	401	CDL	OA6-CA4	-2.53	1.40	1.46
35	E	401	CDL	OB6-CB4	-2.53	1.40	1.46
35	b	602	CDL	OB8-CB7	2.51	1.40	1.33
35	c	401	CDL	OB8-CB7	2.51	1.40	1.33
35	e	401	CDL	OB6-CB4	-2.51	1.40	1.46
33	o	204	PC1	O21-C2	-2.50	1.40	1.46
33	V	201	PC1	O31-C31	2.49	1.40	1.33
33	v	201	PC1	O31-C31	2.49	1.40	1.33
35	b	602	CDL	OA8-CA7	2.48	1.40	1.33
35	C	401	CDL	OB8-CB7	2.48	1.40	1.33
35	B	602	CDL	OB8-CB7	2.48	1.40	1.33
35	V	202	CDL	OA8-CA7	2.48	1.40	1.33
35	B	602	CDL	OA8-CA7	2.47	1.40	1.33
35	v	202	CDL	OA8-CA7	2.47	1.40	1.33
36	C	403	PEE	O3-C30	2.47	1.40	1.33
35	U	201	CDL	OA8-CA7	2.46	1.40	1.33
36	c	403	PEE	O3-C30	2.45	1.40	1.33
35	U	201	CDL	OB8-CB7	2.45	1.40	1.33
33	V	201	PC1	O21-C2	-2.45	1.40	1.46
35	H	302	CDL	OA8-CA7	2.45	1.40	1.33
33	O	204	PC1	O21-C2	-2.45	1.40	1.46
35	u	201	CDL	OB8-CB7	2.45	1.40	1.33
35	h	302	CDL	OA8-CA7	2.44	1.40	1.33
35	O	203	CDL	OB8-CB7	2.44	1.40	1.33
33	o	204	PC1	O31-C31	2.44	1.40	1.33
33	v	201	PC1	O21-C2	-2.44	1.40	1.46
35	u	201	CDL	OA8-CA7	2.44	1.40	1.33
33	O	204	PC1	O31-C31	2.43	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	d	402	CDL	OB8-CB7	2.42	1.40	1.33
35	O	203	CDL	OA8-CA7	2.42	1.40	1.33
35	D	402	CDL	OB8-CB7	2.42	1.40	1.33
35	o	203	CDL	OB8-CB7	2.42	1.40	1.33
35	d	402	CDL	OA6-CA4	-2.41	1.40	1.46
35	b	602	CDL	OA6-CA4	-2.41	1.40	1.46
33	O	201	PC1	O31-C3	-2.41	1.39	1.45
36	j	302	PEE	O3-C30	2.40	1.40	1.33
35	D	402	CDL	OA6-CA4	-2.40	1.40	1.46
35	B	602	CDL	OA6-CA4	-2.40	1.40	1.46
36	J	302	PEE	O3-C30	2.40	1.40	1.33
33	o	201	PC1	O31-C3	-2.39	1.39	1.45
35	v	202	CDL	OB8-CB6	-2.37	1.39	1.45
35	o	203	CDL	OA8-CA7	2.37	1.40	1.33
35	D	402	CDL	OA8-CA6	-2.37	1.39	1.45
35	d	402	CDL	OA8-CA6	-2.36	1.39	1.45
35	E	401	CDL	OA8-CA7	2.35	1.40	1.33
35	B	601	CDL	OA8-CA7	2.35	1.40	1.33
35	e	401	CDL	OA8-CA7	2.34	1.40	1.33
35	v	202	CDL	OB8-CB7	2.34	1.40	1.33
35	b	601	CDL	OA8-CA6	-2.33	1.39	1.45
35	B	601	CDL	OA8-CA6	-2.33	1.39	1.45
36	J	301	PEE	O3-C3	-2.33	1.39	1.45
35	b	601	CDL	OA8-CA7	2.33	1.40	1.33
35	V	202	CDL	OB8-CB6	-2.33	1.39	1.45
35	h	302	CDL	OB8-CB7	2.31	1.40	1.33
35	V	202	CDL	OB8-CB7	2.31	1.40	1.33
35	b	601	CDL	OB8-CB7	2.31	1.40	1.33
36	j	301	PEE	O3-C30	2.30	1.40	1.33
35	H	302	CDL	OB8-CB7	2.30	1.40	1.33
35	B	601	CDL	OB8-CB7	2.29	1.40	1.33
35	c	401	CDL	OB8-CB6	-2.28	1.40	1.45
36	j	301	PEE	O3-C3	-2.28	1.40	1.45
35	d	402	CDL	OA8-CA7	2.28	1.40	1.33
35	D	402	CDL	OA8-CA7	2.28	1.40	1.33
35	B	602	CDL	OA6-CA5	2.26	1.40	1.34
35	C	401	CDL	OB8-CB6	-2.24	1.40	1.45
35	B	601	CDL	OB8-CB6	-2.24	1.40	1.45
35	b	602	CDL	OA6-CA5	2.24	1.40	1.34
36	J	301	PEE	O3-C30	2.24	1.39	1.33
33	O	201	PC1	O31-C31	2.23	1.39	1.33
33	o	201	PC1	O31-C31	2.23	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	O	203	CDL	OA8-CA6	-2.23	1.40	1.45
35	b	601	CDL	OB8-CB6	-2.22	1.40	1.45
35	o	203	CDL	OA8-CA6	-2.22	1.40	1.45
35	c	401	CDL	OA6-CA5	2.20	1.40	1.34
35	O	203	CDL	OB8-CB6	-2.19	1.40	1.45
33	v	201	PC1	O21-C21	2.18	1.40	1.34
33	o	204	PC1	O21-C21	2.17	1.40	1.34
36	j	302	PEE	O3-C3	-2.17	1.40	1.45
33	O	204	PC1	O21-C21	2.17	1.40	1.34
35	d	402	CDL	OA6-CA5	2.17	1.40	1.34
33	V	201	PC1	O21-C21	2.16	1.40	1.34
35	H	302	CDL	OB8-CB6	-2.16	1.40	1.45
35	C	401	CDL	OA6-CA5	2.16	1.40	1.34
35	D	402	CDL	OB8-CB6	-2.15	1.40	1.45
36	J	302	PEE	O2-C10	2.15	1.40	1.34
35	E	401	CDL	OA8-CA6	-2.15	1.40	1.45
35	o	203	CDL	OB8-CB6	-2.15	1.40	1.45
36	C	403	PEE	O3-C3	-2.14	1.40	1.45
35	U	201	CDL	OA8-CA6	-2.14	1.40	1.45
35	h	302	CDL	OB8-CB6	-2.14	1.40	1.45
35	d	402	CDL	OB6-CB5	2.14	1.40	1.34
35	u	201	CDL	OA8-CA6	-2.13	1.40	1.45
36	j	302	PEE	O2-C10	2.13	1.40	1.34
35	h	302	CDL	OA8-CA6	-2.13	1.40	1.45
35	e	401	CDL	OA8-CA6	-2.13	1.40	1.45
35	D	402	CDL	OA6-CA5	2.11	1.40	1.34
35	D	402	CDL	OB6-CB5	2.11	1.40	1.34
35	U	201	CDL	OA6-CA5	2.11	1.40	1.34
35	b	602	CDL	OB8-CB6	-2.11	1.40	1.45
38	D2	601	ADP	C2-N3	2.11	1.35	1.32
35	u	201	CDL	OA6-CA5	2.11	1.40	1.34
35	B	602	CDL	OA8-CA6	-2.11	1.40	1.45
35	e	401	CDL	OB8-CB6	-2.11	1.40	1.45
35	e	401	CDL	OB6-CB5	2.10	1.40	1.34
35	B	602	CDL	OB8-CB6	-2.10	1.40	1.45
36	c	403	PEE	O3-C3	-2.10	1.40	1.45
35	U	201	CDL	OB8-CB6	-2.10	1.40	1.45
35	H	302	CDL	OA8-CA6	-2.10	1.40	1.45
35	o	203	CDL	OB6-CB5	2.10	1.40	1.34
35	d	402	CDL	OB8-CB6	-2.10	1.40	1.45
35	E	401	CDL	OB8-CB6	-2.09	1.40	1.45
35	E	401	CDL	OB6-CB5	2.09	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	b	602	CDL	OA8-CA6	-2.09	1.40	1.45
36	J	302	PEE	O3-C3	-2.09	1.40	1.45
37	C1	601	ATP	C5'-C4'	2.08	1.58	1.51
36	j	301	PEE	O2-C10	2.08	1.40	1.34
35	v	202	CDL	OA8-CA6	-2.08	1.40	1.45
35	B	602	CDL	OB6-CB5	2.07	1.40	1.34
35	V	202	CDL	OA6-CA5	2.07	1.40	1.34
37	E2	601	ATP	C5'-C4'	2.07	1.58	1.51
35	O	203	CDL	OB6-CB5	2.06	1.40	1.34
35	V	202	CDL	OA8-CA6	-2.06	1.40	1.45
35	v	202	CDL	OA6-CA5	2.06	1.40	1.34
37	C2	601	ATP	C5'-C4'	2.05	1.58	1.51
35	b	602	CDL	OB6-CB5	2.05	1.40	1.34
37	E1	601	ATP	C5'-C4'	2.05	1.58	1.51
36	J	301	PEE	O2-C10	2.04	1.40	1.34
33	O	204	PC1	O31-C3	-2.04	1.40	1.45
35	b	601	CDL	OA6-CA5	2.04	1.40	1.34
35	e	401	CDL	OA6-CA5	2.03	1.40	1.34
38	B2	601	ADP	C2-N3	2.02	1.35	1.32
35	u	201	CDL	OB8-CB6	-2.02	1.40	1.45
35	B	601	CDL	OA6-CA5	2.02	1.40	1.34
38	B1	601	ADP	C2-N3	2.02	1.35	1.32
35	E	401	CDL	OA6-CA5	2.02	1.40	1.34
35	H	302	CDL	OA6-CA5	2.02	1.40	1.34
35	b	601	CDL	OB6-CB5	2.01	1.40	1.34
33	o	204	PC1	O31-C3	-2.01	1.40	1.45
33	o	201	PC1	O21-C21	2.01	1.40	1.34
37	C1	601	ATP	C2-N3	2.01	1.35	1.32

All (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
37	A1	601	ATP	C5-C6-N6	7.55	131.82	120.35
37	C2	601	ATP	C5-C6-N6	7.55	131.82	120.35
38	D1	601	ADP	C5-C6-N6	7.54	131.81	120.35
37	E2	601	ATP	C5-C6-N6	7.52	131.77	120.35
38	D2	601	ADP	C5-C6-N6	7.51	131.76	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	A2	601	ATP	C5-C6-N6	7.47	131.71	120.35
37	C1	601	ATP	C5-C6-N6	7.44	131.66	120.35
38	B2	601	ADP	C5-C6-N6	7.43	131.64	120.35
38	B1	601	ADP	C5-C6-N6	7.42	131.63	120.35
37	C1	601	ATP	C1'-N9-C4	5.75	136.74	126.64
37	E2	601	ATP	C1'-N9-C4	5.66	136.59	126.64
37	E1	601	ATP	C1'-N9-C4	5.66	136.59	126.64
38	B1	601	ADP	N3-C2-N1	-5.60	119.92	128.68
38	D2	601	ADP	N3-C2-N1	-5.58	119.95	128.68
37	A2	601	ATP	C1'-N9-C4	5.56	136.41	126.64
37	C2	601	ATP	C1'-N9-C4	5.56	136.40	126.64
37	C1	601	ATP	N3-C2-N1	-5.55	120.01	128.68
37	E1	601	ATP	N3-C2-N1	-5.51	120.06	128.68
38	D1	601	ADP	N3-C2-N1	-5.51	120.07	128.68
38	B2	601	ADP	N3-C2-N1	-5.50	120.08	128.68
37	A1	601	ATP	N3-C2-N1	-5.50	120.08	128.68
37	C2	601	ATP	N3-C2-N1	-5.49	120.09	128.68
37	E2	601	ATP	N3-C2-N1	-5.47	120.13	128.68
37	A2	601	ATP	N3-C2-N1	-5.46	120.15	128.68
37	A1	601	ATP	C1'-N9-C4	5.45	136.21	126.64
38	D1	601	ADP	N6-C6-N1	-5.08	108.03	118.57
38	D2	601	ADP	N6-C6-N1	-5.08	108.03	118.57
37	C2	601	ATP	N6-C6-N1	-5.05	108.09	118.57
37	A1	601	ATP	N6-C6-N1	-5.03	108.13	118.57
38	B1	601	ADP	N6-C6-N1	-5.00	108.19	118.57
37	E1	601	ATP	N6-C6-N1	-4.99	108.22	118.57
38	B2	601	ADP	N6-C6-N1	-4.97	108.25	118.57
37	C1	601	ATP	N6-C6-N1	-4.97	108.27	118.57
37	E2	601	ATP	N6-C6-N1	-4.96	108.27	118.57
37	A2	601	ATP	N6-C6-N1	-4.95	108.30	118.57
33	O	204	PC1	O21-C21-C22	4.63	121.47	111.50
33	o	204	PC1	O21-C21-C22	4.60	121.42	111.50
35	d	402	CDL	OB6-CB5-C51	4.21	120.58	111.50
33	v	201	PC1	O21-C21-C22	4.21	120.58	111.50
33	V	201	PC1	O21-C21-C22	4.20	120.56	111.50
33	O	201	PC1	O21-C21-C22	4.15	120.44	111.50
35	D	402	CDL	OB6-CB5-C51	4.14	120.43	111.50
35	o	203	CDL	OB6-CB5-C51	4.08	120.30	111.50
33	o	201	PC1	O21-C21-C22	4.06	120.24	111.50
35	O	203	CDL	OB6-CB5-C51	4.05	120.22	111.50
35	b	602	CDL	OB6-CB5-C51	4.02	120.16	111.50
35	B	602	CDL	OB6-CB5-C51	3.99	120.10	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	J	302	PEE	O2-C10-C11	3.96	120.03	111.50
35	h	302	CDL	OB6-CB5-C51	3.93	119.97	111.50
35	H	302	CDL	OB6-CB5-C51	3.92	119.95	111.50
36	j	301	PEE	O2-C10-C11	3.76	119.60	111.50
36	j	302	PEE	O2-C10-C11	3.75	119.59	111.50
35	D	402	CDL	OA6-CA5-C11	3.71	119.50	111.50
36	J	301	PEE	O2-C10-C11	3.71	119.49	111.50
35	d	402	CDL	OA6-CA5-C11	3.70	119.48	111.50
38	B2	601	ADP	C3'-C2'-C1'	3.68	106.52	100.98
35	e	401	CDL	OB6-CB5-C51	3.63	119.33	111.50
35	B	601	CDL	OB6-CB5-C51	3.62	119.29	111.50
35	u	201	CDL	OA6-CA5-C11	3.60	119.27	111.50
35	b	601	CDL	OB6-CB5-C51	3.60	119.26	111.50
35	E	401	CDL	OB6-CB5-C51	3.57	119.20	111.50
37	C1	601	ATP	C3'-C2'-C1'	3.56	106.33	100.98
35	b	601	CDL	OA6-CA5-C11	3.55	119.15	111.50
35	U	201	CDL	OA6-CA5-C11	3.53	119.10	111.50
35	B	601	CDL	OA6-CA5-C11	3.52	119.09	111.50
35	e	401	CDL	OA6-CA5-C11	3.42	118.88	111.50
35	E	401	CDL	OA6-CA5-C11	3.40	118.82	111.50
35	b	602	CDL	OA6-CA5-C11	3.38	118.79	111.50
35	u	201	CDL	OB6-CB5-C51	3.37	118.75	111.50
35	B	602	CDL	OA6-CA5-C11	3.35	118.72	111.50
34	x	101	LMT	O5'-C5'-C4'	3.34	116.79	109.75
34	X	101	LMT	O5'-C5'-C4'	3.33	116.77	109.75
35	U	201	CDL	OB6-CB5-C51	3.31	118.64	111.50
35	c	401	CDL	OA6-CA5-C11	3.25	118.51	111.50
37	A2	601	ATP	C3'-C2'-C1'	3.25	105.87	100.98
35	C	401	CDL	OA6-CA5-C11	3.22	118.45	111.50
35	c	401	CDL	OB6-CB5-C51	3.19	118.37	111.50
35	o	203	CDL	OA6-CA5-C11	3.16	118.31	111.50
38	B1	601	ADP	O4'-C1'-C2'	-3.12	102.36	106.93
37	E1	601	ATP	C3'-C2'-C1'	3.12	105.68	100.98
35	O	203	CDL	OA6-CA5-C11	3.11	118.20	111.50
35	v	202	CDL	OB6-CB5-C51	3.11	118.20	111.50
38	D1	601	ADP	C3'-C2'-C1'	3.11	105.66	100.98
35	V	202	CDL	OB6-CB5-C51	3.07	118.11	111.50
35	C	401	CDL	OB6-CB5-C51	3.06	118.10	111.50
35	V	202	CDL	OA6-CA5-C11	3.04	118.05	111.50
38	D2	601	ADP	O4'-C1'-C2'	-3.04	102.49	106.93
35	h	302	CDL	OA6-CA5-C11	3.02	118.01	111.50
35	v	202	CDL	OA6-CA5-C11	2.98	117.93	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	c	403	PEE	O2-C10-C11	2.98	117.92	111.50
36	C	403	PEE	O2-C10-C11	2.96	117.89	111.50
38	D1	601	ADP	C2'-C3'-C4'	2.89	108.27	102.64
35	u	201	CDL	OA8-CA7-C31	2.89	120.97	111.91
38	B2	601	ADP	PA-O3A-PB	-2.88	122.94	132.83
37	A2	601	ATP	PA-O3A-PB	-2.88	122.96	132.83
38	D2	601	ADP	PA-O3A-PB	-2.87	122.99	132.83
38	B1	601	ADP	PA-O3A-PB	-2.86	123.00	132.83
35	H	302	CDL	OA6-CA5-C11	2.86	117.67	111.50
37	C2	601	ATP	PB-O3B-PG	-2.85	123.06	132.83
37	C2	601	ATP	O4'-C1'-C2'	-2.84	102.77	106.93
33	v	201	PC1	O31-C31-C32	2.83	120.80	111.91
35	U	201	CDL	OA8-CA7-C31	2.83	120.79	111.91
33	V	201	PC1	O31-C31-C32	2.82	120.77	111.91
34	d	401	LMT	C1B-O1B-C4'	-2.80	111.02	117.96
34	C	404	LMT	C1B-O1B-C4'	-2.80	111.04	117.96
37	C1	601	ATP	PB-O3B-PG	-2.79	123.24	132.83
37	E2	601	ATP	C3'-C2'-C1'	2.79	105.17	100.98
37	C1	601	ATP	PA-O3A-PB	-2.78	123.28	132.83
38	D1	601	ADP	PA-O3A-PB	-2.78	123.28	132.83
34	D	401	LMT	C1B-O1B-C4'	-2.77	111.11	117.96
35	O	203	CDL	OA8-CA7-C31	2.77	120.59	111.91
35	v	202	CDL	OA8-CA7-C31	2.76	120.55	111.91
37	C2	601	ATP	PA-O3A-PB	-2.75	123.39	132.83
35	o	203	CDL	OA8-CA7-C31	2.73	120.48	111.91
35	V	202	CDL	OA8-CA7-C31	2.72	120.46	111.91
37	E1	601	ATP	PA-O3A-PB	-2.72	123.51	132.83
37	E1	601	ATP	PB-O3B-PG	-2.70	123.55	132.83
35	e	401	CDL	OA8-CA7-C31	2.67	120.28	111.91
37	E2	601	ATP	PB-O3B-PG	-2.65	123.73	132.83
37	A1	601	ATP	PA-O3A-PB	-2.64	123.75	132.83
37	E2	601	ATP	PA-O3A-PB	-2.64	123.76	132.83
35	E	401	CDL	OA8-CA7-C31	2.63	120.15	111.91
37	A2	601	ATP	C2'-C3'-C4'	2.61	107.71	102.64
33	o	204	PC1	O31-C31-C32	2.61	120.09	111.91
35	C	401	CDL	OA8-CA7-C31	2.61	120.09	111.91
35	D	402	CDL	OB8-CB7-C71	2.60	120.07	111.91
36	J	302	PEE	O3-C30-C31	2.60	120.06	111.91
35	d	402	CDL	OB8-CB7-C71	2.59	120.05	111.91
37	A1	601	ATP	PB-O3B-PG	-2.59	123.93	132.83
34	c	404	LMT	C1B-O1B-C4'	-2.59	111.56	117.96
37	A2	601	ATP	PB-O3B-PG	-2.58	123.98	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	h	302	CDL	OB8-CB7-C71	2.54	119.89	111.91
35	H	302	CDL	OB8-CB7-C71	2.54	119.87	111.91
36	C	403	PEE	O3-C30-C31	2.53	119.86	111.91
33	O	201	PC1	C2-O21-C21	-2.53	111.56	117.79
33	O	204	PC1	O31-C31-C32	2.53	119.85	111.91
35	E	401	CDL	OB8-CB7-C71	2.52	119.82	111.91
37	C1	601	ATP	C2'-C3'-C4'	2.52	107.53	102.64
36	c	403	PEE	O3-C30-C31	2.52	119.81	111.91
35	e	401	CDL	OB8-CB7-C71	2.49	119.74	111.91
33	o	201	PC1	C2-O21-C21	-2.48	111.69	117.79
37	E1	601	ATP	C2'-C3'-C4'	2.43	107.36	102.64
35	b	602	CDL	OB8-CB7-C71	2.41	119.48	111.91
38	B2	601	ADP	C2'-C3'-C4'	2.36	107.23	102.64
35	B	602	CDL	OB8-CB7-C71	2.35	119.28	111.91
34	X	101	LMT	C3'-C4'-C5'	2.34	116.30	110.93
34	x	101	LMT	C3'-C4'-C5'	2.34	116.29	110.93
35	u	201	CDL	OB8-CB7-C71	2.33	119.20	111.91
37	E2	601	ATP	C2'-C3'-C4'	2.31	107.14	102.64
36	j	301	PEE	O3-C30-C31	2.31	119.15	111.91
35	b	601	CDL	OB8-CB7-C71	2.29	119.09	111.91
33	O	201	PC1	O31-C31-C32	2.29	119.09	111.91
35	B	601	CDL	OB8-CB7-C71	2.28	119.07	111.91
35	B	602	CDL	OA8-CA7-C31	2.27	119.04	111.91
37	A1	601	ATP	O4'-C1'-C2'	-2.27	103.61	106.93
35	U	201	CDL	OB8-CB7-C71	2.26	118.98	111.91
33	o	201	PC1	O31-C31-C32	2.25	118.96	111.91
36	J	301	PEE	O3-C30-C31	2.24	118.95	111.91
35	b	602	CDL	OA8-CA7-C31	2.22	118.87	111.91
34	D	403	LMT	C1B-O5B-C5B	-2.21	109.36	113.69
35	O	203	CDL	CA4-OA6-CA5	-2.20	112.37	117.79
38	B2	601	ADP	O4'-C1'-C2'	-2.17	103.75	106.93
36	J	302	PEE	C17-C18-C19	-2.16	108.15	124.73
34	d	403	LMT	C1B-O5B-C5B	-2.16	109.45	113.69
35	v	202	CDL	OB8-CB7-C71	2.15	118.66	111.91
35	c	401	CDL	C42-C41-C40	2.15	125.35	114.42
34	H	301	LMT	O5'-C1'-C2'	2.15	114.90	110.35
36	j	302	PEE	C17-C18-C19	-2.14	108.28	124.73
35	H	302	CDL	OA8-CA7-C31	2.14	118.62	111.91
34	h	301	LMT	O5'-C1'-C2'	2.14	114.87	110.35
34	O	202	LMT	O5'-C5'-C4'	2.13	114.25	109.75
34	x	101	LMT	C1B-O1B-C4'	-2.13	112.69	117.96
37	C1	601	ATP	O4'-C1'-C2'	-2.11	103.85	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	o	203	CDL	CA4-OA6-CA5	-2.10	112.63	117.79
35	c	401	CDL	OB8-CB7-C71	2.10	118.49	111.91
35	V	202	CDL	OB8-CB7-C71	2.09	118.48	111.91
36	j	302	PEE	O3-C30-C31	2.08	118.43	111.91
34	X	101	LMT	C1B-O1B-C4'	-2.08	112.83	117.96
34	h	301	LMT	O1B-C4'-C3'	2.08	112.80	107.28
34	o	202	LMT	O5'-C5'-C4'	2.07	114.12	109.75
34	C	402	LMT	C1B-O1B-C4'	-2.06	112.86	117.96
37	C2	601	ATP	C2'-C3'-C4'	2.06	106.65	102.64
35	O	203	CDL	OB8-CB7-C71	2.06	118.37	111.91
35	h	302	CDL	OA8-CA7-C31	2.05	118.34	111.91
34	c	404	LMT	O5'-C5'-C4'	2.05	114.07	109.75
34	C	404	LMT	O5'-C5'-C4'	2.04	114.06	109.75
34	C	404	LMT	C3'-C4'-C5'	2.04	115.61	110.93
34	c	402	LMT	C1B-O1B-C4'	-2.04	112.91	117.96
34	H	301	LMT	O1B-C4'-C3'	2.04	112.71	107.28
35	o	203	CDL	OB8-CB7-C71	2.04	118.31	111.91
37	E2	601	ATP	O4'-C1'-C2'	-2.03	103.96	106.93
36	j	301	PEE	C20-C19-C18	-2.02	109.19	124.73
36	J	301	PEE	C20-C19-C18	-2.02	109.20	124.73
37	A1	601	ATP	C3'-C2'-C1'	2.02	104.02	100.98
35	b	601	CDL	OA8-CA7-C31	2.02	118.24	111.91

There are no chirality outliers.

All (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
33	v	201	PC1	C1-O11-P-O12
33	v	201	PC1	C1-O11-P-O14
33	v	201	PC1	C1-O11-P-O13
33	v	201	PC1	C12-C11-O13-P
33	v	201	PC1	O13-C11-C12-N
33	v	201	PC1	O22-C21-O21-C2
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

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Mol	Chain	Res	Type	Atoms
33	O	204	PC1	C22-C21-O21-C2
33	V	201	PC1	C1-O11-P-O12
33	V	201	PC1	C1-O11-P-O14
33	V	201	PC1	C1-O11-P-O13
33	V	201	PC1	C12-C11-O13-P
33	V	201	PC1	O13-C11-C12-N
33	V	201	PC1	O22-C21-O21-C2
34	h	301	LMT	O5'-C1'-O1'-C1
34	x	101	LMT	C2'-C1'-O1'-C1
34	x	101	LMT	O5'-C1'-O1'-C1
34	d	403	LMT	C2-C1-O1'-C1'
34	H	301	LMT	O5'-C1'-O1'-C1
34	X	101	LMT	C2'-C1'-O1'-C1
34	X	101	LMT	O5'-C1'-O1'-C1
34	D	403	LMT	C2-C1-O1'-C1'
35	o	203	CDL	C11-CA5-OA6-CA4
35	o	203	CDL	CB3-OB5-PB2-OB3
35	u	201	CDL	CA3-OA5-PA1-OA3
35	u	201	CDL	CA3-OA5-PA1-OA4
35	u	201	CDL	CB2-OB2-PB2-OB3
35	h	302	CDL	CB2-C1-CA2-OA2
35	h	302	CDL	CA2-OA2-PA1-OA4
35	h	302	CDL	CB2-OB2-PB2-OB3
35	h	302	CDL	OB7-CB5-OB6-CB4
35	e	401	CDL	CA3-OA5-PA1-OA4
35	e	401	CDL	CB2-OB2-PB2-OB3
35	e	401	CDL	CB2-OB2-PB2-OB4
35	e	401	CDL	CB3-OB5-PB2-OB2
35	e	401	CDL	CB3-OB5-PB2-OB3
35	e	401	CDL	CB3-OB5-PB2-OB4
35	b	601	CDL	OB7-CB5-OB6-CB4
35	b	601	CDL	C51-CB5-OB6-CB4
35	b	602	CDL	CA2-OA2-PA1-OA3
35	b	602	CDL	CA2-OA2-PA1-OA4
35	b	602	CDL	CA3-OA5-PA1-OA3
35	b	602	CDL	C51-CB5-OB6-CB4
35	v	202	CDL	O1-C1-CB2-OB2
35	v	202	CDL	CA2-C1-CB2-OB2
35	v	202	CDL	C1-CB2-OB2-PB2
35	c	401	CDL	CA3-OA5-PA1-OA2
35	c	401	CDL	CA3-OA5-PA1-OA3
35	c	401	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
35	c	401	CDL	CB3-OB5-PB2-OB2
35	c	401	CDL	CB3-OB5-PB2-OB3
35	c	401	CDL	CB3-OB5-PB2-OB4
35	d	402	CDL	O1-C1-CB2-OB2
35	d	402	CDL	CA2-C1-CB2-OB2
35	d	402	CDL	CA2-OA2-PA1-OA3
35	d	402	CDL	CB2-OB2-PB2-OB3
35	d	402	CDL	C51-CB5-OB6-CB4
35	O	203	CDL	C11-CA5-OA6-CA4
35	O	203	CDL	CB3-OB5-PB2-OB3
35	O	203	CDL	CB3-OB5-PB2-OB4
35	U	201	CDL	CA3-OA5-PA1-OA3
35	U	201	CDL	CA3-OA5-PA1-OA4
35	U	201	CDL	CB2-OB2-PB2-OB3
35	H	302	CDL	CB2-C1-CA2-OA2
35	H	302	CDL	CA2-OA2-PA1-OA4
35	H	302	CDL	CB2-OB2-PB2-OB3
35	H	302	CDL	OB7-CB5-OB6-CB4
35	E	401	CDL	CA3-OA5-PA1-OA2
35	E	401	CDL	CA3-OA5-PA1-OA4
35	E	401	CDL	CB2-OB2-PB2-OB3
35	E	401	CDL	CB2-OB2-PB2-OB4
35	E	401	CDL	CB3-OB5-PB2-OB3
35	E	401	CDL	CB3-OB5-PB2-OB4
35	B	601	CDL	OB7-CB5-OB6-CB4
35	B	601	CDL	C51-CB5-OB6-CB4
35	B	602	CDL	CA2-OA2-PA1-OA3
35	B	602	CDL	CA2-OA2-PA1-OA4
35	B	602	CDL	CA3-OA5-PA1-OA3
35	B	602	CDL	C51-CB5-OB6-CB4
35	V	202	CDL	O1-C1-CB2-OB2
35	V	202	CDL	CA2-C1-CB2-OB2
35	V	202	CDL	CA3-OA5-PA1-OA2
35	V	202	CDL	C1-CB2-OB2-PB2
35	C	401	CDL	O1-C1-CA2-OA2
35	C	401	CDL	C1-CA2-OA2-PA1
35	D	402	CDL	O1-C1-CB2-OB2
35	D	402	CDL	CA2-C1-CB2-OB2
35	D	402	CDL	CA2-OA2-PA1-OA3
35	D	402	CDL	CB2-OB2-PB2-OB3
35	D	402	CDL	C51-CB5-OB6-CB4
36	j	302	PEE	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
36	c	403	PEE	O4P-C4-C5-N
36	c	403	PEE	C17-C18-C19-C20
36	c	403	PEE	C1-O3P-P-O1P
36	c	403	PEE	C1-O3P-P-O4P
36	J	302	PEE	O4P-C4-C5-N
36	C	403	PEE	O4P-C4-C5-N
36	C	403	PEE	C17-C18-C19-C20
36	C	403	PEE	C1-O3P-P-O1P
36	C	403	PEE	C1-O3P-P-O4P
37	E2	601	ATP	C5'-O5'-PA-O1A
37	E2	601	ATP	C5'-O5'-PA-O3A
37	C2	601	ATP	C5'-O5'-PA-O1A
37	C2	601	ATP	C5'-O5'-PA-O2A
37	C2	601	ATP	C5'-O5'-PA-O3A
37	E1	601	ATP	C5'-O5'-PA-O1A
37	E1	601	ATP	C5'-O5'-PA-O3A
37	C1	601	ATP	C5'-O5'-PA-O1A
37	C1	601	ATP	C5'-O5'-PA-O2A
37	C1	601	ATP	C5'-O5'-PA-O3A
38	B2	601	ADP	C5'-O5'-PA-O3A
38	D2	601	ADP	C3'-C4'-C5'-O5'
38	B1	601	ADP	C5'-O5'-PA-O3A
38	B1	601	ADP	C3'-C4'-C5'-O5'
35	e	401	CDL	OA9-CA7-OA8-CA6
35	E	401	CDL	OA9-CA7-OA8-CA6
35	h	302	CDL	OB9-CB7-OB8-CB6
35	b	601	CDL	OB9-CB7-OB8-CB6
35	c	401	CDL	OA9-CA7-OA8-CA6
35	H	302	CDL	OB9-CB7-OB8-CB6
35	B	601	CDL	OB9-CB7-OB8-CB6
35	C	401	CDL	OA9-CA7-OA8-CA6
33	o	201	PC1	O22-C21-O21-C2
33	O	201	PC1	O22-C21-O21-C2
35	o	203	CDL	OA7-CA5-OA6-CA4
35	b	602	CDL	OB7-CB5-OB6-CB4
35	d	402	CDL	OB7-CB5-OB6-CB4
35	O	203	CDL	OA7-CA5-OA6-CA4
35	B	602	CDL	OB7-CB5-OB6-CB4
35	D	402	CDL	OB7-CB5-OB6-CB4
35	h	302	CDL	C71-CB7-OB8-CB6
35	e	401	CDL	C31-CA7-OA8-CA6
35	b	601	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
35	c	401	CDL	C31-CA7-OA8-CA6
35	H	302	CDL	C71-CB7-OB8-CB6
35	E	401	CDL	C31-CA7-OA8-CA6
35	B	601	CDL	C71-CB7-OB8-CB6
35	C	401	CDL	C31-CA7-OA8-CA6
33	v	201	PC1	C22-C21-O21-C2
33	V	201	PC1	C22-C21-O21-C2
35	h	302	CDL	C51-CB5-OB6-CB4
35	H	302	CDL	C51-CB5-OB6-CB4
34	X	101	LMT	O5B-C5B-C6B-O6B
34	h	301	LMT	C3'-C4'-O1B-C1B
34	H	301	LMT	C3'-C4'-O1B-C1B
35	B	602	CDL	C31-CA7-OA8-CA6
36	j	301	PEE	C37-C38-C39-C40
36	J	301	PEE	C37-C38-C39-C40
34	D	403	LMT	O5B-C5B-C6B-O6B
33	o	204	PC1	O22-C21-O21-C2
33	O	204	PC1	O22-C21-O21-C2
35	o	203	CDL	OA9-CA7-OA8-CA6
35	O	203	CDL	OA9-CA7-OA8-CA6
35	b	601	CDL	C31-C32-C33-C34
35	B	601	CDL	C31-C32-C33-C34
35	h	302	CDL	O1-C1-CA2-OA2
35	H	302	CDL	O1-C1-CA2-OA2
35	b	602	CDL	C31-CA7-OA8-CA6
34	d	403	LMT	C4B-C5B-C6B-O6B
35	o	203	CDL	CB7-C71-C72-C73
35	O	203	CDL	CB7-C71-C72-C73
34	x	101	LMT	O5B-C5B-C6B-O6B
34	D	403	LMT	C4B-C5B-C6B-O6B
35	c	401	CDL	C40-C41-C42-C43
34	d	403	LMT	O5B-C5B-C6B-O6B
38	D2	601	ADP	O4'-C4'-C5'-O5'
35	o	203	CDL	C31-CA7-OA8-CA6
35	O	203	CDL	C31-CA7-OA8-CA6
34	d	401	LMT	O5B-C5B-C6B-O6B
34	C	404	LMT	O5'-C5'-C6'-O6'
34	D	401	LMT	O5B-C5B-C6B-O6B
35	b	602	CDL	OA9-CA7-OA8-CA6
35	B	602	CDL	OA9-CA7-OA8-CA6
34	X	101	LMT	C4B-C5B-C6B-O6B
34	c	404	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
34	C	404	LMT	O5'-C1'-O1'-C1
34	H	301	LMT	O5'-C5'-C6'-O6'
34	X	101	LMT	O5B-C1B-O1B-C4'
35	C	401	CDL	CB2-C1-CA2-OA2
35	v	202	CDL	C71-CB7-OB8-CB6
35	V	202	CDL	C71-CB7-OB8-CB6
34	C	404	LMT	C4'-C5'-C6'-O6'
35	h	302	CDL	C20-C21-C22-C23
35	H	302	CDL	C20-C21-C22-C23
34	x	101	LMT	C4B-C5B-C6B-O6B
33	o	201	PC1	C31-C32-C33-C34
33	O	201	PC1	C31-C32-C33-C34
34	d	401	LMT	C4B-C5B-C6B-O6B
34	h	301	LMT	O5B-C5B-C6B-O6B
35	C	401	CDL	C51-CB5-OB6-CB4
34	H	301	LMT	C4'-C5'-C6'-O6'
35	u	201	CDL	CA7-C31-C32-C33
35	e	401	CDL	CB5-C51-C52-C53
35	c	401	CDL	CA5-C11-C12-C13
35	U	201	CDL	CA7-C31-C32-C33
34	h	301	LMT	O5'-C5'-C6'-O6'
34	H	301	LMT	O5B-C5B-C6B-O6B
34	D	401	LMT	C4B-C5B-C6B-O6B
35	D	402	CDL	C71-CB7-OB8-CB6
35	h	302	CDL	CB5-C51-C52-C53
35	H	302	CDL	CB5-C51-C52-C53
35	E	401	CDL	CB5-C51-C52-C53
34	x	101	LMT	O5B-C1B-O1B-C4'
35	h	302	CDL	CA5-C11-C12-C13
35	c	401	CDL	CB5-C51-C52-C53
35	H	302	CDL	CA5-C11-C12-C13
35	C	401	CDL	CA5-C11-C12-C13
35	d	402	CDL	C71-CB7-OB8-CB6
35	h	302	CDL	CA4-CA3-OA5-PA1
35	H	302	CDL	CA4-CA3-OA5-PA1
35	u	201	CDL	CB5-C51-C52-C53
35	b	601	CDL	CA7-C31-C32-C33
35	U	201	CDL	CB5-C51-C52-C53
35	B	601	CDL	CA7-C31-C32-C33
35	v	202	CDL	OB9-CB7-OB8-CB6
35	V	202	CDL	OB9-CB7-OB8-CB6
35	c	401	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
35	v	202	CDL	CB7-C71-C72-C73
35	V	202	CDL	CB7-C71-C72-C73
35	v	202	CDL	C63-C64-C65-C66
35	V	202	CDL	C63-C64-C65-C66
35	o	203	CDL	CB3-OB5-PB2-OB2
35	h	302	CDL	CA2-OA2-PA1-OA5
35	e	401	CDL	CA3-OA5-PA1-OA2
35	e	401	CDL	CB2-OB2-PB2-OB5
35	b	602	CDL	CA2-OA2-PA1-OA5
35	d	402	CDL	CB2-OB2-PB2-OB5
35	O	203	CDL	CB3-OB5-PB2-OB2
35	H	302	CDL	CA2-OA2-PA1-OA5
35	E	401	CDL	CB2-OB2-PB2-OB5
35	E	401	CDL	CB3-OB5-PB2-OB2
35	B	602	CDL	CA2-OA2-PA1-OA5
35	C	401	CDL	CA3-OA5-PA1-OA2
35	C	401	CDL	CB3-OB5-PB2-OB2
35	D	402	CDL	CB2-OB2-PB2-OB5
33	o	201	PC1	C21-C22-C23-C24
35	c	401	CDL	C71-CB7-OB8-CB6
35	C	401	CDL	C71-CB7-OB8-CB6
33	O	201	PC1	C21-C22-C23-C24
35	c	401	CDL	CA2-C1-CB2-OB2
35	C	401	CDL	OB7-CB5-OB6-CB4
33	O	201	PC1	C32-C31-O31-C3
33	o	204	PC1	C3A-C3B-C3C-C3D
33	O	204	PC1	C3A-C3B-C3C-C3D
35	b	602	CDL	C38-C39-C40-C41
35	u	201	CDL	C11-CA5-OA6-CA4
35	c	401	CDL	C51-CB5-OB6-CB4
35	U	201	CDL	C11-CA5-OA6-CA4
38	B2	601	ADP	C3'-C4'-C5'-O5'
33	o	201	PC1	C3D-C3E-C3F-C3G
33	V	201	PC1	C35-C36-C37-C38
35	o	203	CDL	C16-C17-C18-C19
35	h	302	CDL	C71-C72-C73-C74
35	b	602	CDL	C77-C78-C79-C80
35	v	202	CDL	C35-C36-C37-C38
35	v	202	CDL	C57-C58-C59-C60
35	c	401	CDL	C17-C18-C19-C20
35	O	203	CDL	C16-C17-C18-C19
35	H	302	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
35	B	602	CDL	C38-C39-C40-C41
35	B	602	CDL	C77-C78-C79-C80
35	V	202	CDL	C35-C36-C37-C38
35	V	202	CDL	C57-C58-C59-C60
35	C	401	CDL	C21-C22-C23-C24
33	o	201	PC1	C32-C31-O31-C3
33	v	201	PC1	C35-C36-C37-C38
33	O	201	PC1	C3D-C3E-C3F-C3G
35	o	203	CDL	C51-C52-C53-C54
35	e	401	CDL	C78-C79-C80-C81
35	c	401	CDL	C52-C53-C54-C55
35	d	402	CDL	C42-C43-C44-C45
35	O	203	CDL	C51-C52-C53-C54
35	C	401	CDL	C35-C36-C37-C38
35	D	402	CDL	C42-C43-C44-C45
35	u	201	CDL	OA7-CA5-OA6-CA4
35	c	401	CDL	OB7-CB5-OB6-CB4
35	U	201	CDL	OA7-CA5-OA6-CA4
35	o	203	CDL	C38-C39-C40-C41
35	c	401	CDL	C53-C54-C55-C56
35	d	402	CDL	C60-C61-C62-C63
35	E	401	CDL	C78-C79-C80-C81
35	D	402	CDL	C60-C61-C62-C63
35	d	402	CDL	C1-CB2-OB2-PB2
35	D	402	CDL	C1-CB2-OB2-PB2
35	o	203	CDL	C12-C13-C14-C15
35	e	401	CDL	C31-C32-C33-C34
35	b	602	CDL	C22-C23-C24-C25
35	b	602	CDL	C40-C41-C42-C43
35	O	203	CDL	C12-C13-C14-C15
35	O	203	CDL	C38-C39-C40-C41
35	H	302	CDL	C56-C57-C58-C59
35	E	401	CDL	C31-C32-C33-C34
35	B	602	CDL	C22-C23-C24-C25
35	B	602	CDL	C40-C41-C42-C43
35	C	401	CDL	C11-C12-C13-C14
35	C	401	CDL	C22-C23-C24-C25
35	C	401	CDL	C33-C34-C35-C36
35	e	401	CDL	O1-C1-CA2-OA2
35	E	401	CDL	O1-C1-CA2-OA2
35	h	302	CDL	C56-C57-C58-C59
35	v	202	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
35	c	401	CDL	C32-C33-C34-C35
33	V	201	PC1	C21-C22-C23-C24
35	B	602	CDL	CA7-C31-C32-C33
33	o	204	PC1	C27-C28-C29-C2A
33	v	201	PC1	C25-C26-C27-C28
33	O	204	PC1	C27-C28-C29-C2A
33	V	201	PC1	C25-C26-C27-C28
34	d	401	LMT	C3-C4-C5-C6
35	u	201	CDL	C41-C42-C43-C44
35	u	201	CDL	C75-C76-C77-C78
35	b	602	CDL	C52-C53-C54-C55
35	c	401	CDL	C21-C22-C23-C24
35	c	401	CDL	C22-C23-C24-C25
35	O	203	CDL	C23-C24-C25-C26
35	U	201	CDL	C41-C42-C43-C44
35	V	202	CDL	C72-C73-C74-C75
35	C	401	CDL	OB9-CB7-OB8-CB6
35	o	203	CDL	C23-C24-C25-C26
35	u	201	CDL	C62-C63-C64-C65
35	e	401	CDL	C58-C59-C60-C61
35	c	401	CDL	C19-C20-C21-C22
35	c	401	CDL	C74-C75-C76-C77
35	U	201	CDL	C75-C76-C77-C78
35	E	401	CDL	C58-C59-C60-C61
35	B	601	CDL	C18-C19-C20-C21
35	B	602	CDL	C52-C53-C54-C55
33	v	201	PC1	C21-C22-C23-C24
34	x	101	LMT	C5-C6-C7-C8
34	X	101	LMT	C5-C6-C7-C8
35	b	601	CDL	C18-C19-C20-C21
35	C	401	CDL	C54-C55-C56-C57
35	c	401	CDL	OB9-CB7-OB8-CB6
35	d	402	CDL	OB9-CB7-OB8-CB6
35	D	402	CDL	OB9-CB7-OB8-CB6
35	h	302	CDL	C22-C23-C24-C25
35	b	601	CDL	C74-C75-C76-C77
35	b	602	CDL	C56-C57-C58-C59
35	c	401	CDL	C72-C73-C74-C75
35	U	201	CDL	C62-C63-C64-C65
35	H	302	CDL	C22-C23-C24-C25
35	B	601	CDL	C74-C75-C76-C77
35	B	602	CDL	C56-C57-C58-C59

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Mol	Chain	Res	Type	Atoms
36	j	301	PEE	C14-C15-C16-C17
36	J	301	PEE	C14-C15-C16-C17
34	X	101	LMT	C3-C4-C5-C6
35	O	203	CDL	C61-C62-C63-C64
35	b	602	CDL	CA7-C31-C32-C33
33	o	204	PC1	C32-C33-C34-C35
33	V	201	PC1	C3B-C3C-C3D-C3E
34	D	401	LMT	C5-C6-C7-C8
35	u	201	CDL	C14-C15-C16-C17
35	u	201	CDL	C23-C24-C25-C26
35	u	201	CDL	C77-C78-C79-C80
35	h	302	CDL	C53-C54-C55-C56
35	e	401	CDL	C81-C82-C83-C84
35	d	402	CDL	C52-C53-C54-C55
35	U	201	CDL	C14-C15-C16-C17
35	U	201	CDL	C23-C24-C25-C26
35	U	201	CDL	C77-C78-C79-C80
35	H	302	CDL	C53-C54-C55-C56
35	E	401	CDL	C40-C41-C42-C43
35	C	401	CDL	C14-C15-C16-C17
35	D	402	CDL	C52-C53-C54-C55
35	D	402	CDL	C82-C83-C84-C85
36	j	301	PEE	C34-C35-C36-C37
36	J	301	PEE	C34-C35-C36-C37
36	C	403	PEE	C22-C23-C24-C25
33	v	201	PC1	C3B-C3C-C3D-C3E
33	O	204	PC1	C32-C33-C34-C35
34	o	202	LMT	C7-C8-C9-C10
34	d	401	LMT	C7-C8-C9-C10
34	O	202	LMT	C7-C8-C9-C10
35	o	203	CDL	C37-C38-C39-C40
35	o	203	CDL	C61-C62-C63-C64
35	u	201	CDL	C35-C36-C37-C38
35	e	401	CDL	C40-C41-C42-C43
35	b	602	CDL	C80-C81-C82-C83
35	c	401	CDL	C55-C56-C57-C58
35	d	402	CDL	C82-C83-C84-C85
35	O	203	CDL	C37-C38-C39-C40
35	O	203	CDL	C83-C84-C85-C86
35	U	201	CDL	C35-C36-C37-C38
35	E	401	CDL	C81-C82-C83-C84
35	B	602	CDL	C80-C81-C82-C83

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Mol	Chain	Res	Type	Atoms
35	C	401	CDL	C74-C75-C76-C77
36	c	403	PEE	C22-C23-C24-C25
34	c	404	LMT	C1-C2-C3-C4
34	x	101	LMT	C3-C4-C5-C6
35	o	203	CDL	C31-C32-C33-C34
35	o	203	CDL	C83-C84-C85-C86
35	e	401	CDL	C37-C38-C39-C40
35	b	601	CDL	C72-C73-C74-C75
35	b	602	CDL	C11-C12-C13-C14
35	b	602	CDL	C73-C74-C75-C76
35	E	401	CDL	C37-C38-C39-C40
35	B	601	CDL	C72-C73-C74-C75
35	B	602	CDL	C11-C12-C13-C14
35	B	602	CDL	C73-C74-C75-C76
35	C	401	CDL	C63-C64-C65-C66
35	d	402	CDL	C80-C81-C82-C83
35	O	203	CDL	C31-C32-C33-C34
35	D	402	CDL	C80-C81-C82-C83
35	b	602	CDL	C71-CB7-OB8-CB6
35	B	602	CDL	C71-CB7-OB8-CB6
36	c	403	PEE	C31-C30-O3-C3
36	C	403	PEE	C31-C30-O3-C3
35	h	302	CDL	C59-C60-C61-C62
35	H	302	CDL	C59-C60-C61-C62
35	u	201	CDL	C79-C80-C81-C82
34	x	101	LMT	C7-C8-C9-C10
34	X	101	LMT	C7-C8-C9-C10
34	D	401	LMT	C11-C10-C9-C8
35	h	302	CDL	C80-C81-C82-C83
35	c	401	CDL	C39-C40-C41-C42
35	U	201	CDL	C79-C80-C81-C82
35	H	302	CDL	C80-C81-C82-C83
35	E	401	CDL	C23-C24-C25-C26
36	c	403	PEE	C23-C24-C25-C26
36	C	403	PEE	C23-C24-C25-C26
34	X	101	LMT	O5'-C5'-C6'-O6'
35	e	401	CDL	C23-C24-C25-C26
35	B	601	CDL	C41-C42-C43-C44
35	C	401	CDL	C58-C59-C60-C61
36	j	302	PEE	C31-C30-O3-C3
36	J	302	PEE	C31-C30-O3-C3
35	d	402	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
35	D	402	CDL	C11-CA5-OA6-CA4
35	b	601	CDL	C41-C42-C43-C44
35	c	401	CDL	C82-C83-C84-C85
35	V	202	CDL	C61-C62-C63-C64
35	C	401	CDL	C32-C33-C34-C35
36	j	301	PEE	C23-C24-C25-C26
36	J	301	PEE	C23-C24-C25-C26
35	v	202	CDL	C61-C62-C63-C64
34	C	404	LMT	C1-C2-C3-C4
33	V	201	PC1	C33-C34-C35-C36
35	C	401	CDL	C20-C21-C22-C23
33	o	201	PC1	O32-C31-O31-C3
33	O	201	PC1	O32-C31-O31-C3
35	e	401	CDL	CB2-C1-CA2-OA2
35	E	401	CDL	CB2-C1-CA2-OA2
33	v	201	PC1	C33-C34-C35-C36
35	C	401	CDL	C15-C16-C17-C18
35	d	402	CDL	OA7-CA5-OA6-CA4
35	D	402	CDL	OA7-CA5-OA6-CA4
35	c	401	CDL	C43-C44-C45-C46
35	B	602	CDL	OB9-CB7-OB8-CB6
36	j	302	PEE	O5-C30-O3-C3
36	C	403	PEE	O5-C30-O3-C3
35	u	201	CDL	C60-C61-C62-C63
35	e	401	CDL	C74-C75-C76-C77
35	c	401	CDL	C51-C52-C53-C54
35	U	201	CDL	C60-C61-C62-C63
35	E	401	CDL	C74-C75-C76-C77
36	C	403	PEE	C21-C22-C23-C24
36	c	403	PEE	C21-C22-C23-C24
34	D	401	LMT	C3-C4-C5-C6
35	b	601	CDL	C36-C37-C38-C39
35	B	601	CDL	C36-C37-C38-C39
35	b	602	CDL	OB9-CB7-OB8-CB6
36	c	403	PEE	O5-C30-O3-C3
34	d	401	LMT	C4-C5-C6-C7
34	C	402	LMT	C3-C4-C5-C6
35	b	601	CDL	C56-C57-C58-C59
35	b	602	CDL	C62-C63-C64-C65
35	B	601	CDL	C56-C57-C58-C59
34	c	402	LMT	C3-C4-C5-C6
36	J	302	PEE	O5-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
35	u	201	CDL	OB7-CB5-OB6-CB4
35	U	201	CDL	OB7-CB5-OB6-CB4
35	B	601	CDL	OA7-CA5-OA6-CA4
35	B	601	CDL	C62-C63-C64-C65
35	B	602	CDL	C62-C63-C64-C65
35	C	401	CDL	C41-C42-C43-C44
36	c	403	PEE	C13-C14-C15-C16
36	C	403	PEE	C13-C14-C15-C16
35	b	601	CDL	C62-C63-C64-C65
35	C	401	CDL	C55-C56-C57-C58
35	D	402	CDL	C73-C74-C75-C76
36	j	301	PEE	C10-C11-C12-C13
36	J	301	PEE	C10-C11-C12-C13
33	O	201	PC1	C26-C27-C28-C29
35	h	302	CDL	C58-C59-C60-C61
35	b	601	CDL	C16-C17-C18-C19
35	b	601	CDL	C78-C79-C80-C81
35	v	202	CDL	C62-C63-C64-C65
35	H	302	CDL	C58-C59-C60-C61
35	B	601	CDL	C16-C17-C18-C19
35	V	202	CDL	C62-C63-C64-C65
33	o	201	PC1	C26-C27-C28-C29
33	o	204	PC1	C37-C38-C39-C3A
33	O	204	PC1	C37-C38-C39-C3A
35	h	302	CDL	C74-C75-C76-C77
35	v	202	CDL	C55-C56-C57-C58
35	d	402	CDL	C73-C74-C75-C76
35	H	302	CDL	C74-C75-C76-C77
35	B	601	CDL	C43-C44-C45-C46
35	B	601	CDL	C78-C79-C80-C81
35	b	601	CDL	C43-C44-C45-C46
35	V	202	CDL	C55-C56-C57-C58
35	D	402	CDL	C40-C41-C42-C43
35	c	401	CDL	CA7-C31-C32-C33
35	u	201	CDL	C51-CB5-OB6-CB4
35	b	601	CDL	C11-CA5-OA6-CA4
35	U	201	CDL	C51-CB5-OB6-CB4
35	B	601	CDL	C11-CA5-OA6-CA4
33	v	201	PC1	C23-C24-C25-C26
33	V	201	PC1	C23-C24-C25-C26
35	d	402	CDL	C40-C41-C42-C43
35	b	601	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
35	h	302	CDL	C76-C77-C78-C79
35	e	401	CDL	C53-C54-C55-C56
35	V	202	CDL	OA6-CA4-CA6-OA8
33	o	204	PC1	C39-C3A-C3B-C3C
33	O	204	PC1	C39-C3A-C3B-C3C
35	e	401	CDL	C14-C15-C16-C17
35	E	401	CDL	C14-C15-C16-C17
35	E	401	CDL	C53-C54-C55-C56
35	b	601	CDL	C58-C59-C60-C61
35	c	401	CDL	C12-C13-C14-C15
35	c	401	CDL	C81-C82-C83-C84
35	H	302	CDL	C76-C77-C78-C79
35	B	601	CDL	C58-C59-C60-C61
36	c	403	PEE	C19-C20-C21-C22
36	C	403	PEE	C19-C20-C21-C22
35	d	402	CDL	C63-C64-C65-C66
34	d	401	LMT	C1-C2-C3-C4
38	B2	601	ADP	O4'-C4'-C5'-O5'
38	B1	601	ADP	O4'-C4'-C5'-O5'
34	C	404	LMT	C3-C4-C5-C6
34	D	401	LMT	C7-C8-C9-C10
35	D	402	CDL	C63-C64-C65-C66
36	c	403	PEE	C36-C37-C38-C39
36	C	403	PEE	C36-C37-C38-C39
34	c	402	LMT	C1-C2-C3-C4
33	o	201	PC1	C1-O11-P-O13
33	v	201	PC1	C11-O13-P-O11
33	V	201	PC1	C11-O13-P-O11
35	u	201	CDL	CA3-OA5-PA1-OA2
35	h	302	CDL	CB2-OB2-PB2-OB5
35	d	402	CDL	CB3-OB5-PB2-OB2
35	U	201	CDL	CA3-OA5-PA1-OA2
35	H	302	CDL	CB2-OB2-PB2-OB5
35	D	402	CDL	CB3-OB5-PB2-OB2
35	D	402	CDL	C36-C37-C38-C39
35	e	401	CDL	CA7-C31-C32-C33
35	E	401	CDL	CA7-C31-C32-C33
34	h	301	LMT	C4'-C5'-C6'-O6'
35	C	401	CDL	OB5-CB3-CB4-CB6
34	c	404	LMT	C2-C3-C4-C5
35	b	601	CDL	C80-C81-C82-C83
35	o	203	CDL	C63-C64-C65-C66

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Mol	Chain	Res	Type	Atoms
35	B	601	CDL	C80-C81-C82-C83
34	C	402	LMT	C1-C2-C3-C4
34	D	401	LMT	C1-C2-C3-C4
35	d	402	CDL	C36-C37-C38-C39
36	j	301	PEE	C41-C42-C43-C44
35	h	302	CDL	C14-C15-C16-C17
35	O	203	CDL	C63-C64-C65-C66
35	H	302	CDL	C14-C15-C16-C17
36	J	301	PEE	C41-C42-C43-C44
33	O	201	PC1	C37-C38-C39-C3A
34	X	101	LMT	C2-C3-C4-C5
33	o	201	PC1	C37-C38-C39-C3A
34	x	101	LMT	C2-C3-C4-C5
34	c	404	LMT	C3-C4-C5-C6
35	b	602	CDL	C51-C52-C53-C54
35	c	401	CDL	C44-C45-C46-C47
34	C	404	LMT	C2-C3-C4-C5
35	v	202	CDL	C59-C60-C61-C62
35	B	601	CDL	C63-C64-C65-C66
35	B	602	CDL	C51-C52-C53-C54
35	o	203	CDL	CB3-CB4-CB6-OB8
35	b	601	CDL	C63-C64-C65-C66
35	b	602	CDL	CB3-CB4-CB6-OB8
35	v	202	CDL	CA3-CA4-CA6-OA8
35	O	203	CDL	CB3-CB4-CB6-OB8
35	B	602	CDL	CB3-CB4-CB6-OB8
35	V	202	CDL	CA3-CA4-CA6-OA8
35	C	401	CDL	CB3-CB4-CB6-OB8
36	J	302	PEE	C17-C18-C19-C20
34	D	401	LMT	O5'-C5'-C6'-O6'
35	c	401	CDL	C31-C32-C33-C34
35	V	202	CDL	C59-C60-C61-C62
35	u	201	CDL	C84-C85-C86-C87
35	U	201	CDL	C84-C85-C86-C87
35	B	602	CDL	C44-C45-C46-C47
33	o	204	PC1	C3E-C3F-C3G-C3H
33	O	204	PC1	C3E-C3F-C3G-C3H
35	b	602	CDL	C44-C45-C46-C47
33	V	201	PC1	C36-C37-C38-C39
34	D	403	LMT	C3-C4-C5-C6
35	C	401	CDL	C84-C85-C86-C87
33	v	201	PC1	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
34	d	403	LMT	C3-C4-C5-C6
36	J	302	PEE	C40-C41-C42-C43
34	d	401	LMT	O5'-C5'-C6'-O6'
36	j	302	PEE	C40-C41-C42-C43
36	J	302	PEE	C23-C24-C25-C26
35	V	202	CDL	C44-C45-C46-C47
36	j	302	PEE	C23-C24-C25-C26
35	h	302	CDL	CB3-CB4-OB6-CB5
35	d	402	CDL	CA6-CA4-OA6-CA5
35	H	302	CDL	CB3-CB4-OB6-CB5
35	D	402	CDL	CA6-CA4-OA6-CA5
35	u	201	CDL	C38-C39-C40-C41
35	C	401	CDL	C19-C20-C21-C22
36	c	403	PEE	C42-C43-C44-C45
36	C	403	PEE	C42-C43-C44-C45
35	v	202	CDL	C44-C45-C46-C47
35	U	201	CDL	C38-C39-C40-C41
35	C	401	CDL	C34-C35-C36-C37
33	v	201	PC1	C38-C39-C3A-C3B
33	V	201	PC1	C38-C39-C3A-C3B
35	u	201	CDL	C58-C59-C60-C61
35	b	601	CDL	C32-C33-C34-C35
35	v	202	CDL	C74-C75-C76-C77
35	U	201	CDL	C58-C59-C60-C61
35	H	302	CDL	C64-C65-C66-C67
35	o	203	CDL	C71-CB7-OB8-CB6
35	O	203	CDL	C71-CB7-OB8-CB6
33	V	201	PC1	O11-C1-C2-O21
35	b	601	CDL	OA5-CA3-CA4-OA6
35	b	602	CDL	OA5-CA3-CA4-OA6
35	B	601	CDL	OA5-CA3-CA4-OA6
36	j	302	PEE	C17-C18-C19-C20
35	C	401	CDL	CA7-C31-C32-C33
34	D	401	LMT	C6-C7-C8-C9
35	h	302	CDL	C64-C65-C66-C67
36	j	302	PEE	C21-C22-C23-C24
35	E	401	CDL	C42-C43-C44-C45
35	B	602	CDL	C58-C59-C60-C61
34	h	301	LMT	C4B-C5B-C6B-O6B
35	C	401	CDL	C60-C61-C62-C63
36	J	302	PEE	C21-C22-C23-C24
34	d	401	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
35	V	202	CDL	C74-C75-C76-C77
35	o	203	CDL	OB6-CB4-CB6-OB8
35	e	401	CDL	OA6-CA4-CA6-OA8
35	v	202	CDL	OA6-CA4-CA6-OA8
35	O	203	CDL	OB6-CB4-CB6-OB8
35	E	401	CDL	OA6-CA4-CA6-OA8
35	e	401	CDL	C42-C43-C44-C45
35	B	601	CDL	C32-C33-C34-C35
35	h	302	CDL	C34-C35-C36-C37
35	b	601	CDL	C83-C84-C85-C86
35	H	302	CDL	C34-C35-C36-C37
35	b	602	CDL	C58-C59-C60-C61
35	B	601	CDL	C83-C84-C85-C86
35	b	601	CDL	C52-C53-C54-C55
35	c	401	CDL	C15-C16-C17-C18
35	B	601	CDL	C17-C18-C19-C20
35	b	601	CDL	C31-CA7-OA8-CA6
35	d	402	CDL	C31-CA7-OA8-CA6
35	B	601	CDL	C31-CA7-OA8-CA6
35	D	402	CDL	C31-CA7-OA8-CA6
35	c	401	CDL	C36-C37-C38-C39
35	O	203	CDL	C35-C36-C37-C38
34	x	101	LMT	O5'-C5'-C6'-O6'
35	o	203	CDL	C35-C36-C37-C38
35	B	602	CDL	C31-C32-C33-C34
35	h	302	CDL	C24-C25-C26-C27
35	b	601	CDL	C17-C18-C19-C20
35	b	602	CDL	C31-C32-C33-C34
35	H	302	CDL	C24-C25-C26-C27
35	C	401	CDL	C75-C76-C77-C78
35	c	401	CDL	C14-C15-C16-C17
36	J	302	PEE	C13-C14-C15-C16
35	c	401	CDL	C13-C14-C15-C16
35	B	601	CDL	C52-C53-C54-C55
35	e	401	CDL	OB5-CB3-CB4-CB6
35	E	401	CDL	OB5-CB3-CB4-CB6
35	O	203	CDL	C59-C60-C61-C62
35	u	201	CDL	C64-C65-C66-C67
35	V	202	CDL	C11-C12-C13-C14
36	j	302	PEE	C13-C14-C15-C16
34	c	402	LMT	O1'-C1-C2-C3
34	C	402	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
35	U	201	CDL	C64-C65-C66-C67
35	o	203	CDL	C59-C60-C61-C62
35	v	202	CDL	C11-C12-C13-C14
35	C	401	CDL	C13-C14-C15-C16
35	C	401	CDL	C61-C62-C63-C64
36	J	302	PEE	C30-C31-C32-C33
35	c	401	CDL	C63-C64-C65-C66
35	v	202	CDL	C1-CA2-OA2-PA1
35	V	202	CDL	C52-C53-C54-C55
34	o	202	LMT	C2-C1-O1'-C1'
34	O	202	LMT	C2-C1-O1'-C1'
35	v	202	CDL	C52-C53-C54-C55
35	c	401	CDL	C59-C60-C61-C62
35	o	203	CDL	CA3-CA4-CA6-OA8
35	c	401	CDL	CB3-CB4-CB6-OB8
35	O	203	CDL	CA3-CA4-CA6-OA8
33	O	204	PC1	C26-C27-C28-C29
35	D	402	CDL	C71-C72-C73-C74
36	c	403	PEE	C34-C35-C36-C37
36	C	403	PEE	C34-C35-C36-C37
36	j	302	PEE	C30-C31-C32-C33
35	d	402	CDL	C71-C72-C73-C74
35	V	202	CDL	C15-C16-C17-C18
33	o	204	PC1	C26-C27-C28-C29
35	e	401	CDL	C32-C33-C34-C35
35	E	401	CDL	C32-C33-C34-C35
33	O	201	PC1	C1-O11-P-O13
35	u	201	CDL	CB2-OB2-PB2-OB5
35	v	202	CDL	CA3-OA5-PA1-OA2
35	U	201	CDL	CB2-OB2-PB2-OB5
34	D	401	LMT	O1'-C1-C2-C3
35	D	402	CDL	C56-C57-C58-C59
34	c	404	LMT	C4'-C5'-C6'-O6'
35	d	402	CDL	C56-C57-C58-C59
35	V	202	CDL	C33-C34-C35-C36
33	o	201	PC1	O11-C1-C2-O21
33	o	204	PC1	O11-C1-C2-O21
33	v	201	PC1	O11-C1-C2-O21
33	O	201	PC1	O11-C1-C2-O21
33	O	204	PC1	O11-C1-C2-O21
35	b	602	CDL	OB5-CB3-CB4-OB6
35	c	401	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
35	B	602	CDL	OB5-CB3-CB4-OB6
35	c	401	CDL	C20-C21-C22-C23
33	O	201	PC1	C34-C35-C36-C37
35	v	202	CDL	C33-C34-C35-C36
33	V	201	PC1	C2B-C2C-C2D-C2E
35	v	202	CDL	C15-C16-C17-C18
35	C	401	CDL	C62-C63-C64-C65
35	b	601	CDL	OA9-CA7-OA8-CA6
35	B	601	CDL	OA9-CA7-OA8-CA6
33	o	201	PC1	C34-C35-C36-C37
33	v	201	PC1	C2B-C2C-C2D-C2E
35	c	401	CDL	C34-C35-C36-C37
35	h	302	CDL	C36-C37-C38-C39
35	e	401	CDL	C71-C72-C73-C74
35	E	401	CDL	C71-C72-C73-C74
35	h	302	CDL	C1-CA2-OA2-PA1
35	O	203	CDL	CA4-CA3-OA5-PA1
35	H	302	CDL	C1-CA2-OA2-PA1
35	V	202	CDL	C1-CA2-OA2-PA1
35	o	203	CDL	OB9-CB7-OB8-CB6
35	O	203	CDL	OB9-CB7-OB8-CB6
35	b	602	CDL	C63-C64-C65-C66
35	H	302	CDL	C36-C37-C38-C39
35	B	602	CDL	C63-C64-C65-C66
35	o	203	CDL	C44-C45-C46-C47
35	O	203	CDL	C44-C45-C46-C47
34	H	301	LMT	C4B-C5B-C6B-O6B
35	C	401	CDL	C31-C32-C33-C34
35	d	402	CDL	CA7-C31-C32-C33
35	D	402	CDL	CA7-C31-C32-C33
35	c	401	CDL	OB5-CB3-CB4-CB6
35	h	302	CDL	C78-C79-C80-C81
35	c	401	CDL	C75-C76-C77-C78
35	d	402	CDL	OA9-CA7-OA8-CA6
35	o	203	CDL	C72-C73-C74-C75
35	O	203	CDL	C72-C73-C74-C75
35	H	302	CDL	C78-C79-C80-C81
34	H	301	LMT	C5'-C4'-O1B-C1B
34	c	402	LMT	C6-C7-C8-C9
35	C	401	CDL	C56-C57-C58-C59
35	D	402	CDL	OA9-CA7-OA8-CA6
34	C	402	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
35	b	602	CDL	CB6-CB4-OB6-CB5
35	B	602	CDL	CB6-CB4-OB6-CB5
35	b	601	CDL	C61-C62-C63-C64
35	u	201	CDL	C11-C12-C13-C14
34	h	301	LMT	C5'-C4'-O1B-C1B
34	C	402	LMT	C11-C10-C9-C8
35	o	203	CDL	CA4-CA3-OA5-PA1
35	c	401	CDL	C1-CA2-OA2-PA1
35	V	202	CDL	CB3-CB4-CB6-OB8
35	E	401	CDL	C17-C18-C19-C20
35	e	401	CDL	OB5-CB3-CB4-OB6
35	b	601	CDL	OB5-CB3-CB4-OB6
35	v	202	CDL	OA5-CA3-CA4-OA6
35	B	602	CDL	OA5-CA3-CA4-OA6
35	C	401	CDL	OB5-CB3-CB4-OB6
33	o	204	PC1	C23-C24-C25-C26
33	O	204	PC1	C23-C24-C25-C26
35	h	302	CDL	C16-C17-C18-C19
35	U	201	CDL	C11-C12-C13-C14
35	H	302	CDL	C16-C17-C18-C19
35	B	601	CDL	C61-C62-C63-C64
34	c	402	LMT	C11-C10-C9-C8
34	x	101	LMT	C9-C10-C11-C12
35	e	401	CDL	C59-C60-C61-C62
35	d	402	CDL	C38-C39-C40-C41
35	D	402	CDL	C38-C39-C40-C41
35	E	401	CDL	C59-C60-C61-C62
35	h	302	CDL	OB6-CB4-CB6-OB8
35	b	602	CDL	OB6-CB4-CB6-OB8
35	v	202	CDL	OB6-CB4-CB6-OB8
35	c	401	CDL	OB6-CB4-CB6-OB8
35	H	302	CDL	OB6-CB4-CB6-OB8
35	B	602	CDL	OB6-CB4-CB6-OB8
34	X	101	LMT	C9-C10-C11-C12
35	O	203	CDL	C43-C44-C45-C46
36	c	403	PEE	C40-C41-C42-C43
35	o	203	CDL	C43-C44-C45-C46
35	e	401	CDL	C17-C18-C19-C20
36	J	301	PEE	C12-C13-C14-C15
35	d	402	CDL	C41-C42-C43-C44
35	D	402	CDL	C41-C42-C43-C44
36	j	301	PEE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
35	B	602	CDL	C71-C72-C73-C74
36	C	403	PEE	C40-C41-C42-C43
34	D	401	LMT	C4-C5-C6-C7
35	b	602	CDL	C71-C72-C73-C74
36	j	302	PEE	C44-C45-C46-C47
35	d	402	CDL	CA2-OA2-PA1-OA5
35	D	402	CDL	CA2-OA2-PA1-OA5
35	b	601	CDL	O1-C1-CA2-OA2
35	B	601	CDL	O1-C1-CA2-OA2
34	x	101	LMT	C4-C5-C6-C7
36	J	302	PEE	C44-C45-C46-C47
34	X	101	LMT	C4-C5-C6-C7
34	C	402	LMT	C3'-C4'-O1B-C1B
33	o	201	PC1	C1-O11-P-O12
33	v	201	PC1	C11-O13-P-O14
33	O	201	PC1	C1-O11-P-O12
33	V	201	PC1	C11-O13-P-O14
35	o	203	CDL	CB3-OB5-PB2-OB4
35	h	302	CDL	CA2-OA2-PA1-OA3
35	h	302	CDL	CB2-OB2-PB2-OB4
35	e	401	CDL	CA3-OA5-PA1-OA3
35	d	402	CDL	CB3-OB5-PB2-OB4
35	H	302	CDL	CA2-OA2-PA1-OA3
35	H	302	CDL	CB2-OB2-PB2-OB4
35	E	401	CDL	CA3-OA5-PA1-OA3
35	C	401	CDL	CA3-OA5-PA1-OA3
35	C	401	CDL	CA3-OA5-PA1-OA4
35	C	401	CDL	CB3-OB5-PB2-OB3
35	D	402	CDL	CB3-OB5-PB2-OB4
37	E2	601	ATP	C5'-O5'-PA-O2A
37	E1	601	ATP	C5'-O5'-PA-O2A
38	B2	601	ADP	C5'-O5'-PA-O1A
38	B1	601	ADP	C5'-O5'-PA-O1A
35	D	402	CDL	C11-C12-C13-C14
33	v	201	PC1	O11-C1-C2-C3
33	V	201	PC1	O11-C1-C2-C3
35	o	203	CDL	OA5-CA3-CA4-CA6
35	v	202	CDL	OA5-CA3-CA4-CA6
35	V	202	CDL	OA5-CA3-CA4-CA6
35	D	402	CDL	OA5-CA3-CA4-CA6
35	d	402	CDL	C11-C12-C13-C14
33	o	201	PC1	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
33	O	201	PC1	C38-C39-C3A-C3B
35	E	401	CDL	C20-C21-C22-C23
35	e	401	CDL	C20-C21-C22-C23
33	o	204	PC1	C12-C11-O13-P
33	O	204	PC1	C12-C11-O13-P
36	j	302	PEE	C14-C15-C16-C17
35	C	401	CDL	C17-C18-C19-C20
35	C	401	CDL	C43-C44-C45-C46
36	J	302	PEE	C14-C15-C16-C17
35	c	401	CDL	C54-C55-C56-C57
35	B	602	CDL	C59-C60-C61-C62
35	V	202	CDL	OA5-CA3-CA4-OA6
35	B	602	CDL	C15-C16-C17-C18
33	o	204	PC1	C3B-C3C-C3D-C3E
35	b	602	CDL	C59-C60-C61-C62
33	O	201	PC1	C2D-C2E-C2F-C2G
33	O	204	PC1	C3B-C3C-C3D-C3E
36	j	302	PEE	C41-C42-C43-C44
33	o	201	PC1	C2D-C2E-C2F-C2G
34	c	402	LMT	C3'-C4'-O1B-C1B
35	b	602	CDL	C15-C16-C17-C18
33	o	204	PC1	O13-C11-C12-N
33	O	204	PC1	O13-C11-C12-N
35	v	202	CDL	CB3-CB4-CB6-OB8
35	U	201	CDL	C18-C19-C20-C21
35	o	203	CDL	OA6-CA4-CA6-OA8
35	O	203	CDL	OA6-CA4-CA6-OA8
35	V	202	CDL	OB6-CB4-CB6-OB8
35	C	401	CDL	OB6-CB4-CB6-OB8
34	d	403	LMT	O1'-C1-C2-C3
36	J	302	PEE	C41-C42-C43-C44
35	u	201	CDL	C18-C19-C20-C21
34	D	403	LMT	O1'-C1-C2-C3
35	C	401	CDL	C53-C54-C55-C56
35	e	401	CDL	C1-CB2-OB2-PB2
35	E	401	CDL	C1-CB2-OB2-PB2
35	B	602	CDL	C83-C84-C85-C86
35	b	602	CDL	C83-C84-C85-C86
35	H	302	CDL	C84-C85-C86-C87
33	v	201	PC1	C26-C27-C28-C29
35	U	201	CDL	C16-C17-C18-C19
35	V	202	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
33	V	201	PC1	C26-C27-C28-C29
35	b	601	CDL	C60-C61-C62-C63
35	v	202	CDL	C37-C38-C39-C40
35	O	203	CDL	C19-C20-C21-C22
35	u	201	CDL	C16-C17-C18-C19
35	h	302	CDL	C84-C85-C86-C87
35	v	202	CDL	C81-C82-C83-C84
35	V	202	CDL	C81-C82-C83-C84
33	O	204	PC1	O31-C31-C32-C33
36	J	301	PEE	O4-C10-O2-C2
34	C	402	LMT	C5'-C4'-O1B-C1B
35	u	201	CDL	C33-C34-C35-C36
35	c	401	CDL	C23-C24-C25-C26
33	o	204	PC1	O31-C31-C32-C33
35	U	201	CDL	C33-C34-C35-C36
36	j	301	PEE	C20-C21-C22-C23
36	J	301	PEE	C20-C21-C22-C23
35	u	201	CDL	C36-C37-C38-C39
35	C	401	CDL	C83-C84-C85-C86
35	b	602	CDL	CA3-CA4-OA6-CA5
35	v	202	CDL	CA3-CA4-OA6-CA5
33	o	204	PC1	O11-C1-C2-C3
33	O	204	PC1	O11-C1-C2-C3
35	b	601	CDL	OA5-CA3-CA4-CA6
35	B	601	CDL	OA5-CA3-CA4-CA6
35	B	601	CDL	C60-C61-C62-C63
36	j	301	PEE	O4-C10-O2-C2
36	j	302	PEE	C16-C17-C18-C19
36	J	302	PEE	C16-C17-C18-C19
35	c	401	CDL	C80-C81-C82-C83
35	d	402	CDL	C74-C75-C76-C77
35	D	402	CDL	C74-C75-C76-C77
35	E	401	CDL	OB5-CB3-CB4-OB6
35	o	203	CDL	C19-C20-C21-C22
35	U	201	CDL	C36-C37-C38-C39
35	H	302	CDL	C39-C40-C41-C42
33	v	201	PC1	C2F-C2G-C2H-C2I
33	V	201	PC1	C2F-C2G-C2H-C2I
35	d	402	CDL	OB6-CB4-CB6-OB8
35	D	402	CDL	OB6-CB4-CB6-OB8
33	o	204	PC1	C1-O11-P-O13
33	O	204	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
35	o	203	CDL	CA2-OA2-PA1-OA5
35	O	203	CDL	CA2-OA2-PA1-OA5
36	c	403	PEE	C4-O4P-P-O3P
36	C	403	PEE	C4-O4P-P-O3P
35	v	202	CDL	C24-C25-C26-C27
33	O	204	PC1	C2B-C2C-C2D-C2E
35	V	202	CDL	C24-C25-C26-C27
36	j	301	PEE	O5-C30-O3-C3
35	B	601	CDL	C76-C77-C78-C79
36	j	301	PEE	C21-C22-C23-C24
36	J	301	PEE	C21-C22-C23-C24
33	o	204	PC1	C2B-C2C-C2D-C2E
34	c	402	LMT	C5'-C4'-O1B-C1B
35	B	601	CDL	C15-C16-C17-C18
35	h	302	CDL	C39-C40-C41-C42
35	b	601	CDL	C76-C77-C78-C79
33	v	201	PC1	O32-C31-O31-C3
33	V	201	PC1	O32-C31-O31-C3
33	O	201	PC1	C39-C3A-C3B-C3C
33	V	201	PC1	C32-C31-O31-C3
36	j	301	PEE	C2-C1-O3P-P
36	J	301	PEE	C2-C1-O3P-P
35	b	601	CDL	C15-C16-C17-C18
36	J	302	PEE	C34-C35-C36-C37
36	C	403	PEE	C33-C34-C35-C36
35	C	401	CDL	C39-C40-C41-C42
33	v	201	PC1	C32-C31-O31-C3
33	O	204	PC1	C25-C26-C27-C28
36	J	301	PEE	O5-C30-O3-C3
35	c	401	CDL	C35-C36-C37-C38
33	o	201	PC1	C39-C3A-C3B-C3C
33	o	204	PC1	C25-C26-C27-C28
36	c	403	PEE	C33-C34-C35-C36
35	d	402	CDL	OA5-CA3-CA4-CA6
35	O	203	CDL	OA5-CA3-CA4-CA6
36	j	301	PEE	O4P-C4-C5-N
36	J	301	PEE	O4P-C4-C5-N
35	b	602	CDL	C13-C14-C15-C16
35	O	203	CDL	C17-C18-C19-C20
35	e	401	CDL	OA5-CA3-CA4-OA6
35	B	601	CDL	OB5-CB3-CB4-OB6
35	o	203	CDL	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
35	V	202	CDL	C76-C77-C78-C79
34	d	401	LMT	O1'-C1-C2-C3
35	e	401	CDL	C62-C63-C64-C65
36	j	302	PEE	C34-C35-C36-C37
36	J	302	PEE	C11-C12-C13-C14
35	u	201	CDL	C44-C45-C46-C47
35	c	401	CDL	C11-C12-C13-C14
33	v	201	PC1	C39-C3A-C3B-C3C
35	U	201	CDL	C44-C45-C46-C47
35	B	602	CDL	C13-C14-C15-C16
35	v	202	CDL	C76-C77-C78-C79
34	c	402	LMT	C7-C8-C9-C10
34	O	202	LMT	C5-C6-C7-C8
35	E	401	CDL	C62-C63-C64-C65
36	j	302	PEE	C11-C12-C13-C14
33	V	201	PC1	C39-C3A-C3B-C3C
36	j	301	PEE	C31-C30-O3-C3
33	o	204	PC1	C29-C2A-C2B-C2C
34	C	402	LMT	C7-C8-C9-C10
33	O	204	PC1	C29-C2A-C2B-C2C
35	d	402	CDL	C16-C17-C18-C19
33	O	201	PC1	C3A-C3B-C3C-C3D
35	h	302	CDL	C63-C64-C65-C66
35	D	402	CDL	C16-C17-C18-C19
35	C	401	CDL	CB5-C51-C52-C53
33	o	201	PC1	C3A-C3B-C3C-C3D
35	d	402	CDL	C32-C33-C34-C35
36	J	301	PEE	C11-C10-O2-C2
35	d	402	CDL	CB3-CB4-CB6-OB8
35	D	402	CDL	CB3-CB4-CB6-OB8
34	o	202	LMT	C5-C6-C7-C8
36	C	403	PEE	C11-C12-C13-C14
35	d	402	CDL	C75-C76-C77-C78
36	J	301	PEE	C31-C30-O3-C3
34	c	404	LMT	O5'-C5'-C6'-O6'
33	o	204	PC1	C24-C25-C26-C27
35	D	402	CDL	C32-C33-C34-C35
35	H	302	CDL	C63-C64-C65-C66
35	C	401	CDL	CB7-C71-C72-C73
35	D	402	CDL	C75-C76-C77-C78
35	h	302	CDL	CA3-CA4-OA6-CA5
35	h	302	CDL	CA6-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
35	c	401	CDL	CA6-CA4-OA6-CA5
35	d	402	CDL	CB3-CB4-OB6-CB5
35	H	302	CDL	CA3-CA4-OA6-CA5
35	B	602	CDL	CA3-CA4-OA6-CA5
35	V	202	CDL	CA3-CA4-OA6-CA5
35	D	402	CDL	CB3-CB4-OB6-CB5
35	e	401	CDL	C55-C56-C57-C58
35	e	401	CDL	OB7-CB5-OB6-CB4
35	E	401	CDL	OB7-CB5-OB6-CB4
36	c	403	PEE	C11-C12-C13-C14
35	b	602	CDL	C17-C18-C19-C20
35	B	602	CDL	C17-C18-C19-C20
35	E	401	CDL	OA5-CA3-CA4-OA6
35	C	401	CDL	C16-C17-C18-C19
33	o	201	PC1	O11-C1-C2-C3
33	O	201	PC1	O11-C1-C2-C3
35	e	401	CDL	OA5-CA3-CA4-CA6
35	b	601	CDL	OB5-CB3-CB4-CB6
35	E	401	CDL	OA5-CA3-CA4-CA6
33	O	204	PC1	C24-C25-C26-C27
36	j	301	PEE	C11-C10-O2-C2
36	j	301	PEE	C22-C23-C24-C25
35	E	401	CDL	C55-C56-C57-C58
36	j	301	PEE	C42-C43-C44-C45
36	J	301	PEE	C22-C23-C24-C25
35	E	401	CDL	OA7-CA5-OA6-CA4
35	B	602	CDL	C21-C22-C23-C24
35	o	203	CDL	C52-C51-CB5-OB6
35	D	402	CDL	C64-C65-C66-C67
35	d	402	CDL	C64-C65-C66-C67
36	J	301	PEE	C19-C20-C21-C22
35	e	401	CDL	C35-C36-C37-C38
35	b	602	CDL	C21-C22-C23-C24
35	c	401	CDL	C41-C42-C43-C44
36	c	403	PEE	C12-C13-C14-C15
36	J	301	PEE	C13-C14-C15-C16
36	J	301	PEE	C42-C43-C44-C45
35	D	402	CDL	C24-C25-C26-C27
36	j	301	PEE	C13-C14-C15-C16
35	e	401	CDL	C84-C85-C86-C87
36	C	403	PEE	C12-C13-C14-C15
36	j	301	PEE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
36	J	301	PEE	C36-C37-C38-C39
35	O	203	CDL	C52-C51-CB5-OB6
35	E	401	CDL	C35-C36-C37-C38
37	C1	601	ATP	PB-O3A-PA-O2A
36	j	301	PEE	C19-C20-C21-C22
34	c	404	LMT	C5-C6-C7-C8
35	C	401	CDL	C36-C37-C38-C39
35	c	401	CDL	C83-C84-C85-C86
35	u	201	CDL	C32-C31-CA7-OA8
35	U	201	CDL	C32-C31-CA7-OA8
34	H	301	LMT	C5-C6-C7-C8
35	C	401	CDL	C82-C83-C84-C85
35	d	402	CDL	C24-C25-C26-C27
35	u	201	CDL	C43-C44-C45-C46
35	E	401	CDL	C84-C85-C86-C87
35	V	202	CDL	C34-C35-C36-C37
34	h	301	LMT	C5-C6-C7-C8
36	c	403	PEE	C38-C39-C40-C41
36	C	403	PEE	C38-C39-C40-C41
35	H	302	CDL	CB7-C71-C72-C73
35	v	202	CDL	C34-C35-C36-C37
35	U	201	CDL	C43-C44-C45-C46
35	h	302	CDL	CB7-C71-C72-C73
34	C	404	LMT	C5-C6-C7-C8
35	b	602	CDL	OA5-CA3-CA4-CA6
35	b	602	CDL	OB5-CB3-CB4-CB6
35	B	601	CDL	OB5-CB3-CB4-CB6
35	B	602	CDL	OA5-CA3-CA4-CA6
35	B	602	CDL	OB5-CB3-CB4-CB6
36	c	403	PEE	C18-C19-C20-C21
36	C	403	PEE	C18-C19-C20-C21
35	b	602	CDL	C60-C61-C62-C63
35	h	302	CDL	OA6-CA4-CA6-OA8
35	b	602	CDL	C72-C71-CB7-OB8
35	B	602	CDL	C72-C71-CB7-OB8
35	O	203	CDL	C34-C35-C36-C37
36	j	301	PEE	C32-C33-C34-C35
35	b	602	CDL	CA3-OA5-PA1-OA2
35	o	203	CDL	C34-C35-C36-C37
35	U	201	CDL	C54-C55-C56-C57
33	O	201	PC1	C2F-C2G-C2H-C2I
35	u	201	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
34	o	202	LMT	C9-C10-C11-C12
36	J	301	PEE	C32-C33-C34-C35
35	u	201	CDL	C52-C51-CB5-OB6
35	U	201	CDL	C52-C51-CB5-OB6
35	c	401	CDL	CA3-CA4-OA6-CA5
35	H	302	CDL	CA6-CA4-OA6-CA5
35	C	401	CDL	CA6-CA4-OA6-CA5
36	j	302	PEE	C3-C2-O2-C10
33	o	201	PC1	C2F-C2G-C2H-C2I
35	e	401	CDL	OA7-CA5-OA6-CA4
35	o	203	CDL	C32-C31-CA7-OA8
33	v	201	PC1	C32-C33-C34-C35
33	V	201	PC1	C32-C33-C34-C35
34	O	202	LMT	C9-C10-C11-C12
35	B	602	CDL	C60-C61-C62-C63
35	O	203	CDL	C32-C31-CA7-OA8
35	e	401	CDL	CA3-CA4-CA6-OA8
35	C	401	CDL	C81-C82-C83-C84
35	v	202	CDL	C82-C83-C84-C85
35	V	202	CDL	C82-C83-C84-C85
35	o	203	CDL	C77-C78-C79-C80
36	j	302	PEE	O3-C30-C31-C32
35	B	602	CDL	C41-C42-C43-C44
35	H	302	CDL	OA6-CA4-CA6-OA8
33	o	204	PC1	C28-C29-C2A-C2B
36	J	302	PEE	O3-C30-C31-C32
35	O	203	CDL	C80-C81-C82-C83
35	V	202	CDL	C83-C84-C85-C86
35	b	602	CDL	C41-C42-C43-C44
35	e	401	CDL	C51-CB5-OB6-CB4
35	c	401	CDL	C56-C57-C58-C59
35	b	601	CDL	C40-C41-C42-C43
35	v	202	CDL	C83-C84-C85-C86
35	O	203	CDL	C77-C78-C79-C80
35	C	401	CDL	C80-C81-C82-C83
35	b	601	CDL	C32-C31-CA7-OA8
37	C2	601	ATP	PB-O3A-PA-O2A
37	C1	601	ATP	PB-O3A-PA-O1A
36	C	403	PEE	C41-C42-C43-C44
36	c	403	PEE	C41-C42-C43-C44
35	E	401	CDL	C51-CB5-OB6-CB4
35	B	602	CDL	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
35	B	601	CDL	C32-C31-CA7-OA8
35	o	203	CDL	C80-C81-C82-C83
35	H	302	CDL	C42-C43-C44-C45
33	o	204	PC1	C2C-C2D-C2E-C2F
35	b	602	CDL	C19-C20-C21-C22
35	D	402	CDL	C31-C32-C33-C34
35	d	402	CDL	C31-C32-C33-C34
35	B	602	CDL	C32-C31-CA7-OA8
33	O	204	PC1	C28-C29-C2A-C2B
35	u	201	CDL	C52-C51-CB5-OB7
35	B	602	CDL	C72-C71-CB7-OB9
35	b	602	CDL	C32-C31-CA7-OA8
35	e	401	CDL	C15-C16-C17-C18
35	E	401	CDL	C36-C37-C38-C39
35	h	302	CDL	C42-C43-C44-C45
35	b	602	CDL	C72-C71-CB7-OB9
35	O	203	CDL	C79-C80-C81-C82
35	B	601	CDL	C40-C41-C42-C43
35	E	401	CDL	CA3-CA4-CA6-OA8
34	h	301	LMT	O1'-C1-C2-C3
35	e	401	CDL	C36-C37-C38-C39
35	e	401	CDL	C80-C81-C82-C83
35	E	401	CDL	C72-C73-C74-C75
35	o	203	CDL	C79-C80-C81-C82
36	J	302	PEE	O5-C30-C31-C32
34	H	301	LMT	O1'-C1-C2-C3
33	o	201	PC1	C11-O13-P-O14
33	v	201	PC1	C11-O13-P-O12
33	O	201	PC1	C11-O13-P-O14
33	V	201	PC1	C11-O13-P-O12
33	V	201	PC1	C11-C12-N-C15
35	v	202	CDL	CA2-OA2-PA1-OA3
35	v	202	CDL	CB2-OB2-PB2-OB4
35	v	202	CDL	CB3-OB5-PB2-OB3
35	c	401	CDL	CB2-OB2-PB2-OB3
35	V	202	CDL	CA2-OA2-PA1-OA3
35	V	202	CDL	CB2-OB2-PB2-OB4
35	E	401	CDL	C15-C16-C17-C18
35	E	401	CDL	C80-C81-C82-C83
35	U	201	CDL	C52-C51-CB5-OB7
35	h	302	CDL	C72-C71-CB7-OB8
35	U	201	CDL	C72-C71-CB7-OB8

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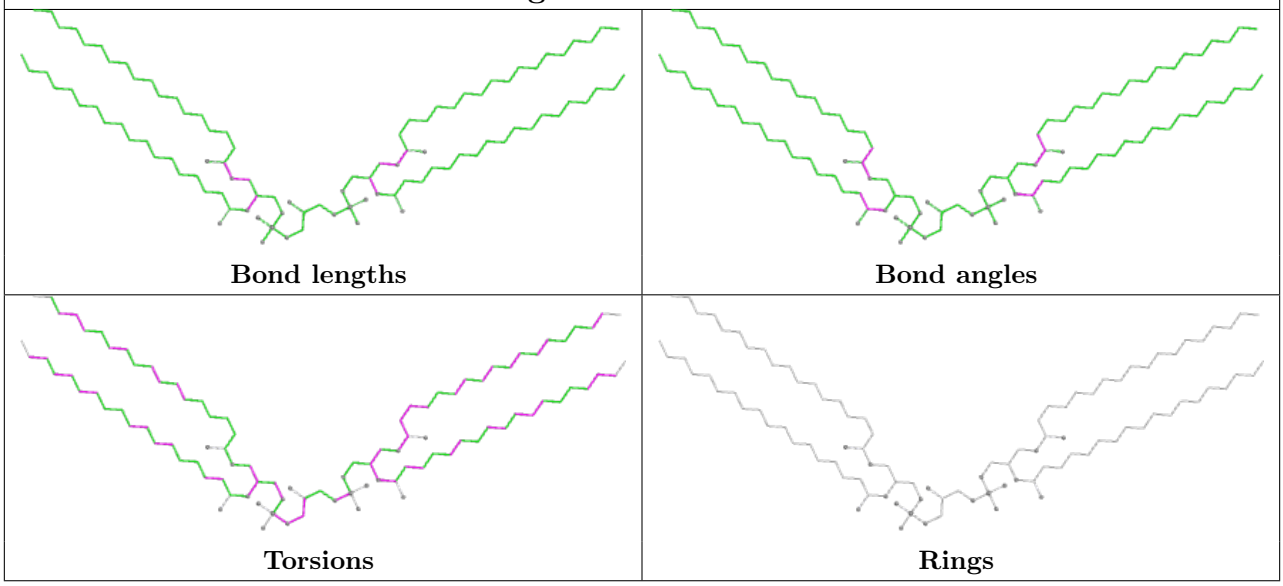
Mol	Chain	Res	Type	Atoms
35	U	201	CDL	OA5-CA3-CA4-CA6
36	j	302	PEE	O5-C30-C31-C32
33	o	204	PC1	C22-C23-C24-C25
35	e	401	CDL	C72-C73-C74-C75
33	O	204	PC1	C2C-C2D-C2E-C2F
35	b	602	CDL	CA6-CA4-OA6-CA5
36	j	302	PEE	C1-C2-O2-C10
36	J	302	PEE	C3-C2-O2-C10
35	u	201	CDL	C72-C71-CB7-OB8
35	H	302	CDL	C72-C71-CB7-OB8
35	c	401	CDL	C16-C17-C18-C19
36	j	302	PEE	C42-C43-C44-C45
35	v	202	CDL	CA7-C31-C32-C33
35	V	202	CDL	CA7-C31-C32-C33
35	D	402	CDL	C33-C34-C35-C36
33	v	201	PC1	C11-C12-N-C14
33	O	204	PC1	C22-C23-C24-C25
33	V	201	PC1	C28-C29-C2A-C2B
35	C	401	CDL	C64-C65-C66-C67
35	c	401	CDL	C58-C59-C60-C61
35	c	401	CDL	C60-C61-C62-C63
36	J	302	PEE	C42-C43-C44-C45
35	u	201	CDL	C72-C71-CB7-OB9
35	b	601	CDL	C32-C31-CA7-OA9
35	b	602	CDL	C32-C31-CA7-OA9
35	U	201	CDL	C72-C71-CB7-OB9
35	B	602	CDL	C32-C31-CA7-OA9
35	D	402	CDL	C12-C13-C14-C15
35	B	601	CDL	C32-C31-CA7-OA9
33	V	201	PC1	O31-C31-C32-C33
33	v	201	PC1	C28-C29-C2A-C2B
35	d	402	CDL	C33-C34-C35-C36
35	C	401	CDL	C37-C38-C39-C40
35	h	302	CDL	C43-C44-C45-C46
36	j	301	PEE	O2-C10-C11-C12
36	J	301	PEE	O2-C10-C11-C12
33	v	201	PC1	C11-C12-N-C15
33	V	201	PC1	C11-C12-N-C14
33	o	201	PC1	C3E-C3F-C3G-C3H
35	H	302	CDL	C43-C44-C45-C46
33	v	201	PC1	O31-C31-C32-C33

There are no ring outliers.

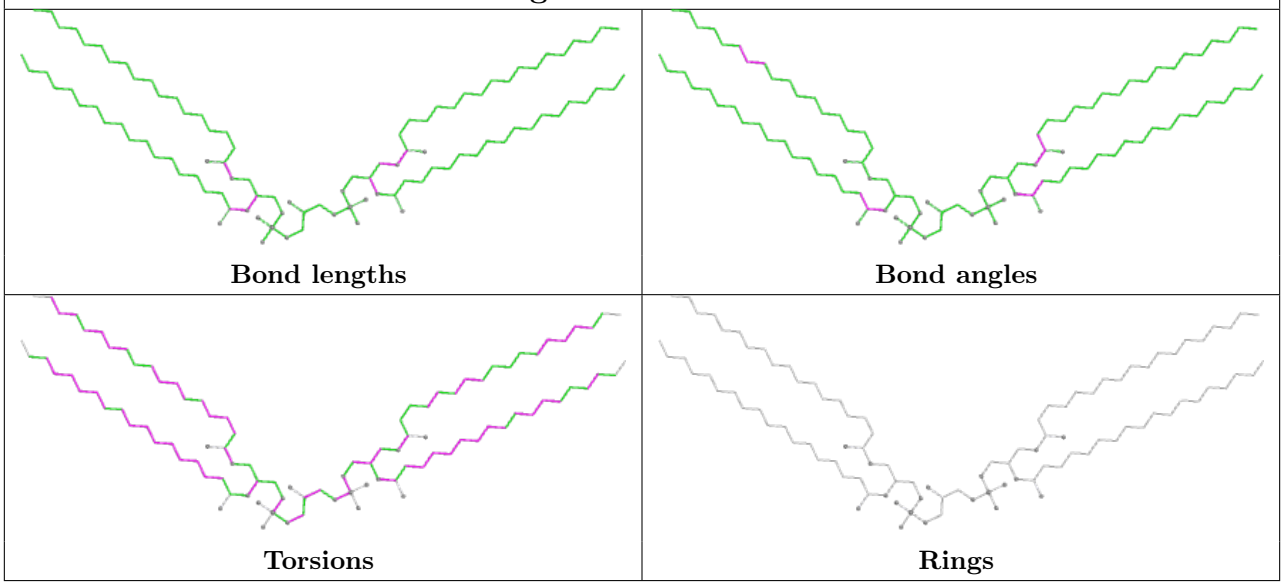
No monomer is involved in short contacts.

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.

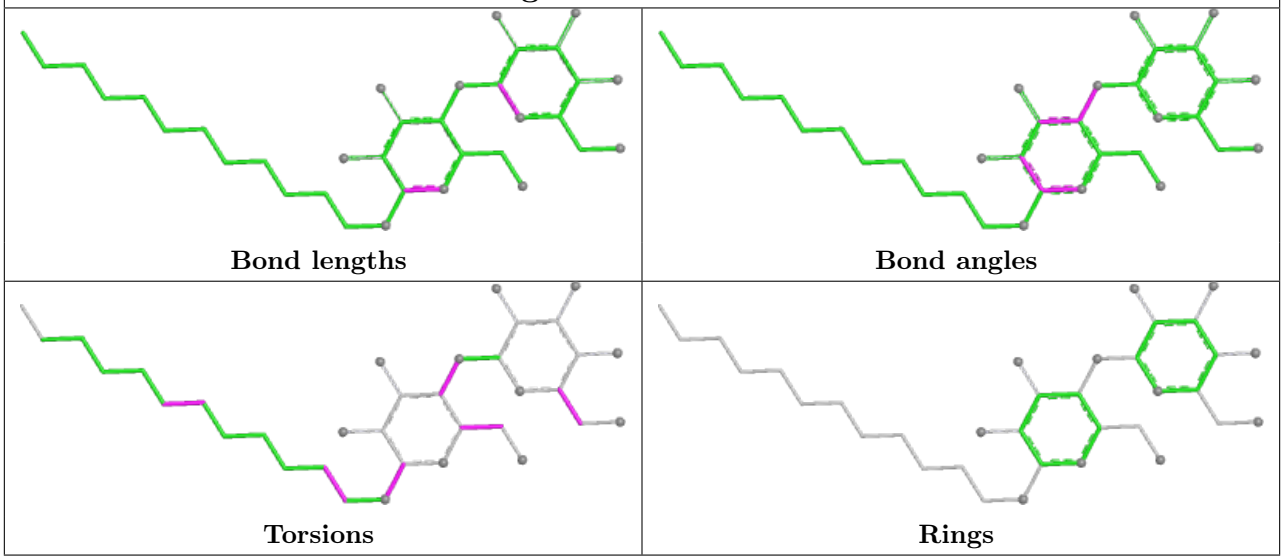
Ligand CDL h 302



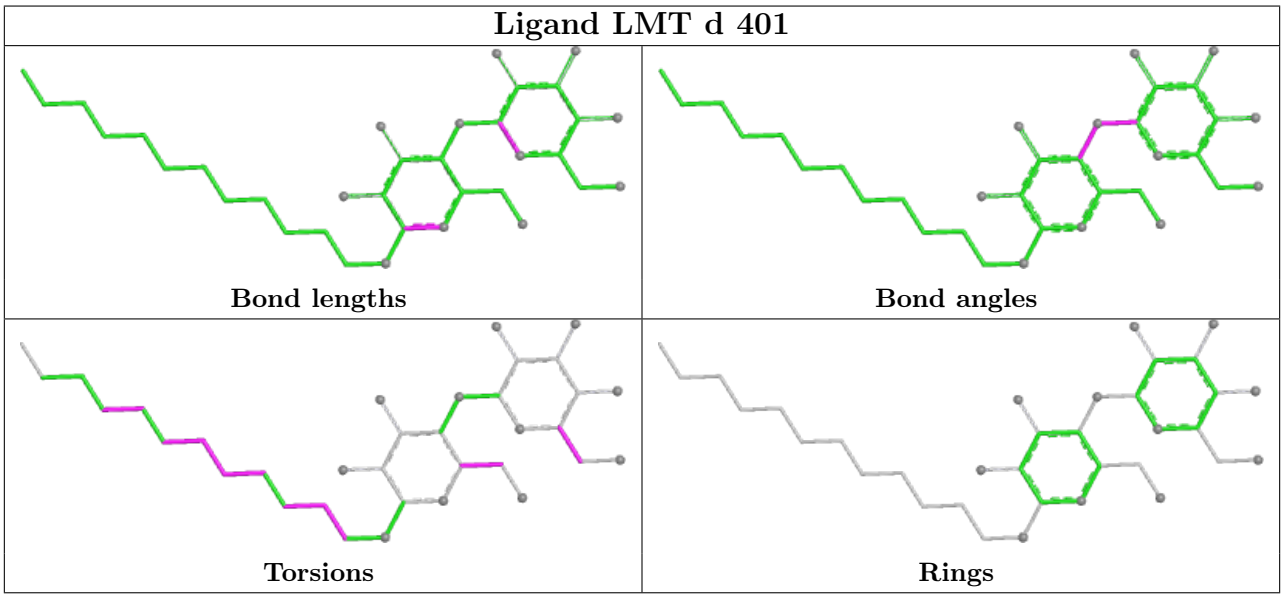
Ligand CDL c 401



Ligand LMT H 301



Ligand LMT d 401



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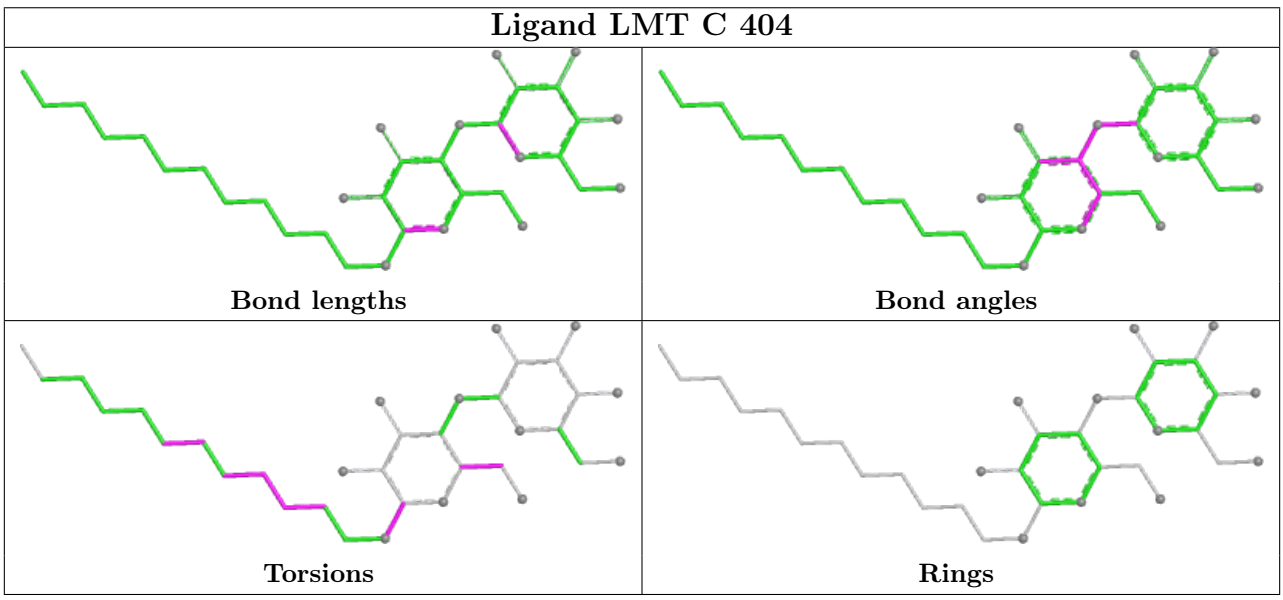
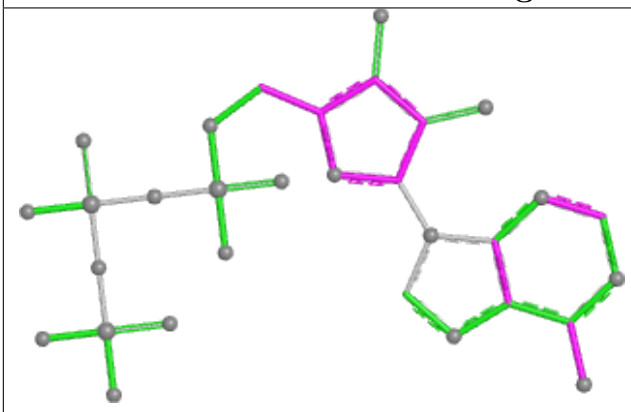
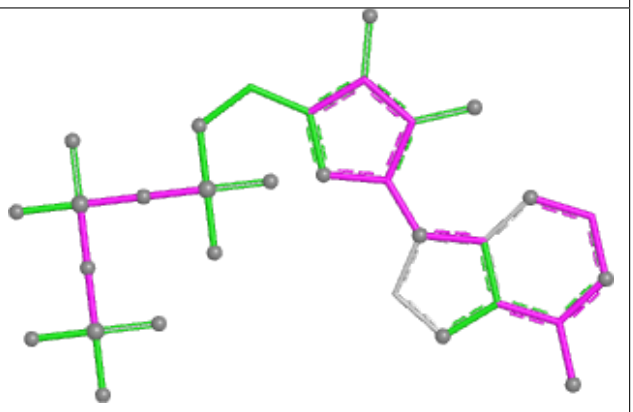


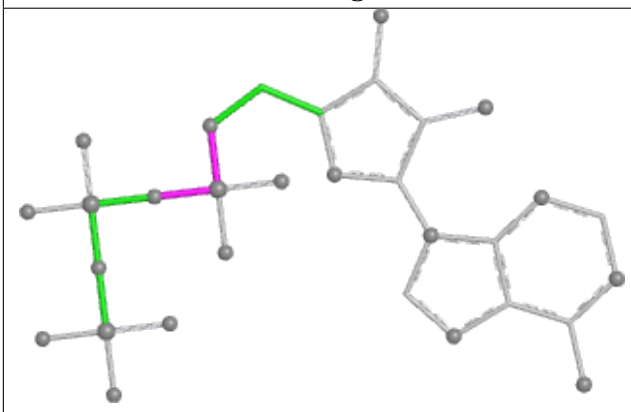
Ligand ATP C1 601



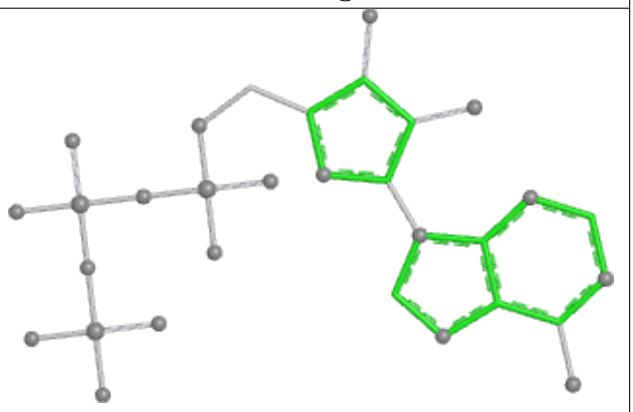
Bond lengths



Bond angles

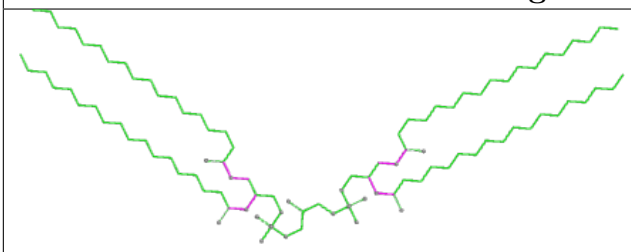


Torsions

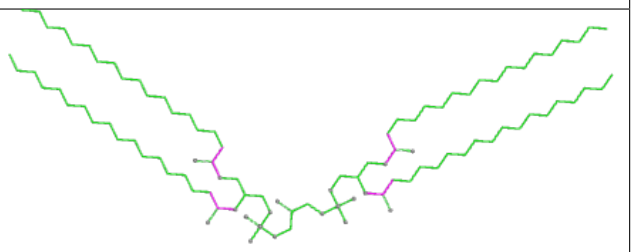


Rings

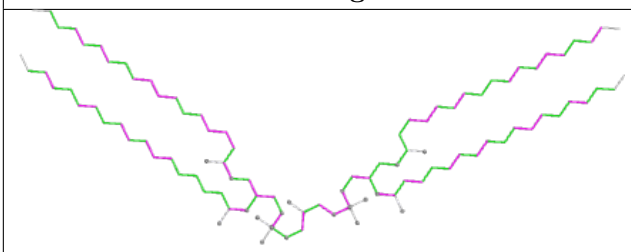
Ligand CDL e 401



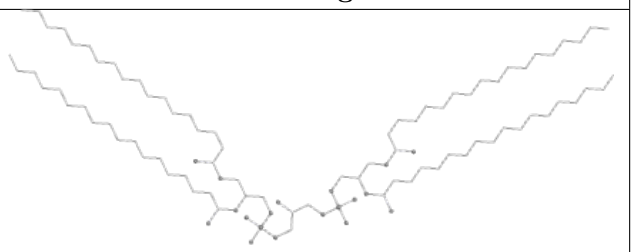
Bond lengths



Bond angles

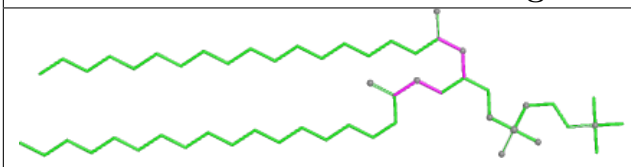


Torsions



Rings

Ligand PC1 O 204



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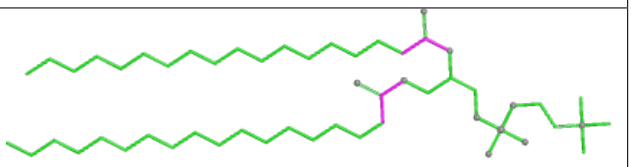
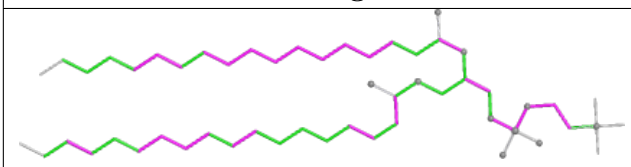


Bond angles



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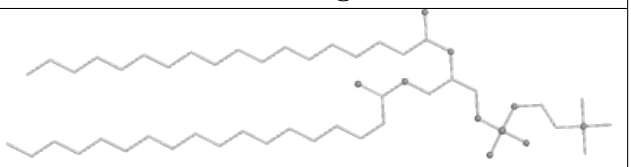
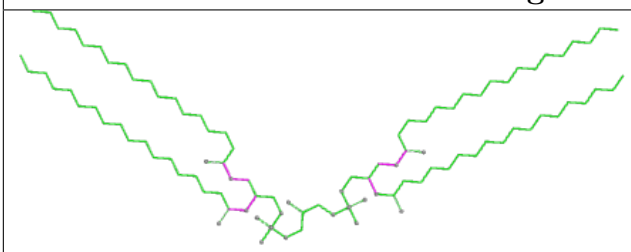


Rings

Ligand CDL u 201



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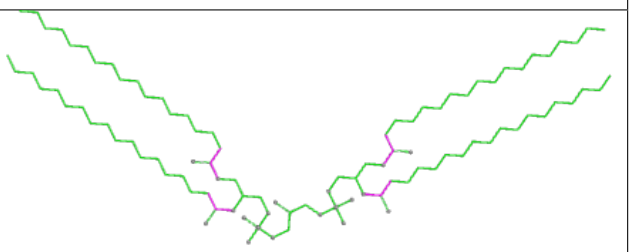

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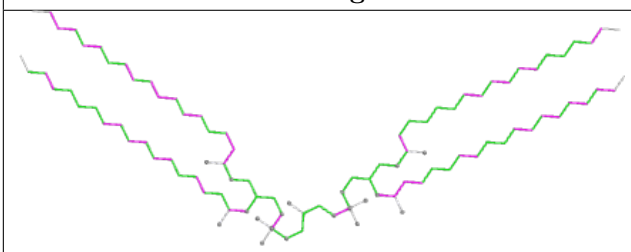

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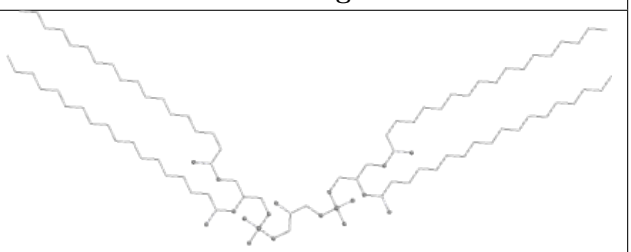
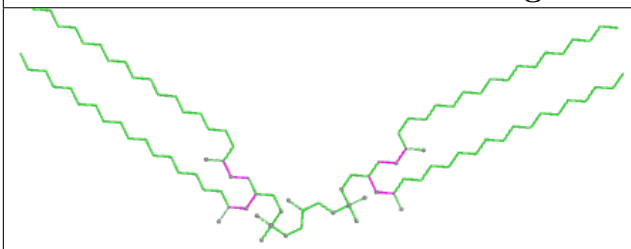


Rings

Ligand CDL B 602



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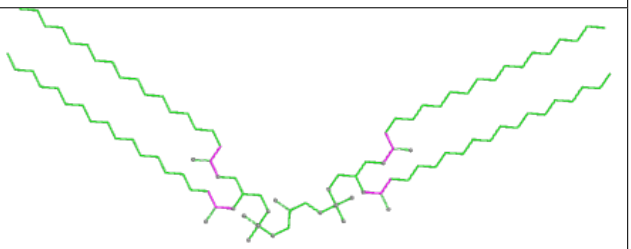

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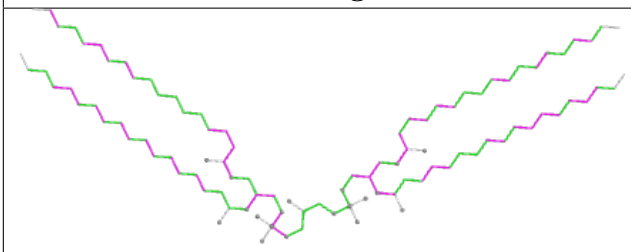

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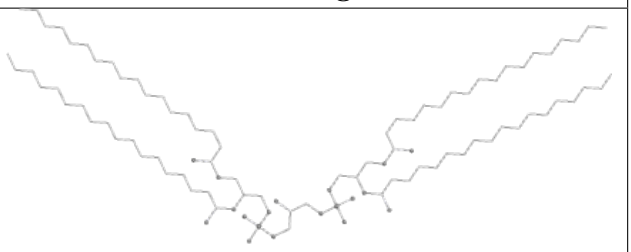

Rings

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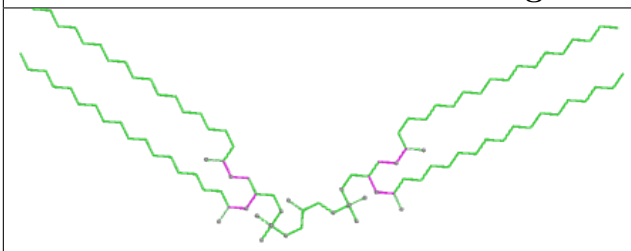

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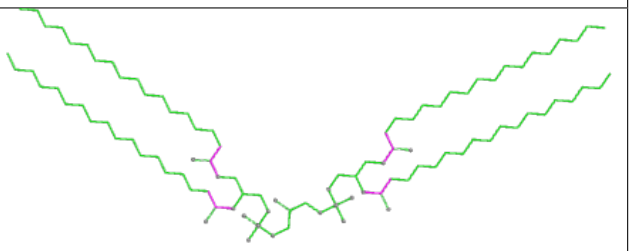

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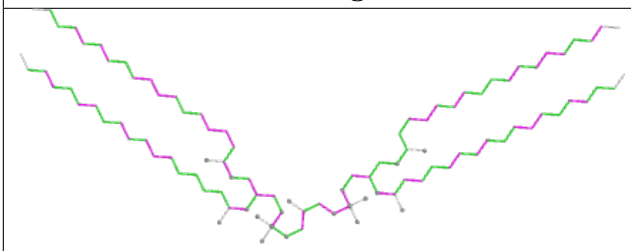

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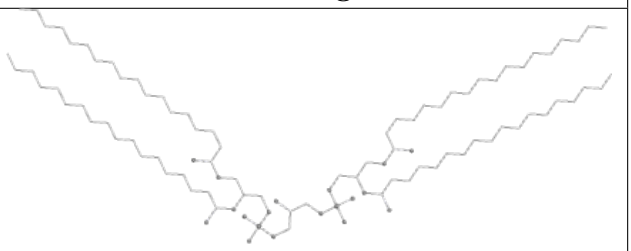
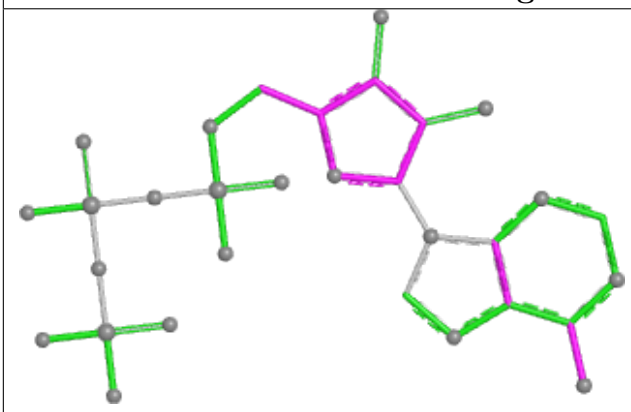


Rings

Ligand ATP E1 601



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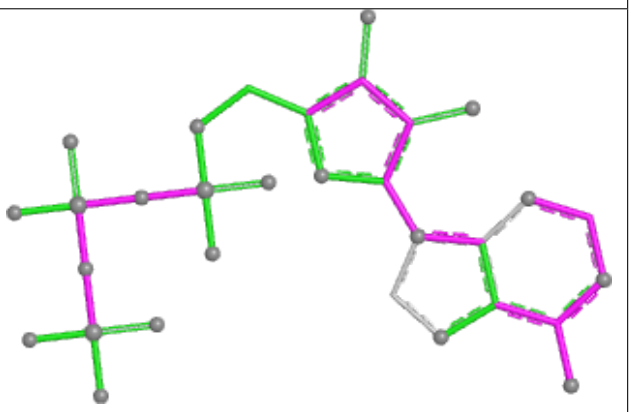

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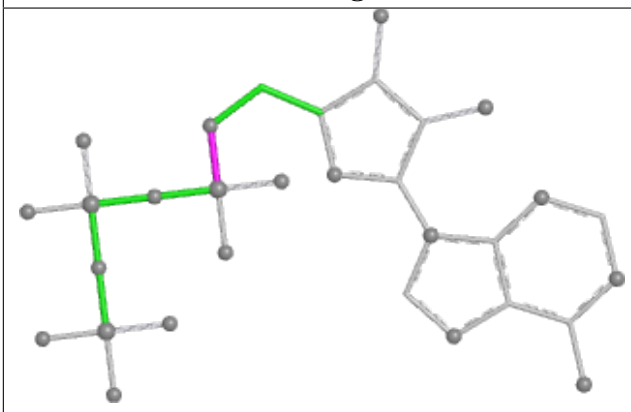

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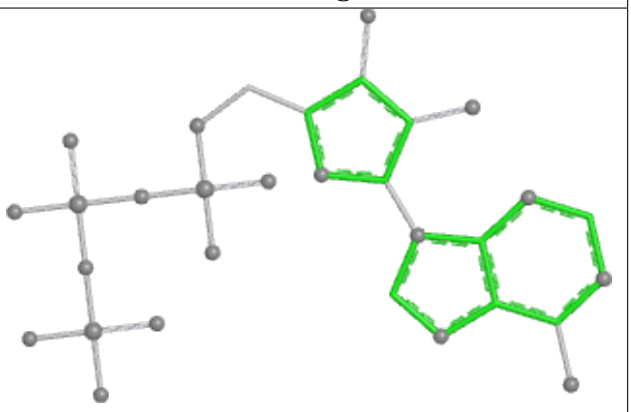
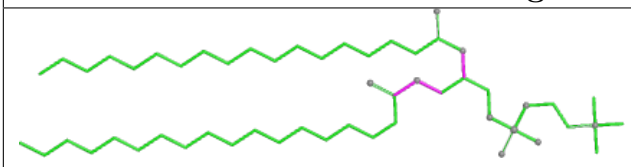
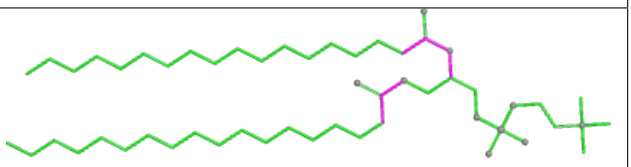
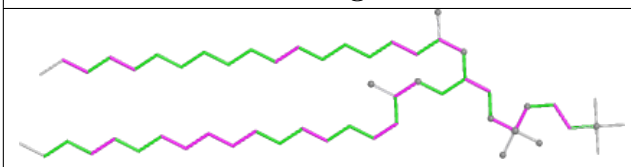
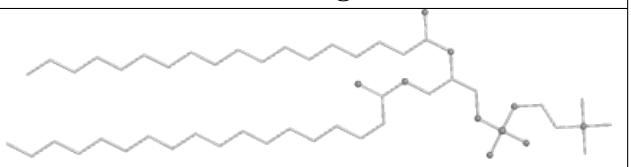
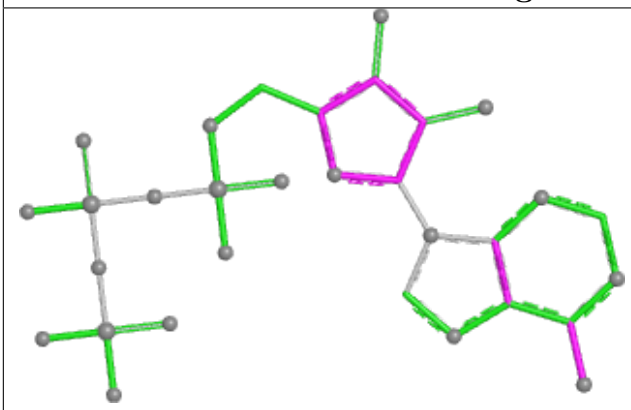
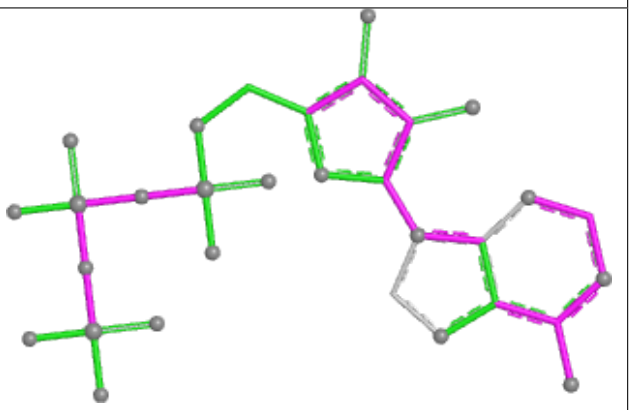
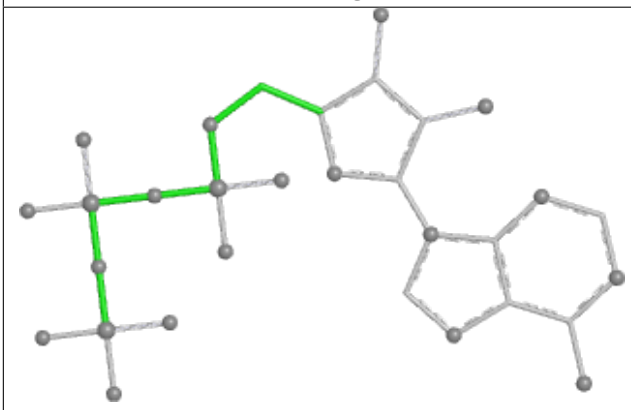
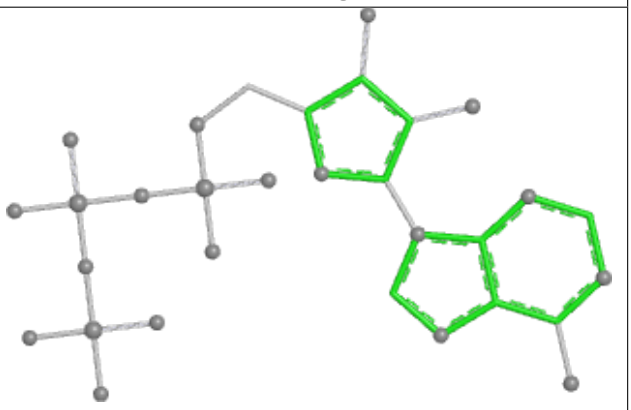
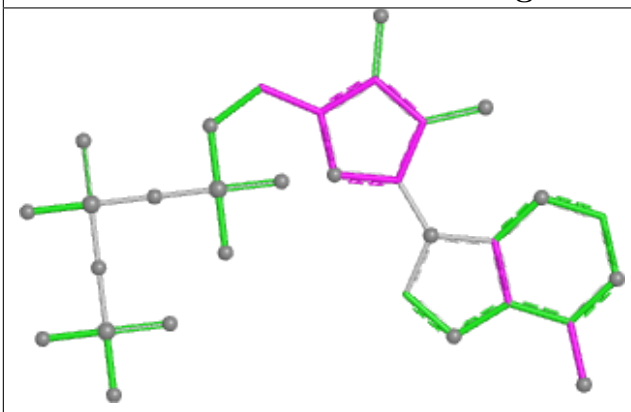


Rings

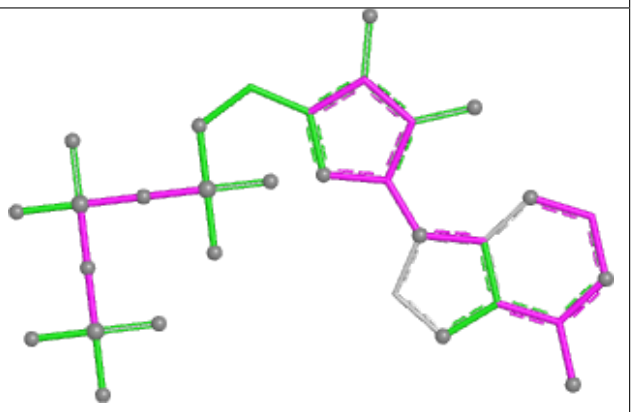
Ligand PC1 O 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP A2 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

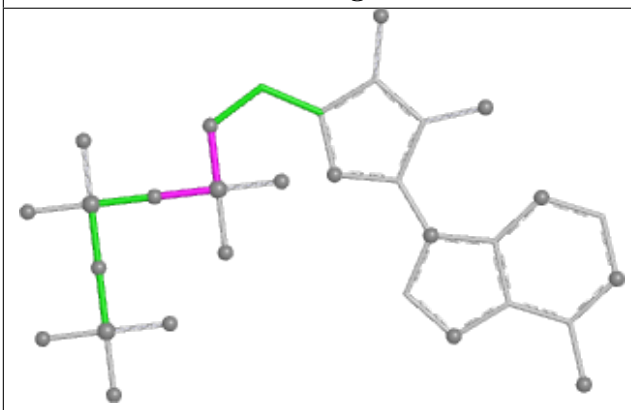
Ligand ATP C2 601



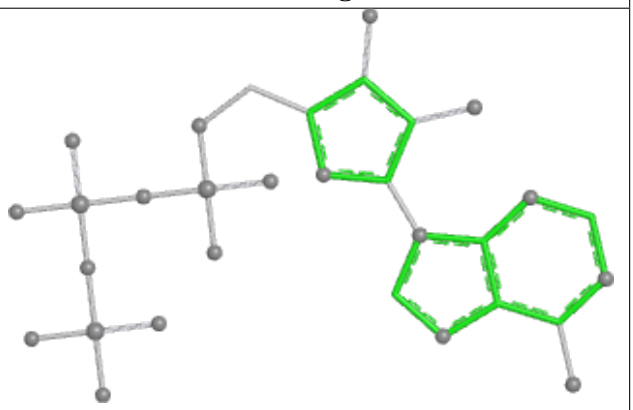
Bond lengths



Bond angles

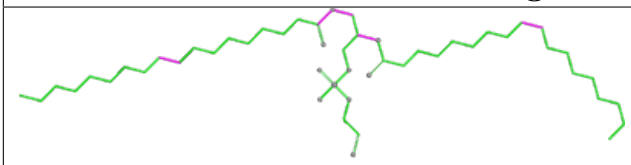


Torsions

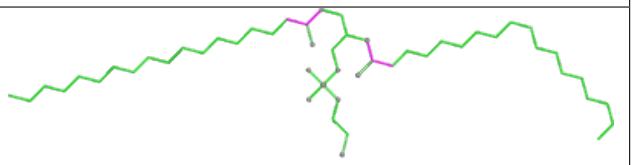


Rings

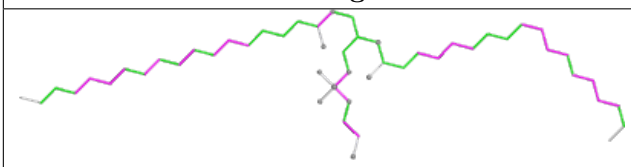
Ligand PEE C 403



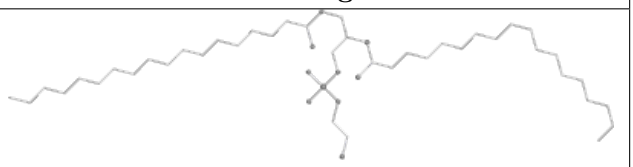
Bond lengths



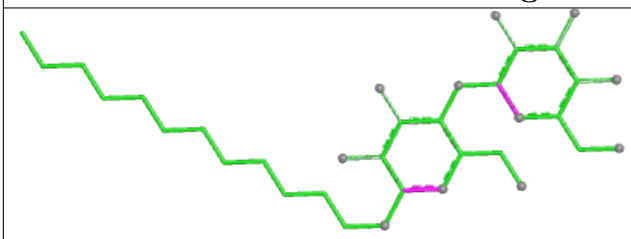
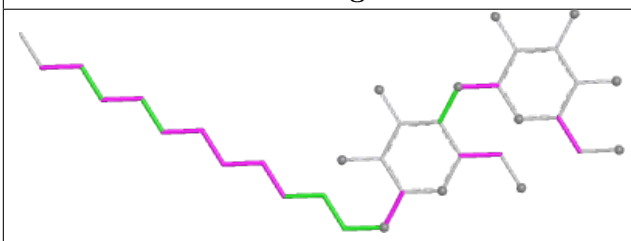
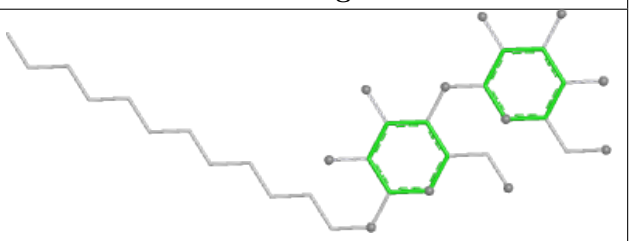
Bond angles

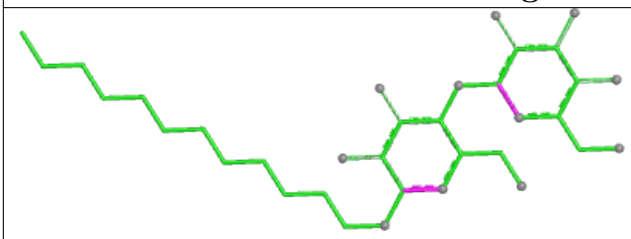
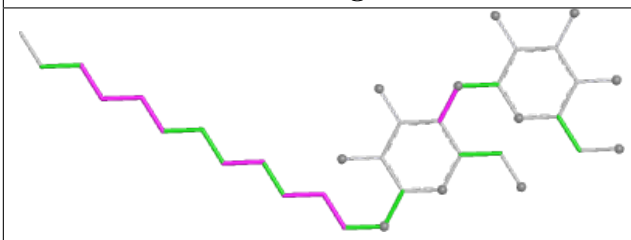
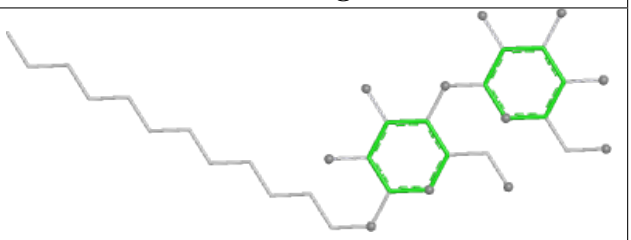


Torsions

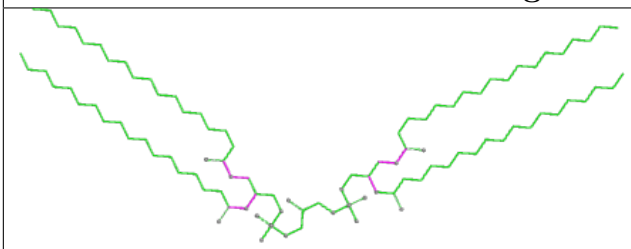


Rings

Ligand LMT X 101	
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand LMT C 402	
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand CDL V 202



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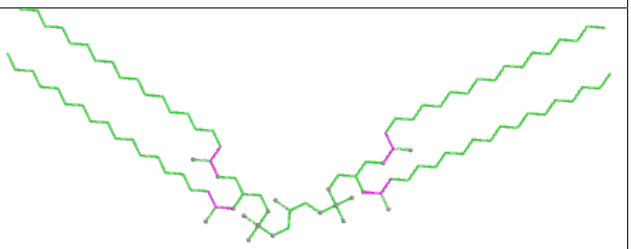

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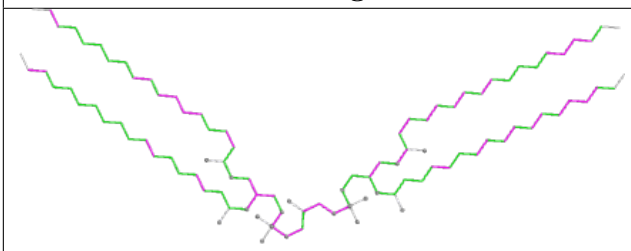

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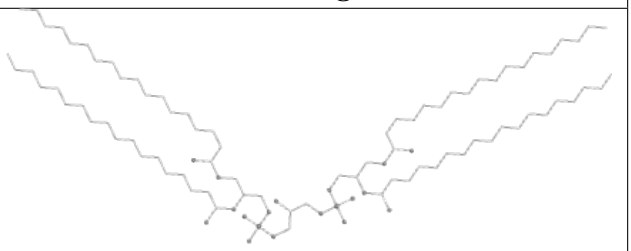
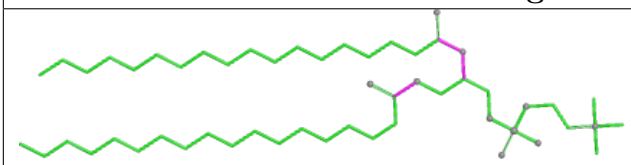


Rings

Ligand PC1 V 201



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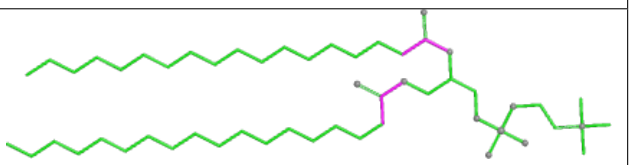

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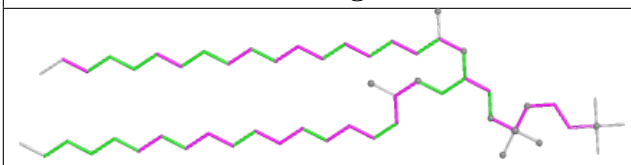

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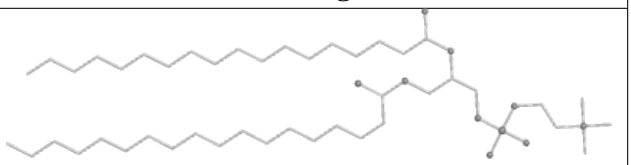
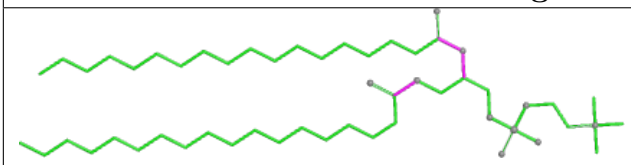


Rings

Ligand PC1 v 201



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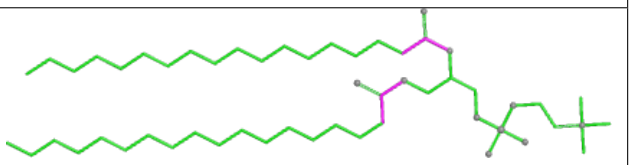

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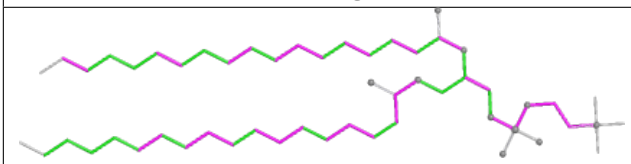

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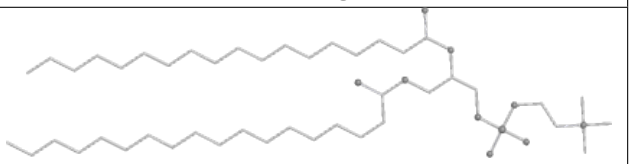

Rings

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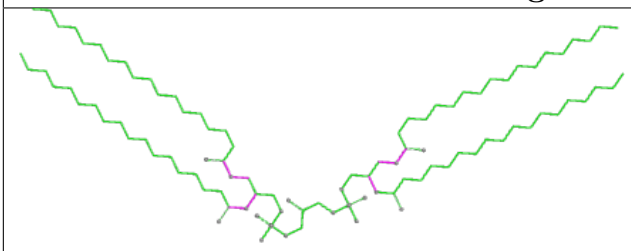
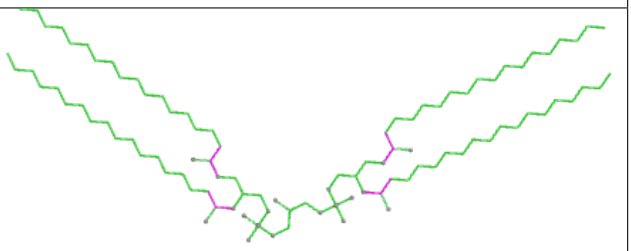
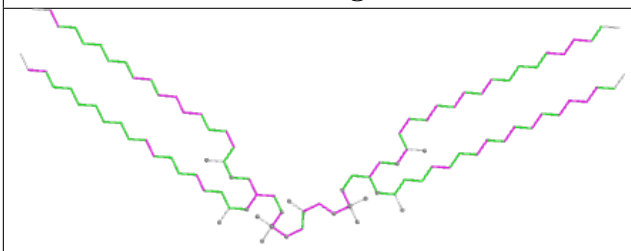
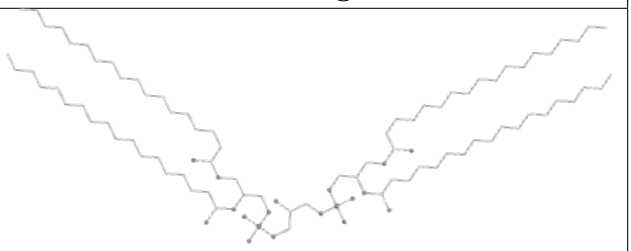
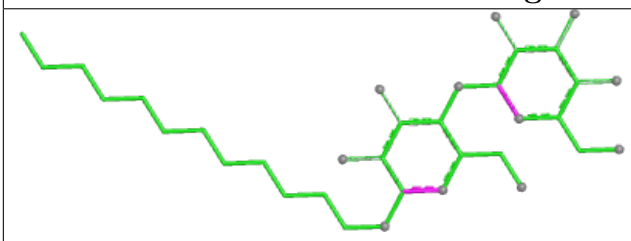
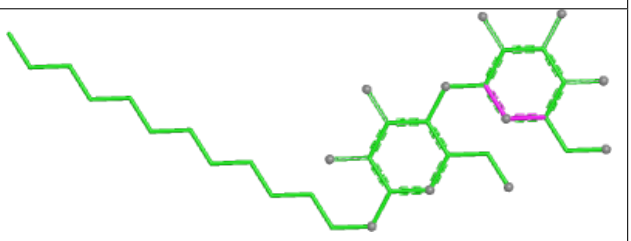
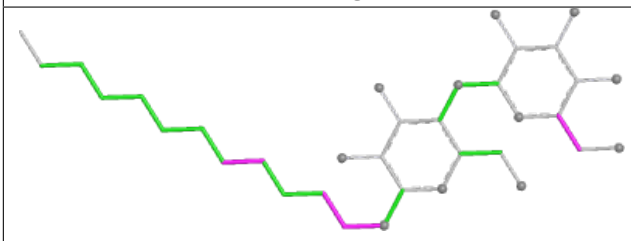
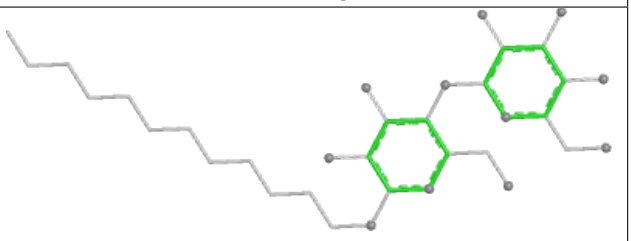
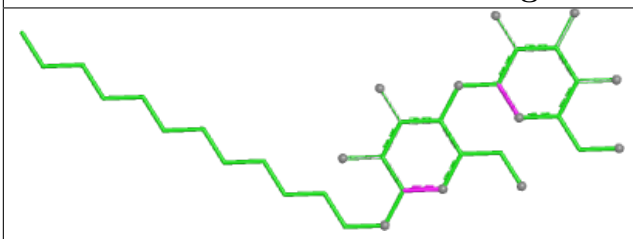
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT d 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT O 202



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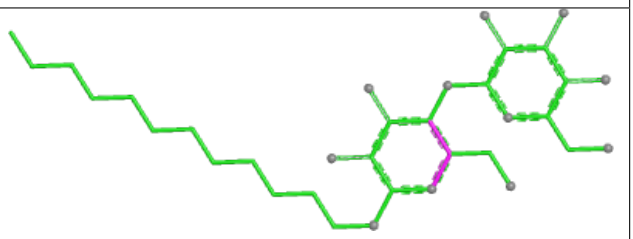

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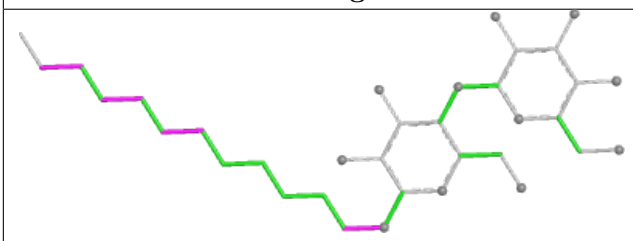

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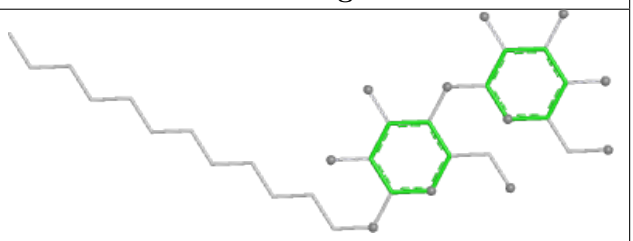
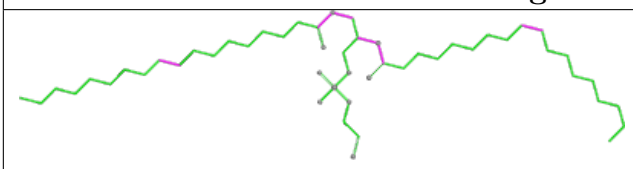


Rings

Ligand PEE J 302



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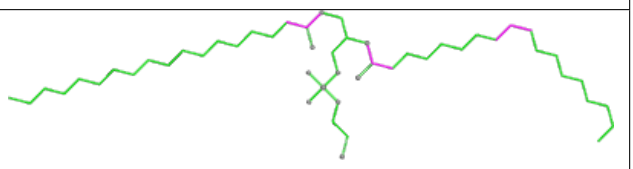

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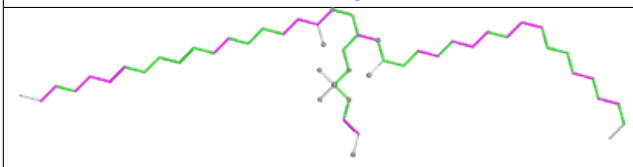

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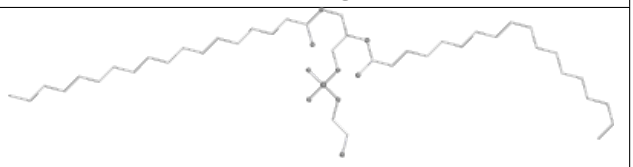
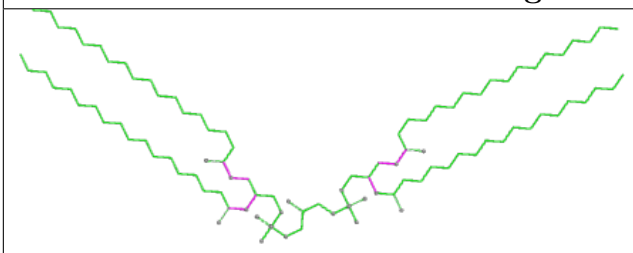


Rings

Ligand CDL B 601



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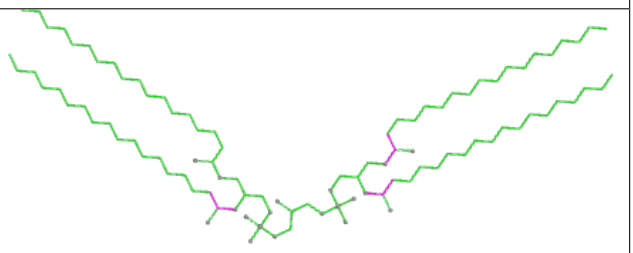

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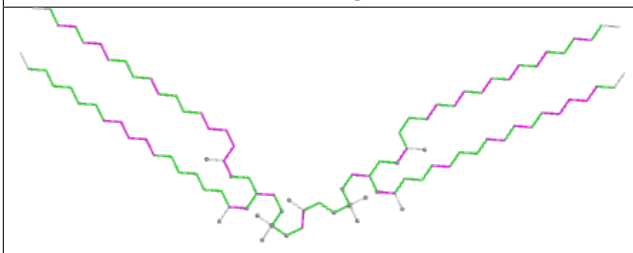

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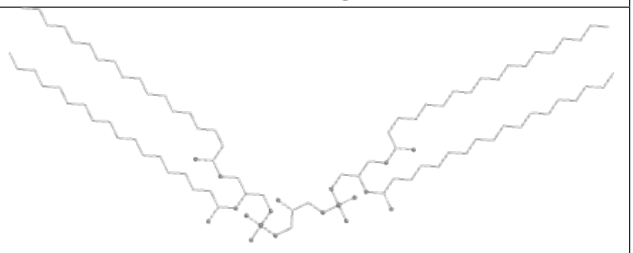
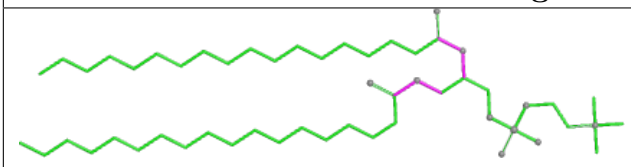


Rings

Ligand PC1 o 201



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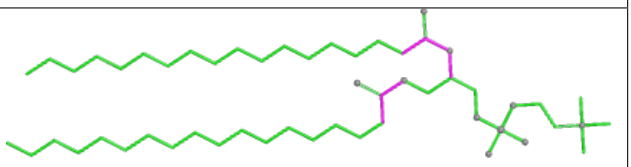

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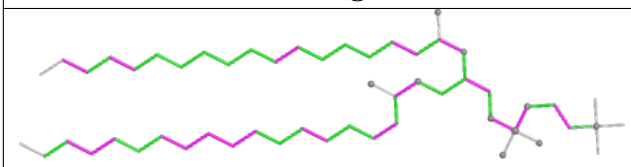

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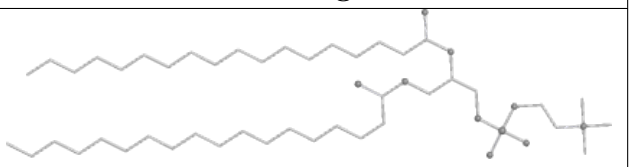
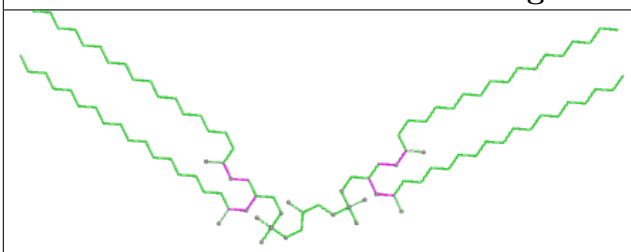


Rings

Ligand CDL d 402



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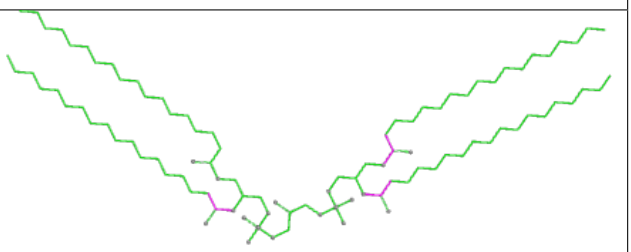

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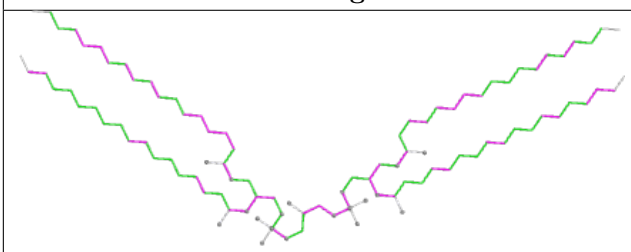

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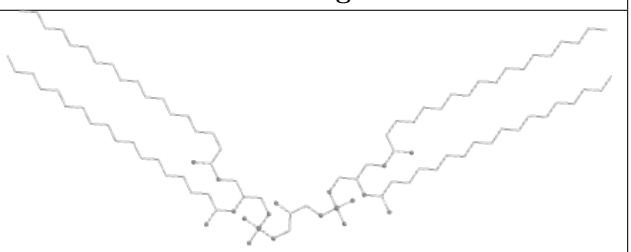
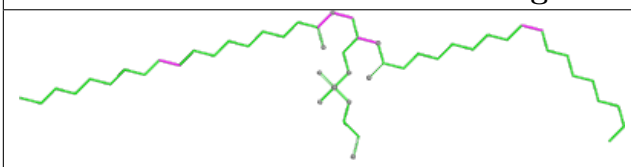


Rings

Ligand PEE c 403



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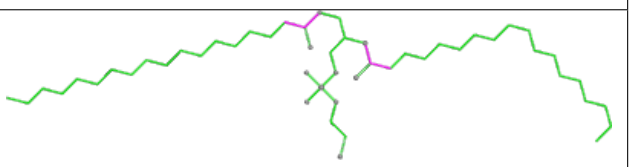

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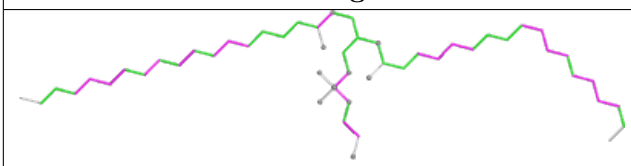

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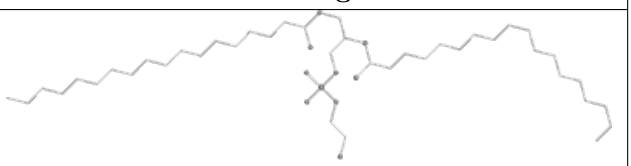
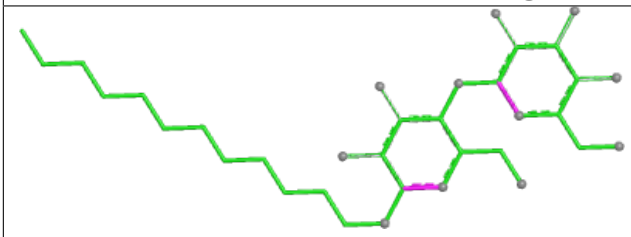
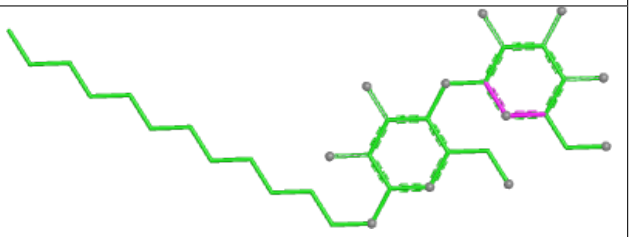
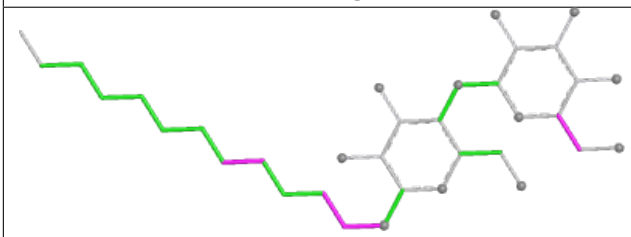
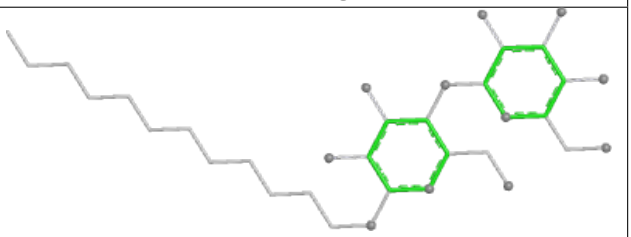
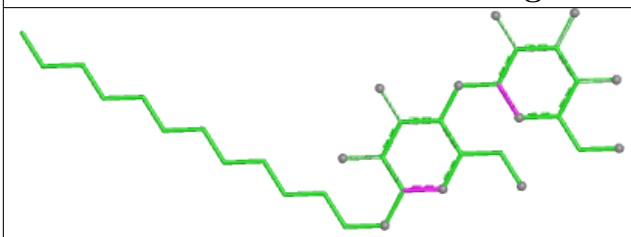
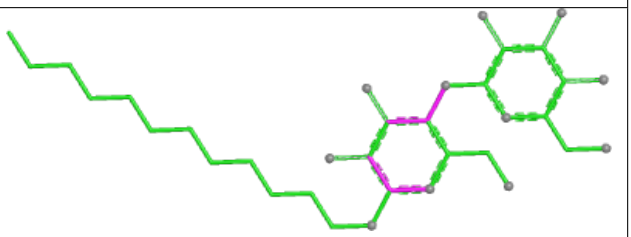
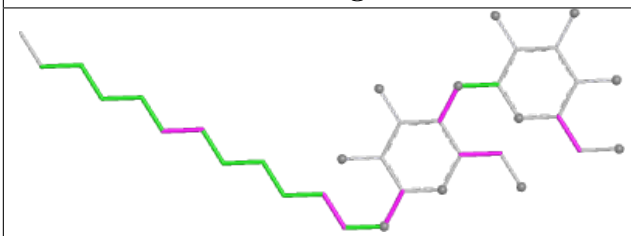
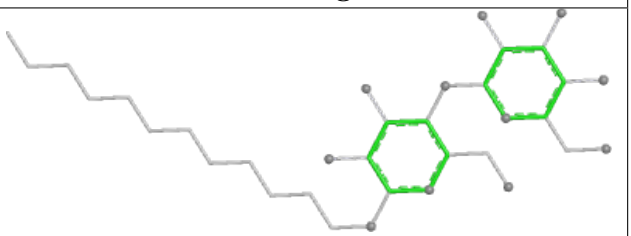
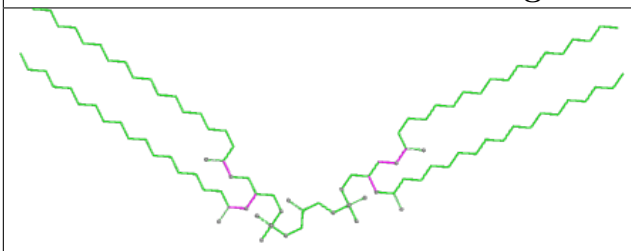


Rings

Ligand LMT D 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT h 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL C 401



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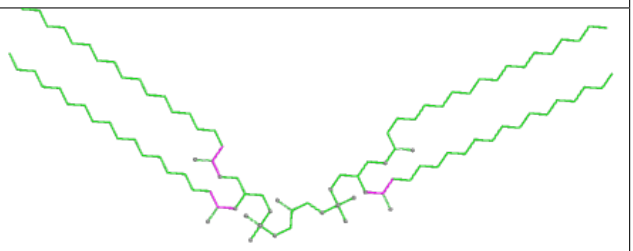

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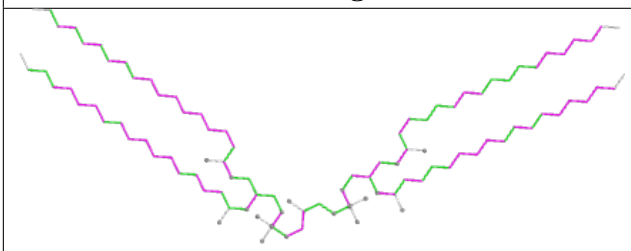

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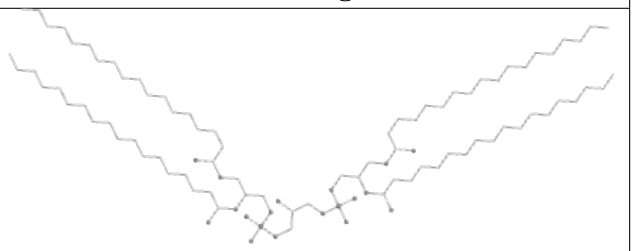
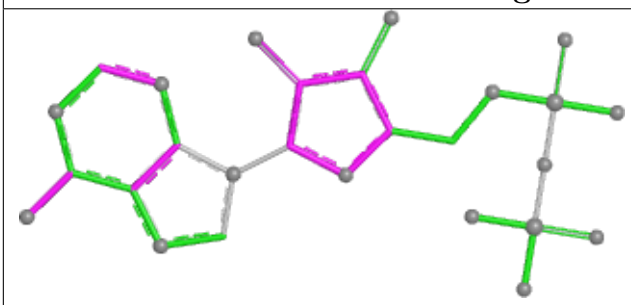


Rings

Ligand ADP B1 601



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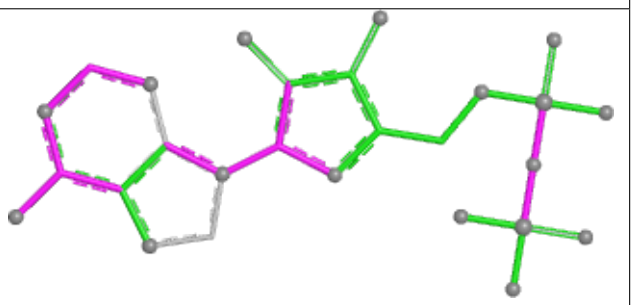

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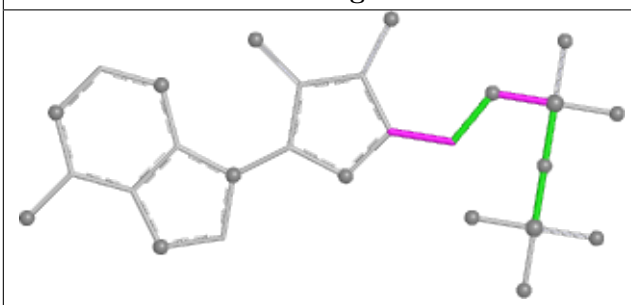

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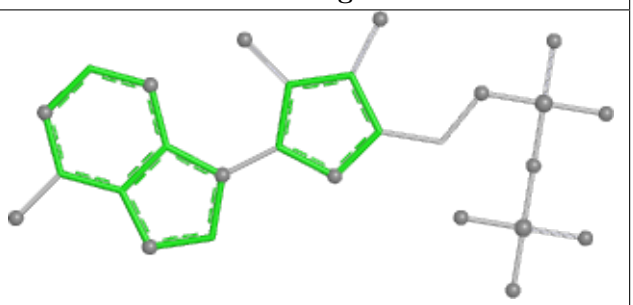
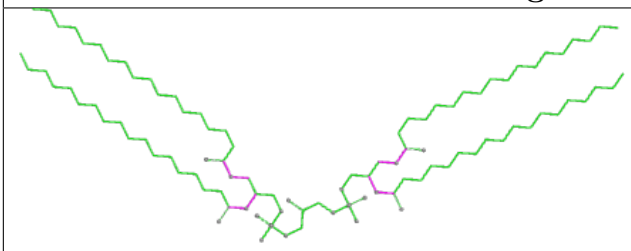


Rings

Ligand CDL b 601



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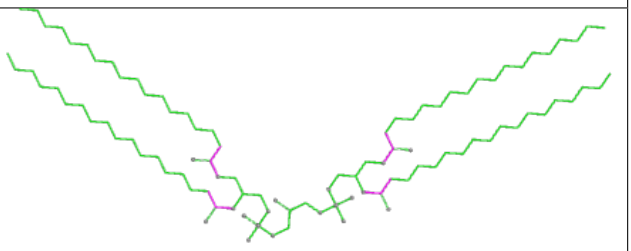

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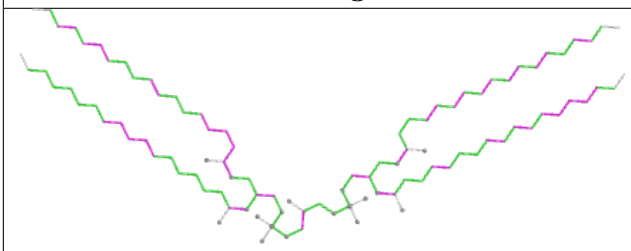

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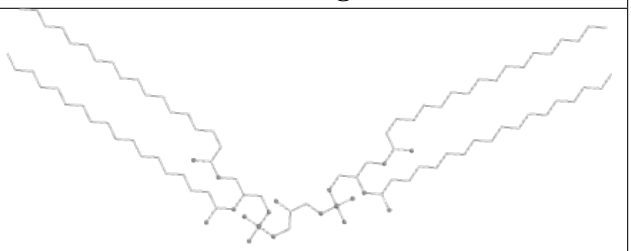
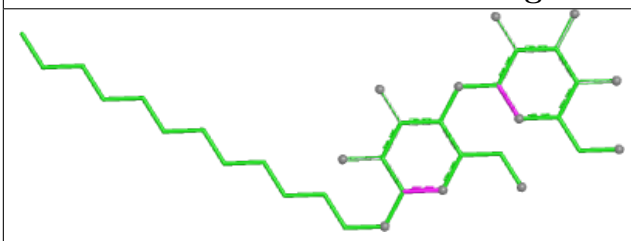


Rings

Ligand LMT x 101



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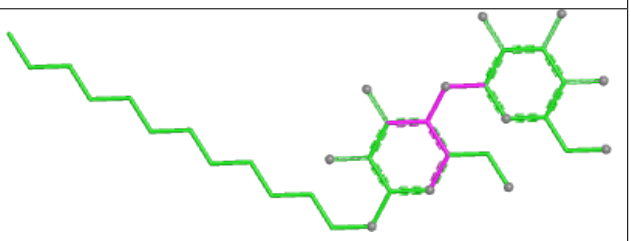

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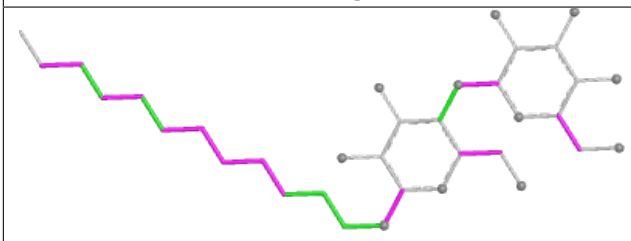

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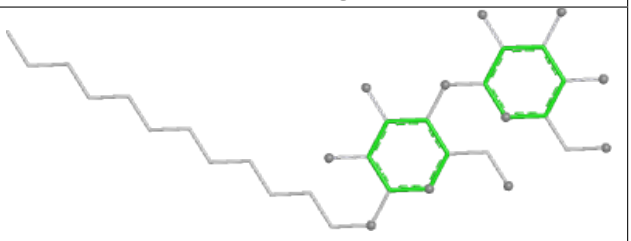
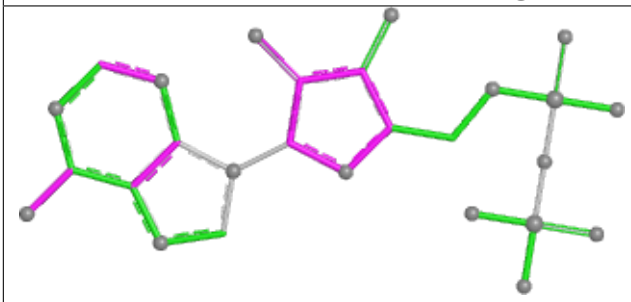
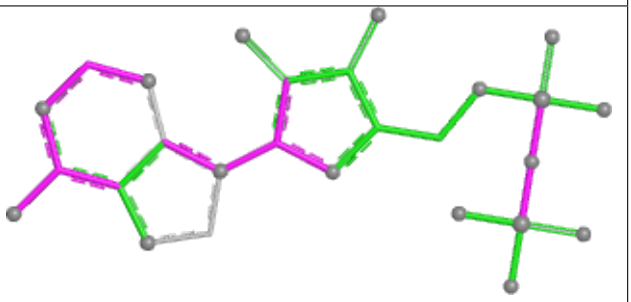
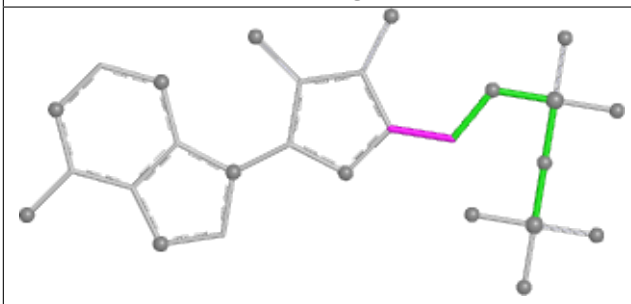
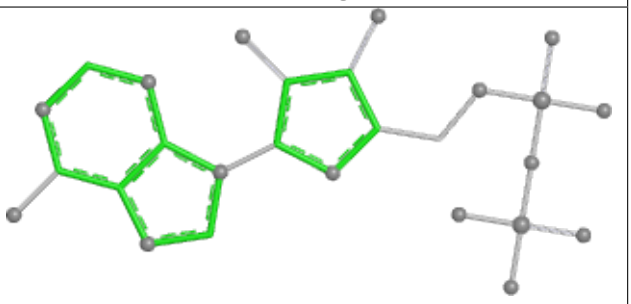


Rings

Ligand ADP D2 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

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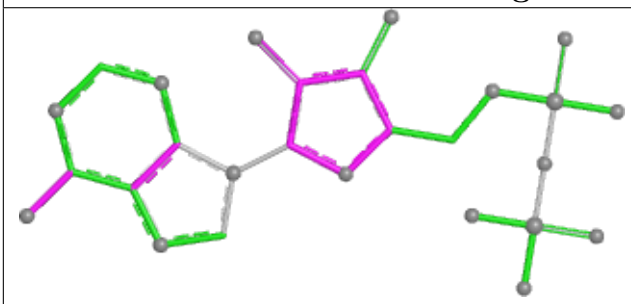
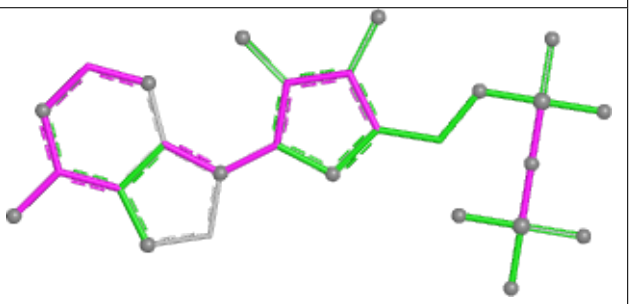
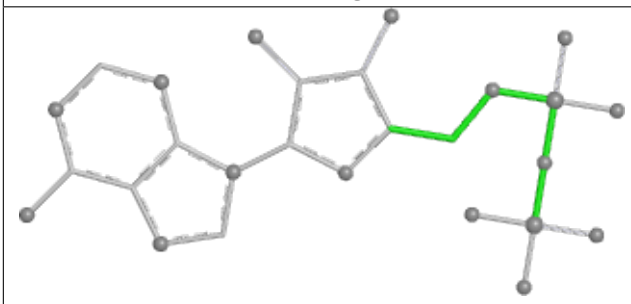
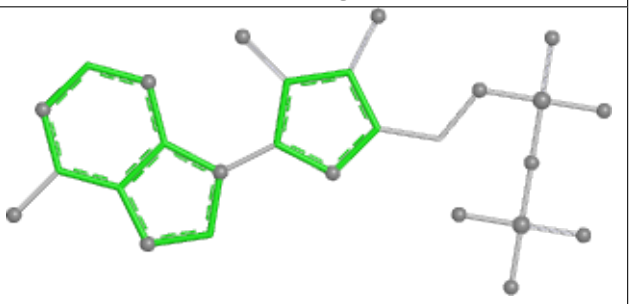
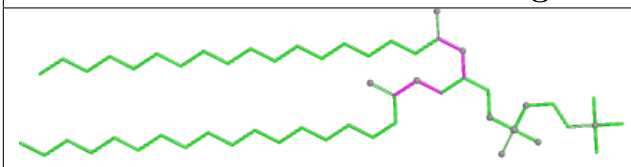
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 o 204



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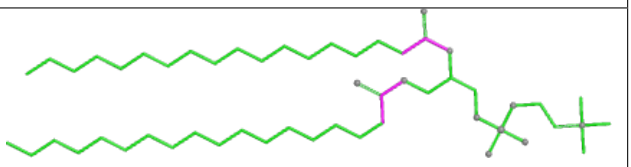

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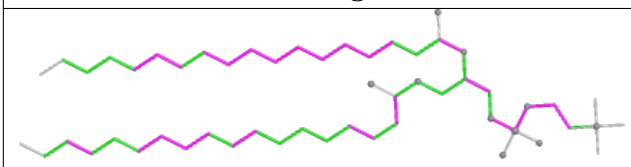

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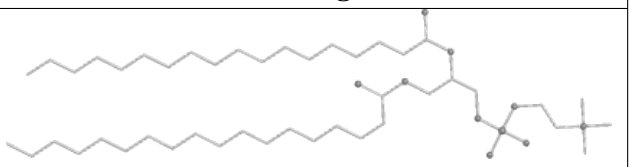
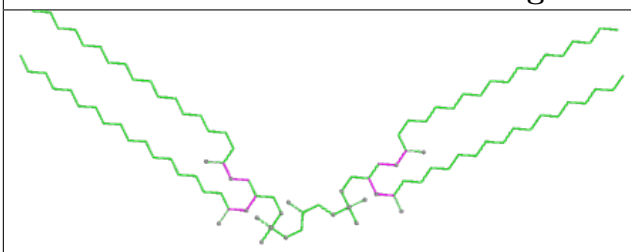


Rings

Ligand CDL b 602



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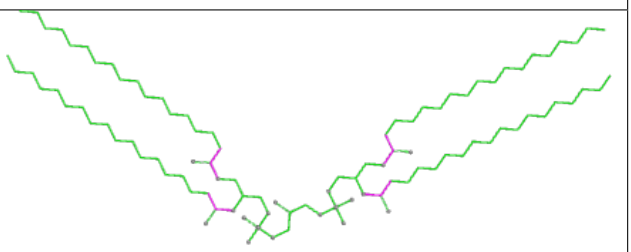

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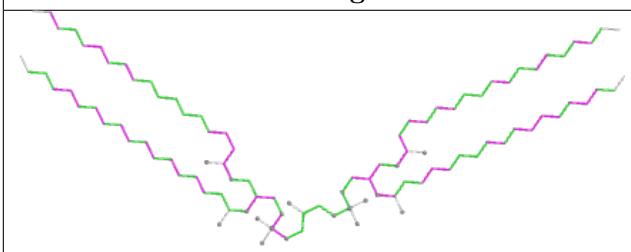

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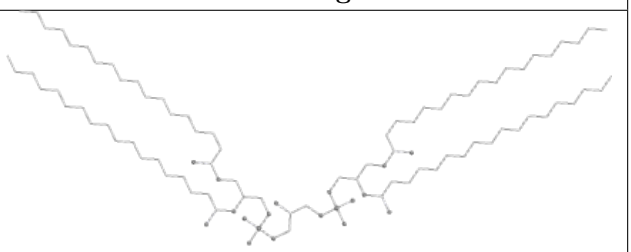

Rings

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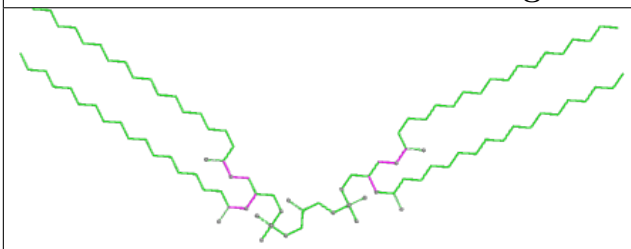

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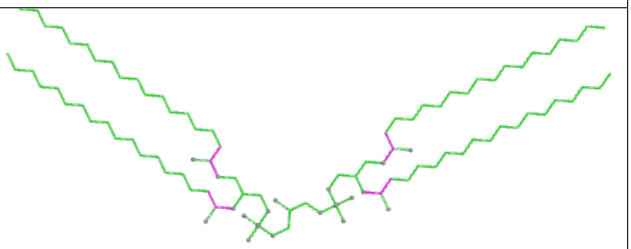
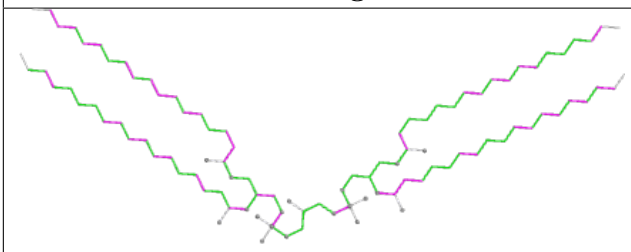


Bond angles



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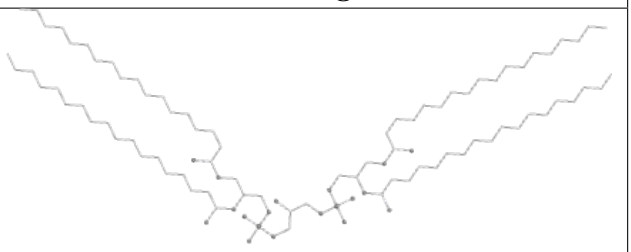
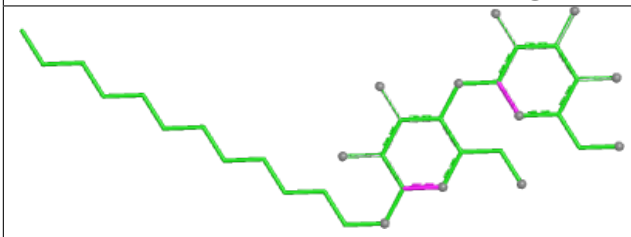
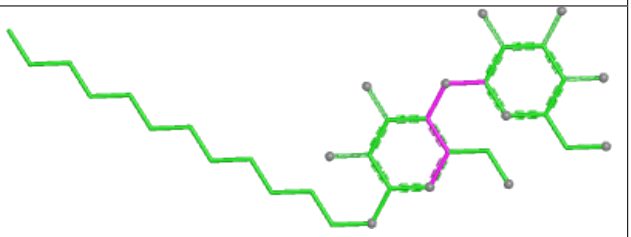
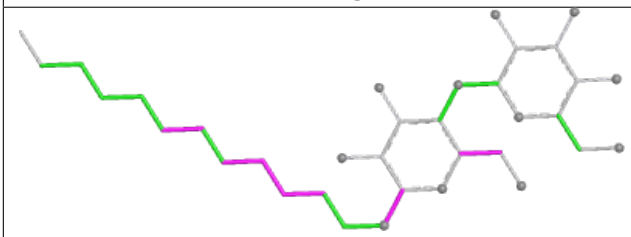
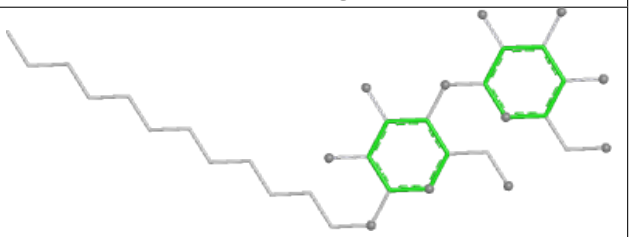
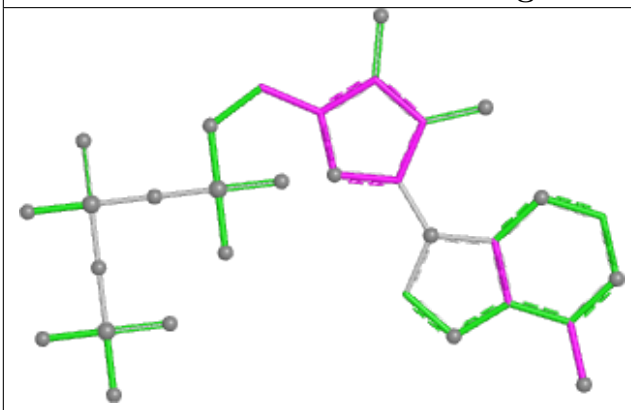
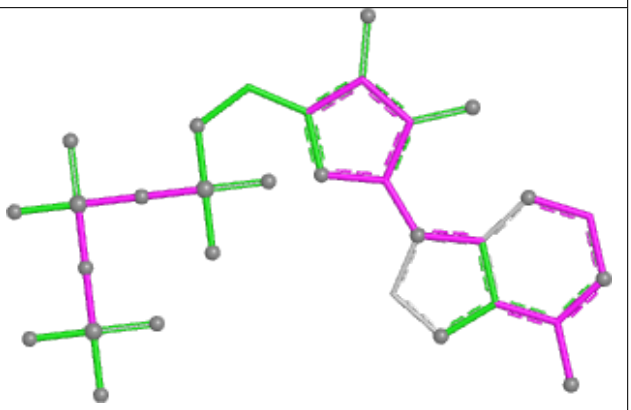
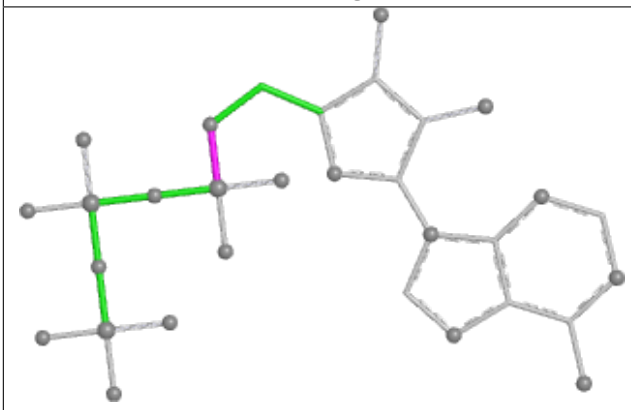
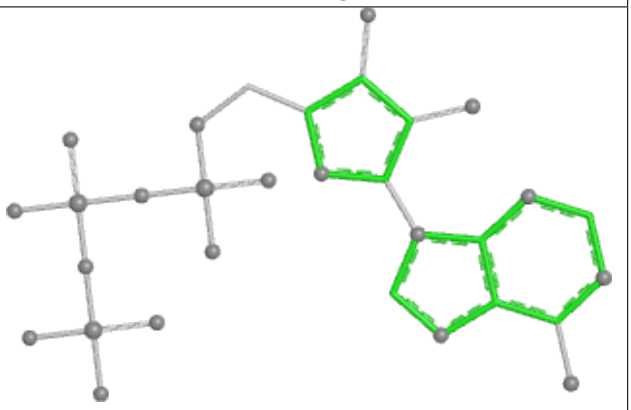
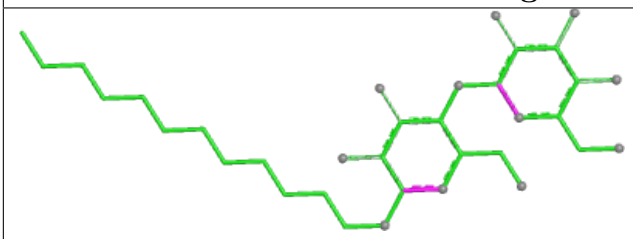


Rings

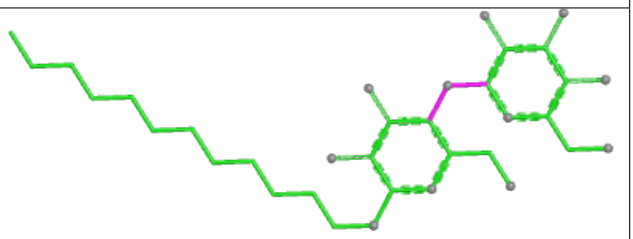
Ligand LMT c 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP E2 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

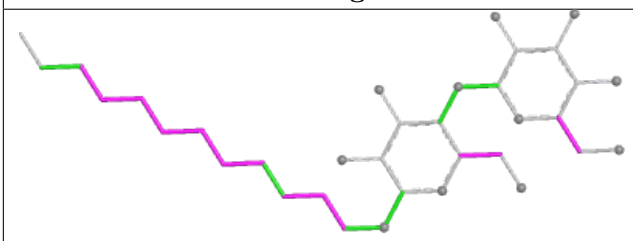
Ligand LMT D 401



Bond lengths



Bond angles



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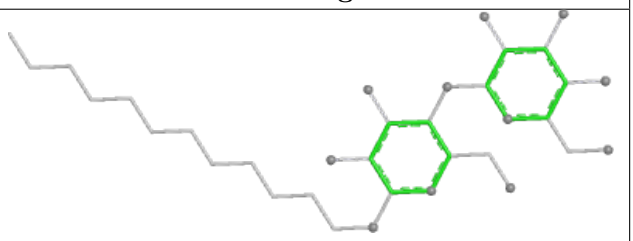
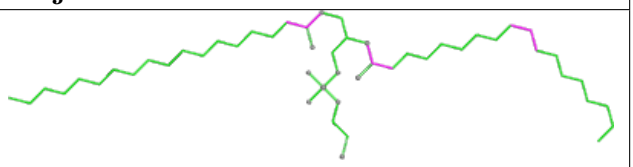


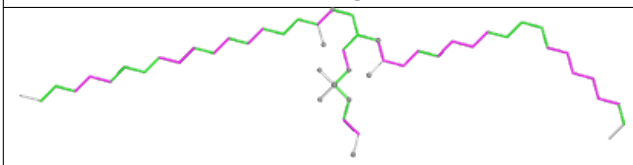
Rings

Ligand PEE j 301

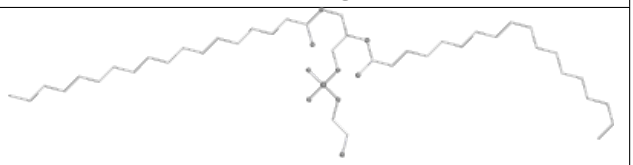
Bond lengths



Bond angles

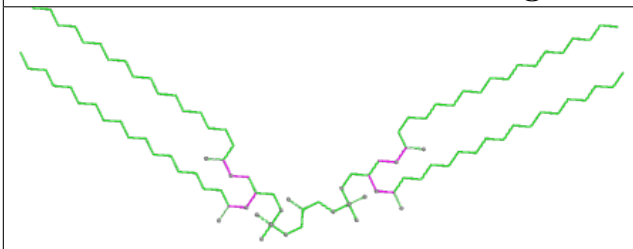


Torsions

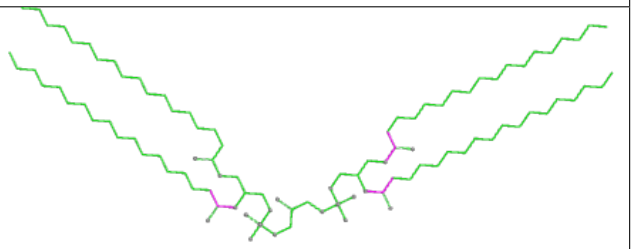


Rings

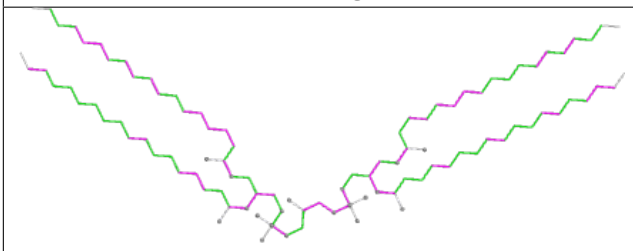
Ligand CDL D 402



Bond lengths



Bond angles



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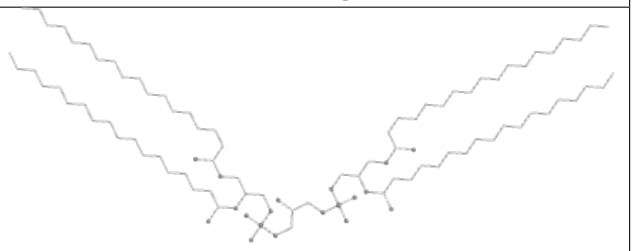
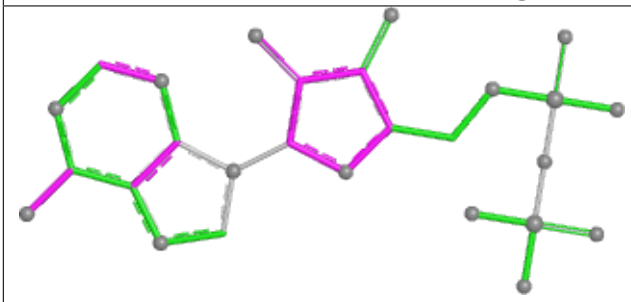
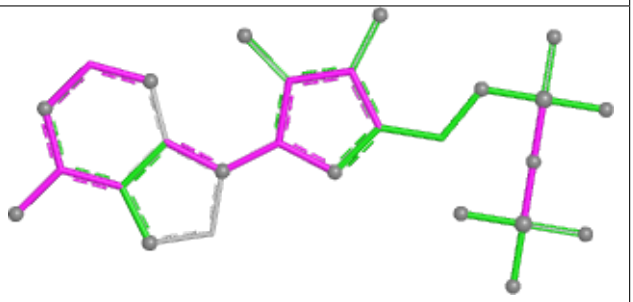


Rings

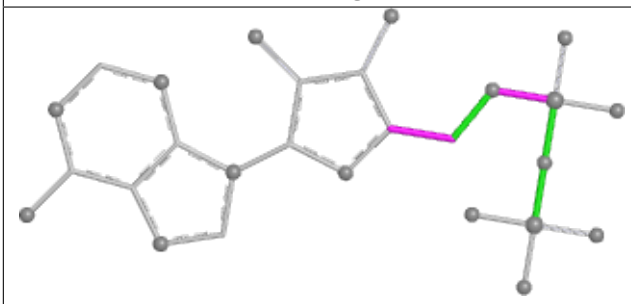
Ligand ADP B2 601



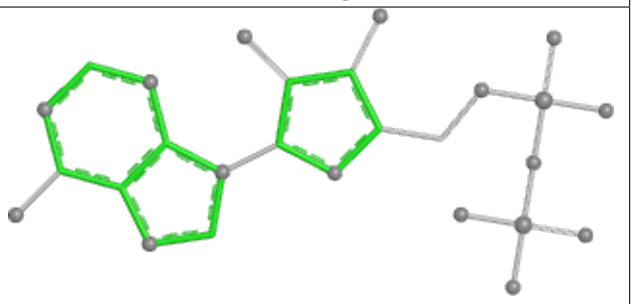
Bond lengths



Bond angles

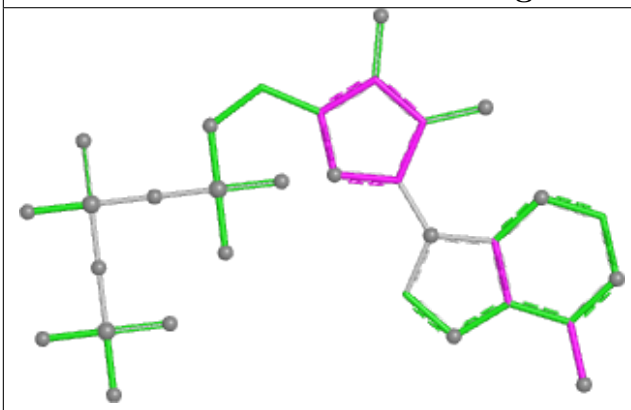


Torsions

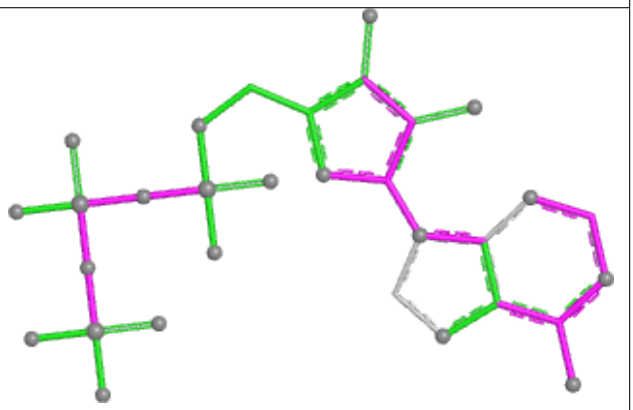


Rings

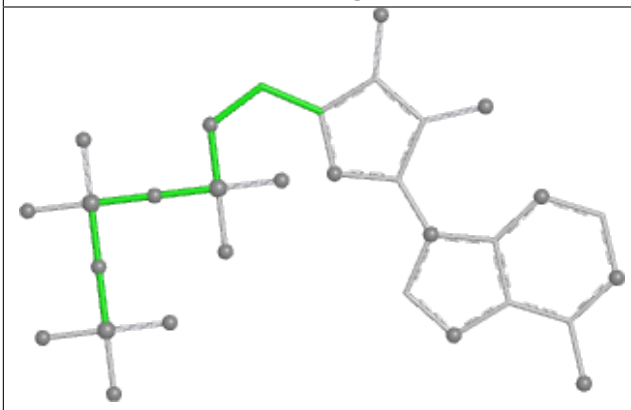
Ligand ATP A1 601



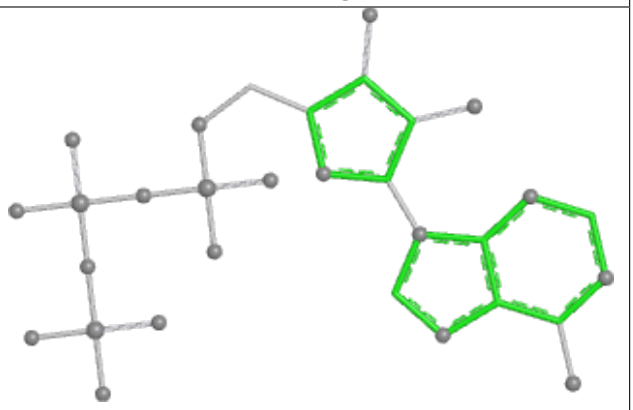
Bond lengths



Bond angles

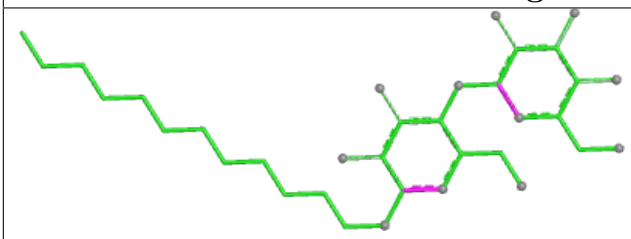


Torsions

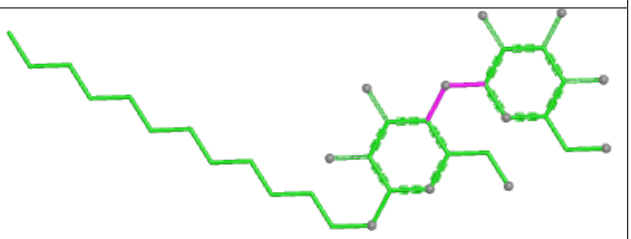


Rings

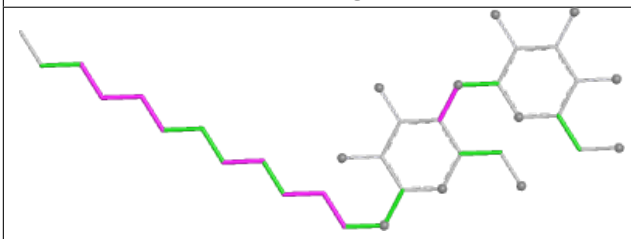
Ligand LMT c 402



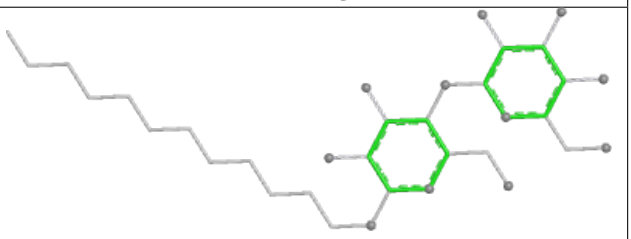
Bond lengths



Bond angles

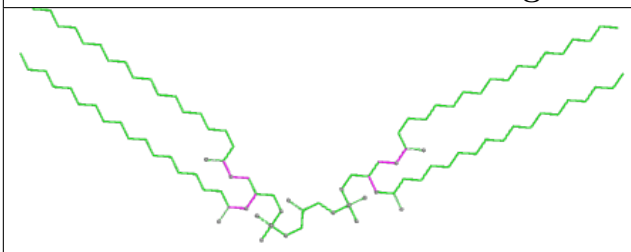


Torsions

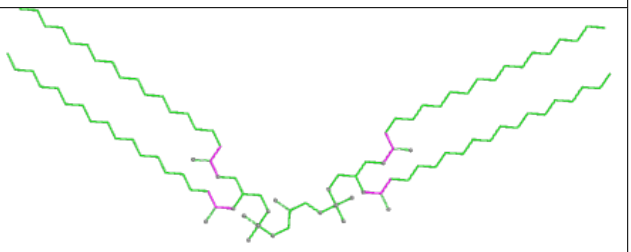


Rings

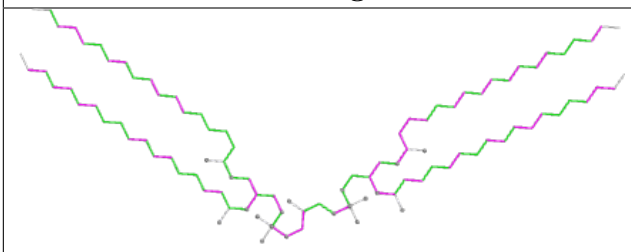
Ligand CDL H 302



Bond lengths



Bond angles



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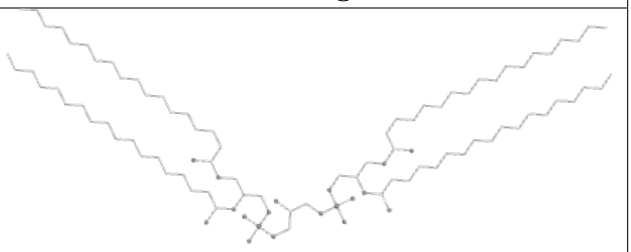
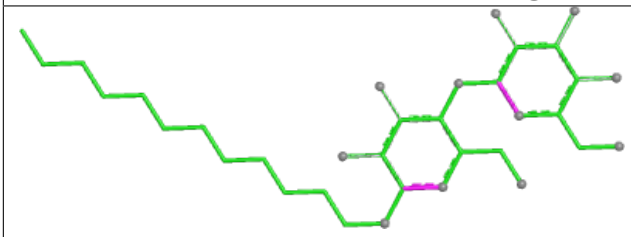
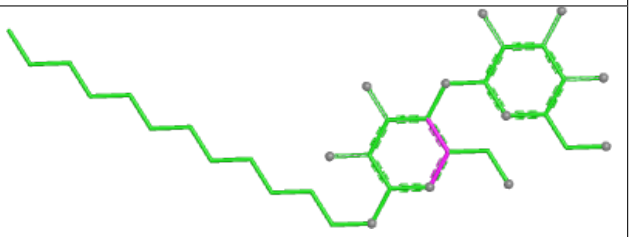
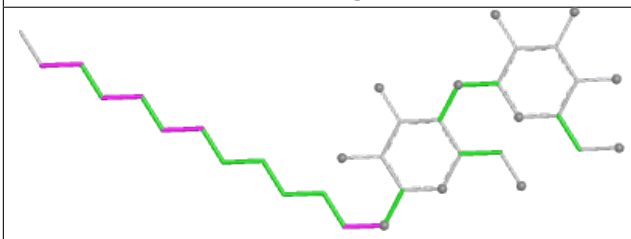
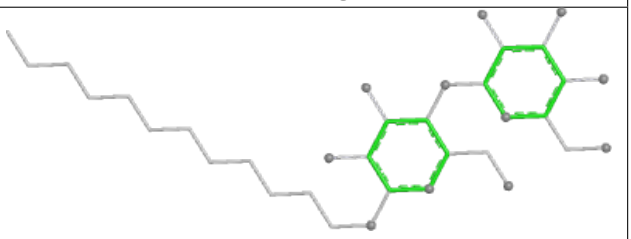
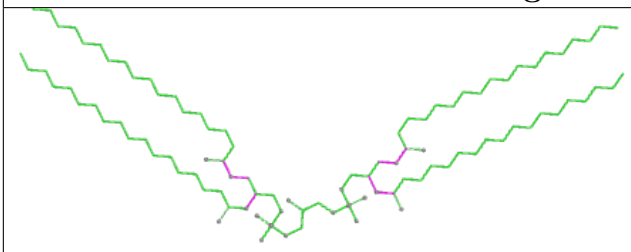
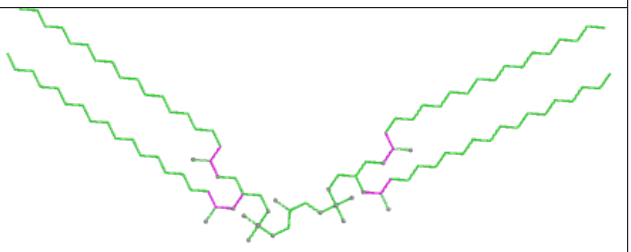
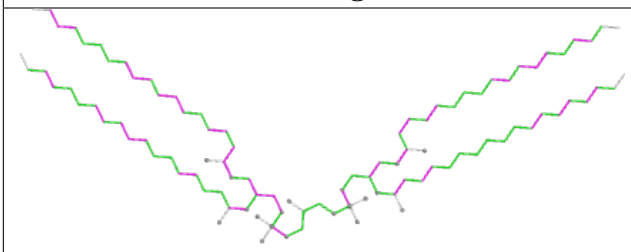
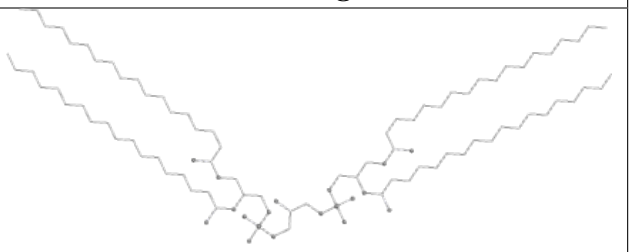
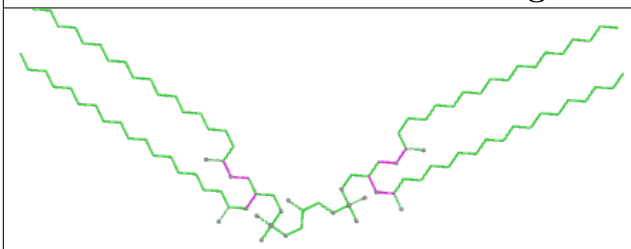


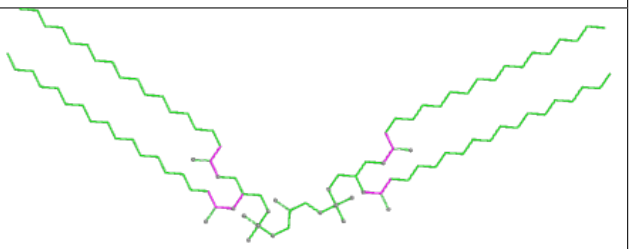
Rings

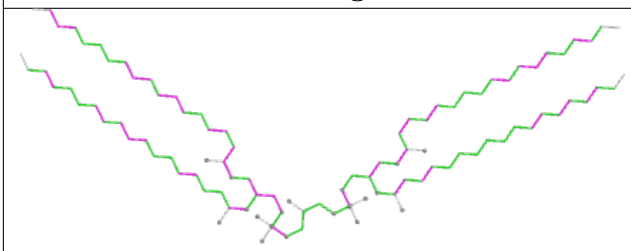
Ligand LMT o 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

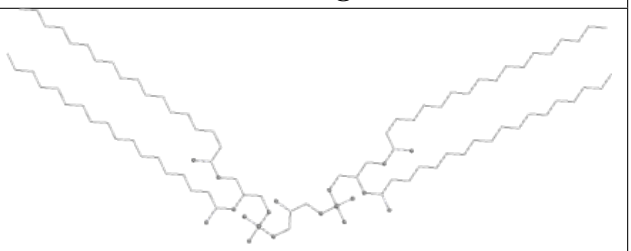
Ligand CDL O 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL o 203

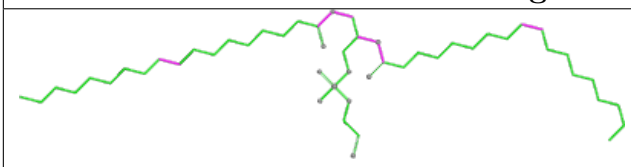

Bond lengths

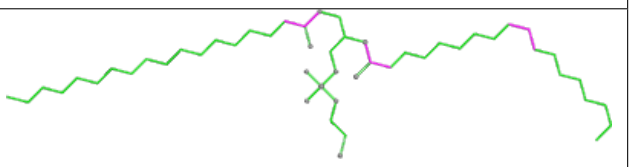

Bond angles

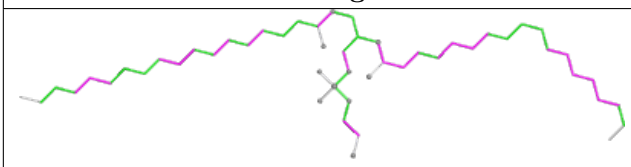

Torsions

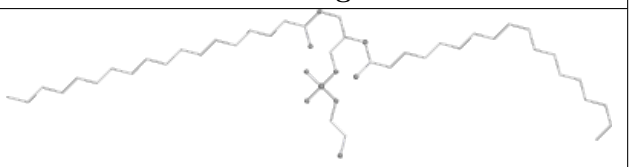

Rings

Ligand PEE J 301

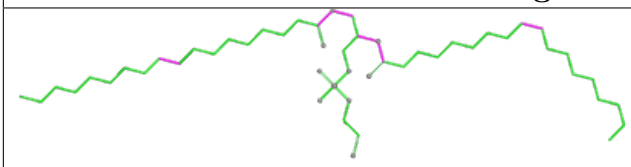

Bond lengths

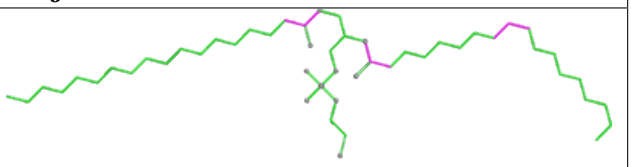

Bond angles

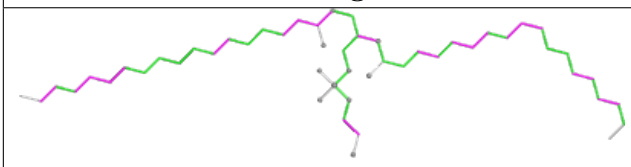

Torsions

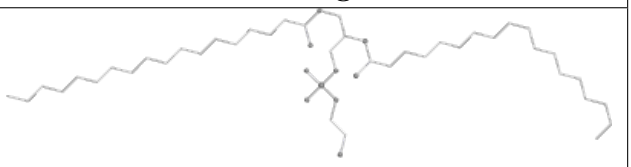

Rings

Ligand PEE j 302


Bond lengths


Bond angles


Torsions


Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

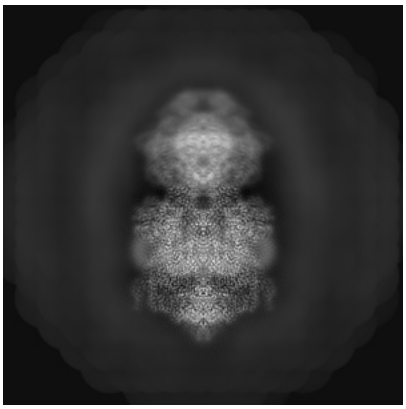
6 Map visualisation

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.

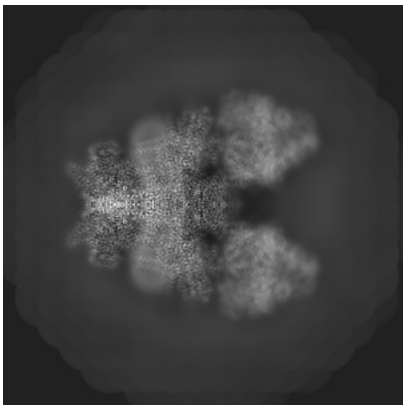
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

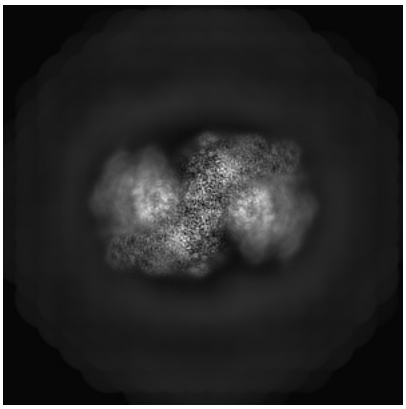
6.1.1 Primary map



X

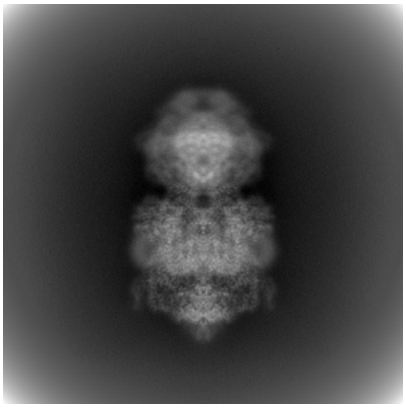


Y

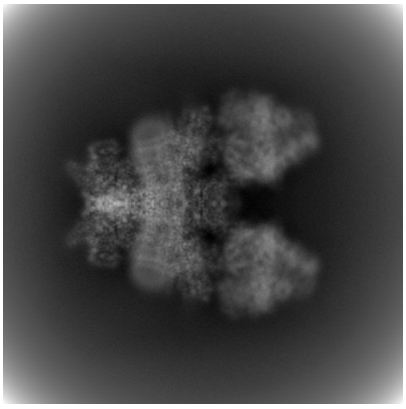


Z

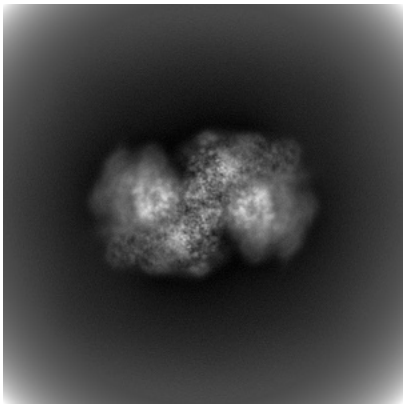
6.1.2 Raw map



X



Y

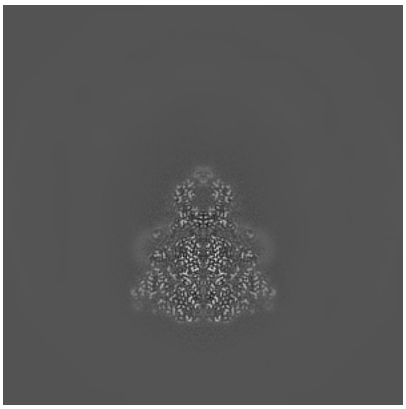


Z

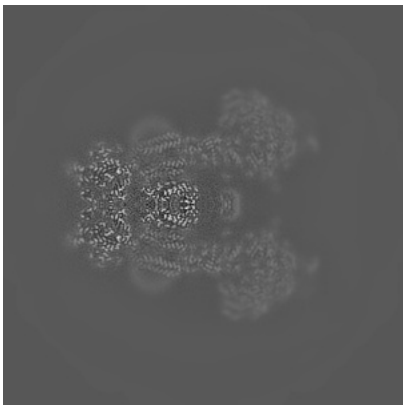
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

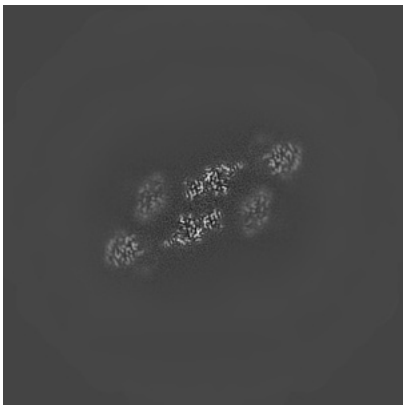
6.2.1 Primary map



X Index: 280

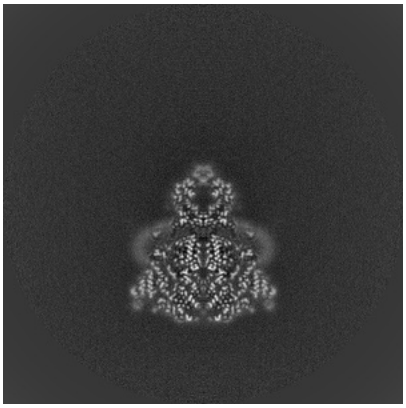


Y Index: 280

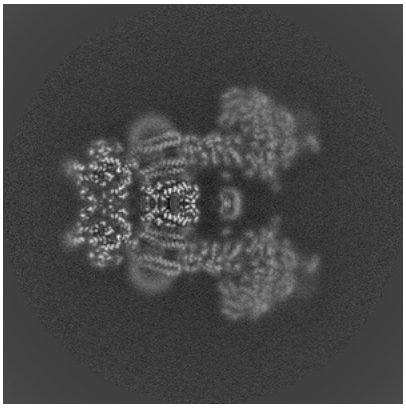


Z Index: 280

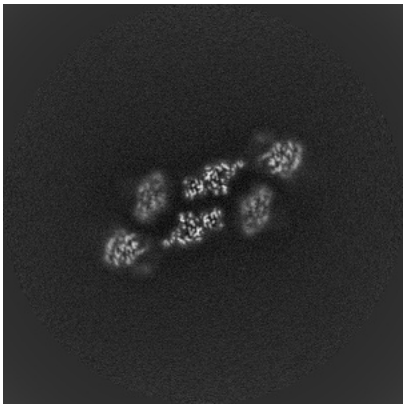
6.2.2 Raw map



X Index: 280



Y Index: 280

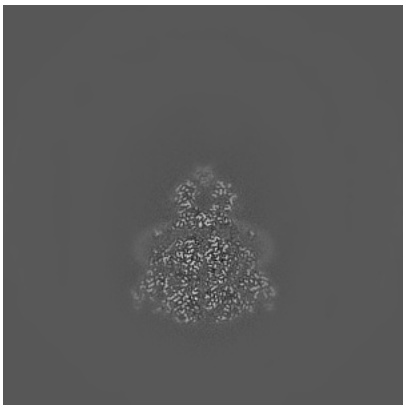


Z Index: 280

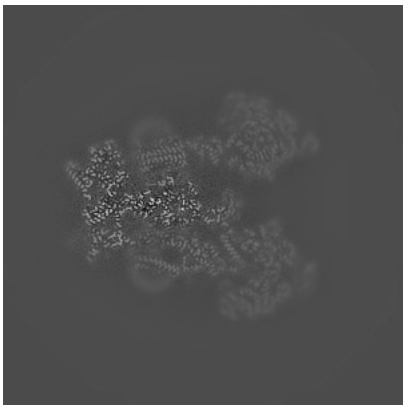
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

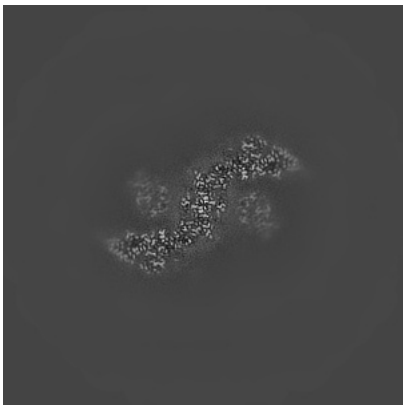
6.3.1 Primary map



X Index: 282

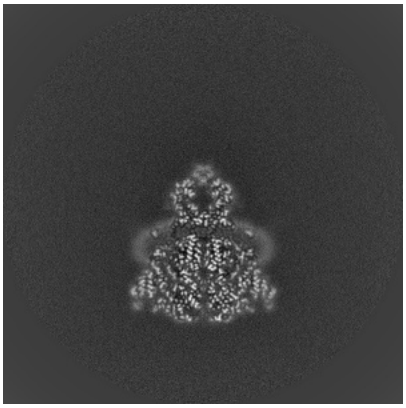


Y Index: 289

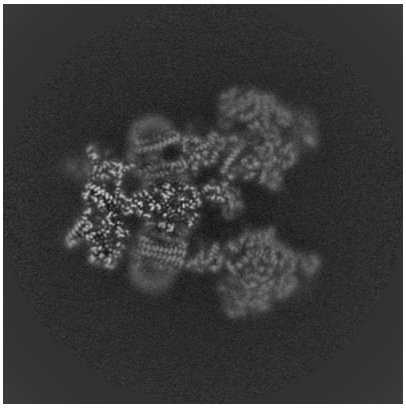


Z Index: 253

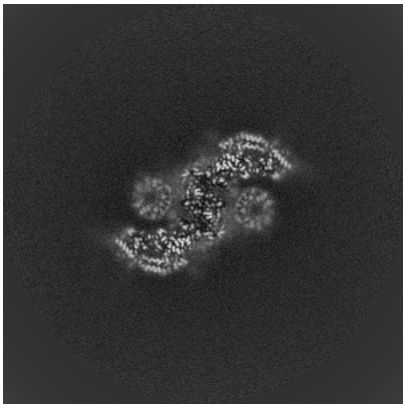
6.3.2 Raw map



X Index: 279



Y Index: 271

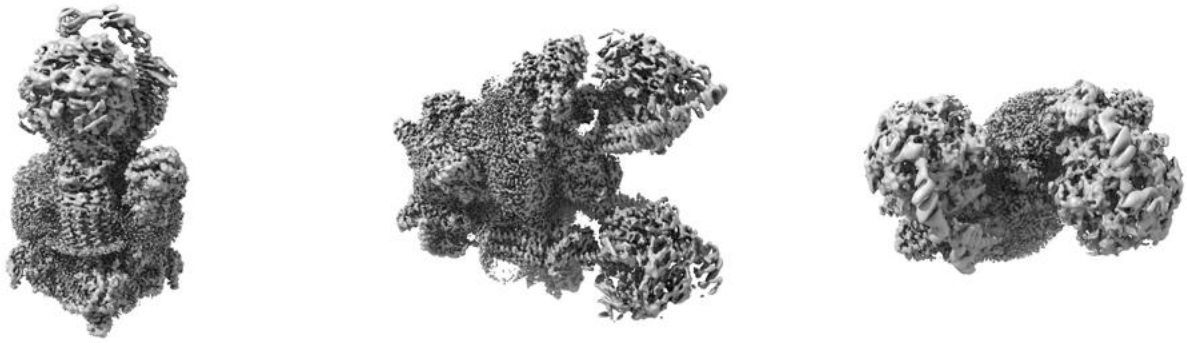


Z Index: 248

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

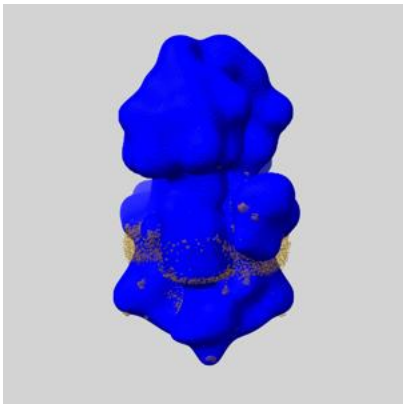
6.5 Mask visualisation (i)

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

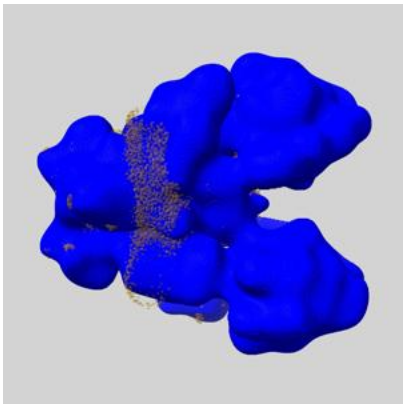
A mask typically either:

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

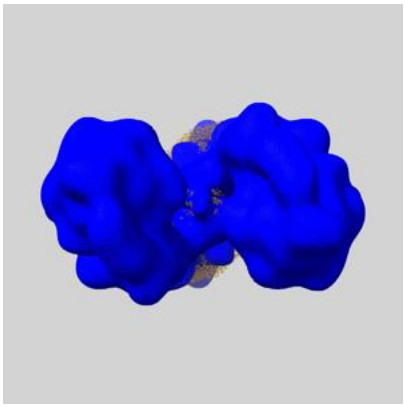
6.5.1 emd_10524_msk_1.map (i)



X



Y

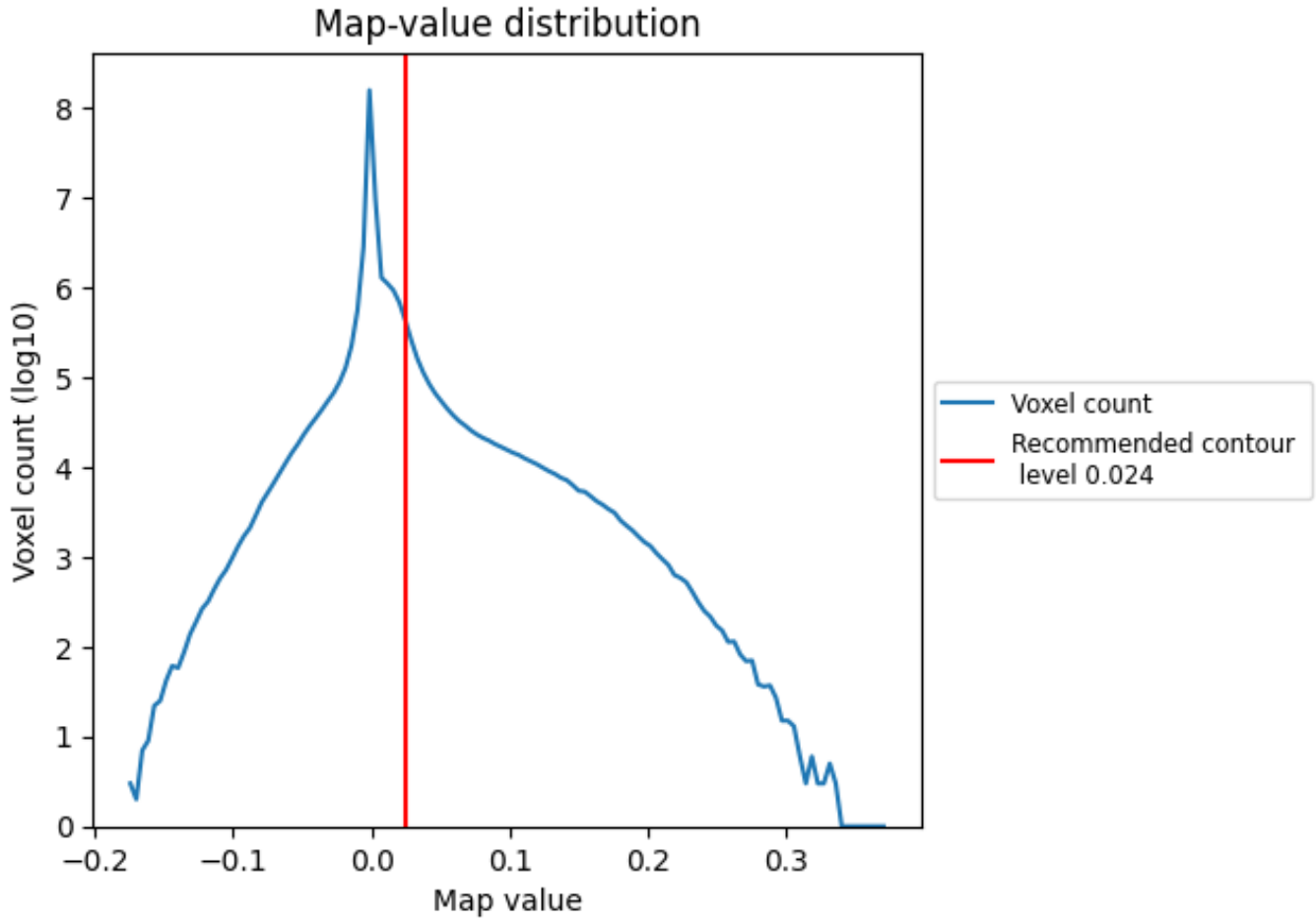


Z

7 Map analysis

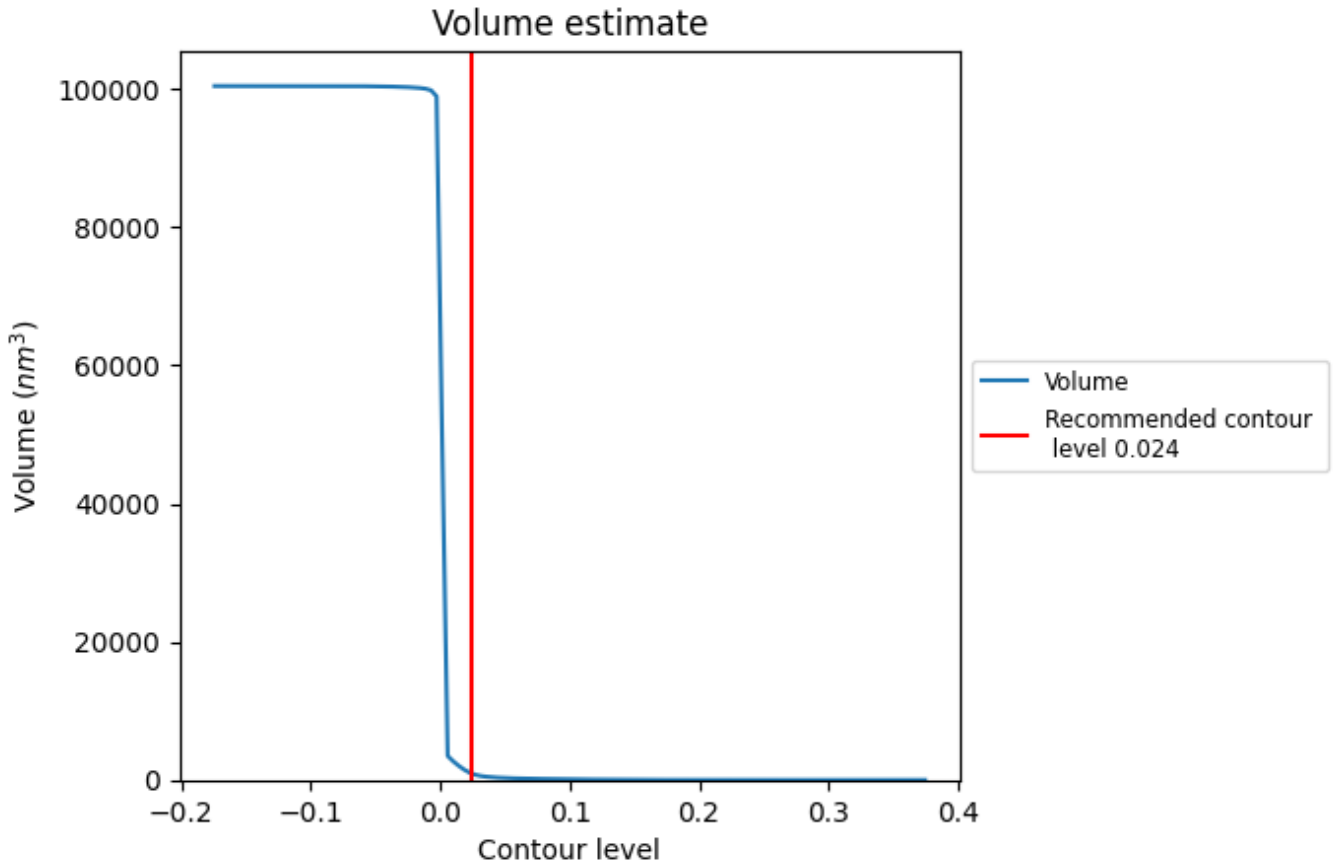
This section contains the results of statistical analysis of the map.

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.

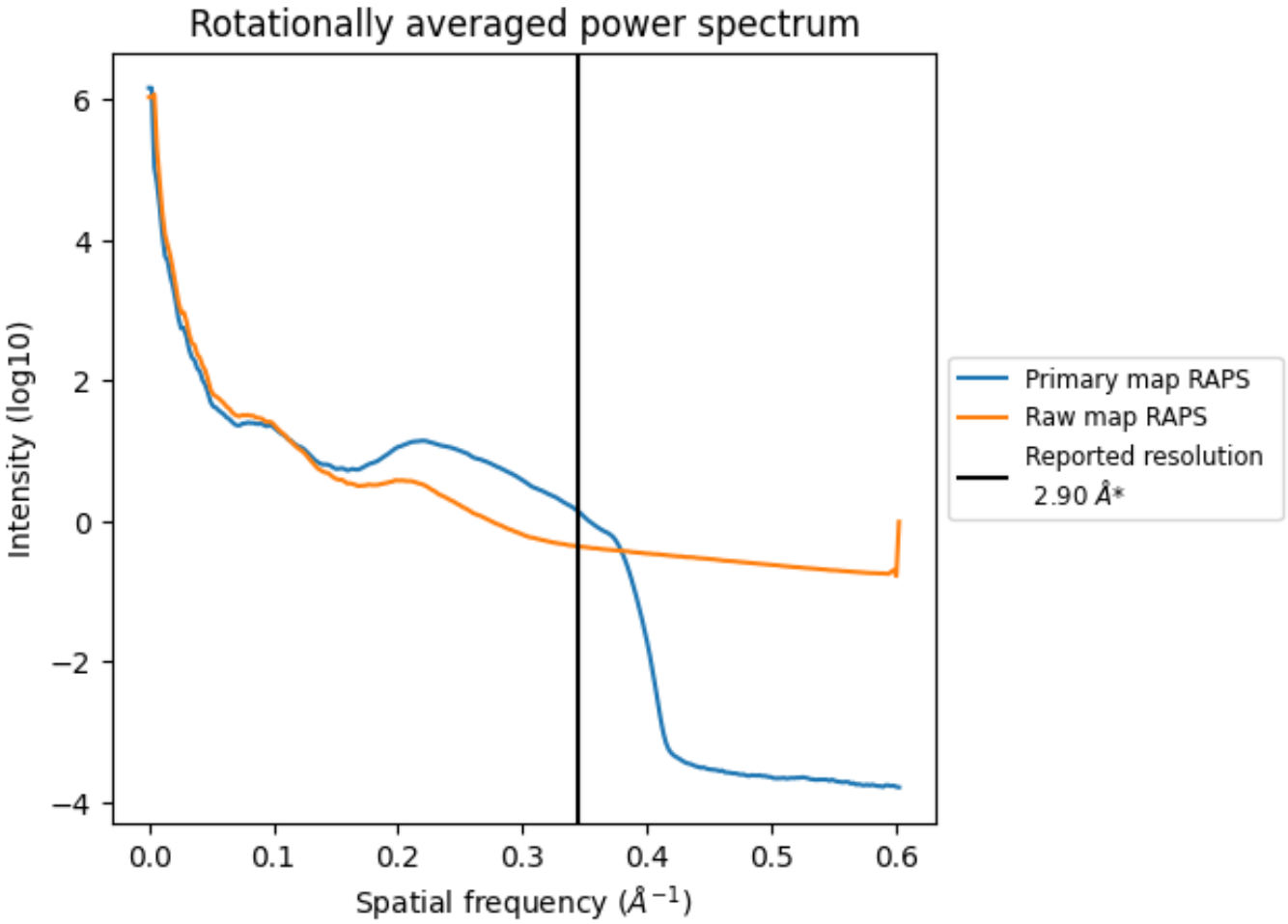
7.2 Volume estimate



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)

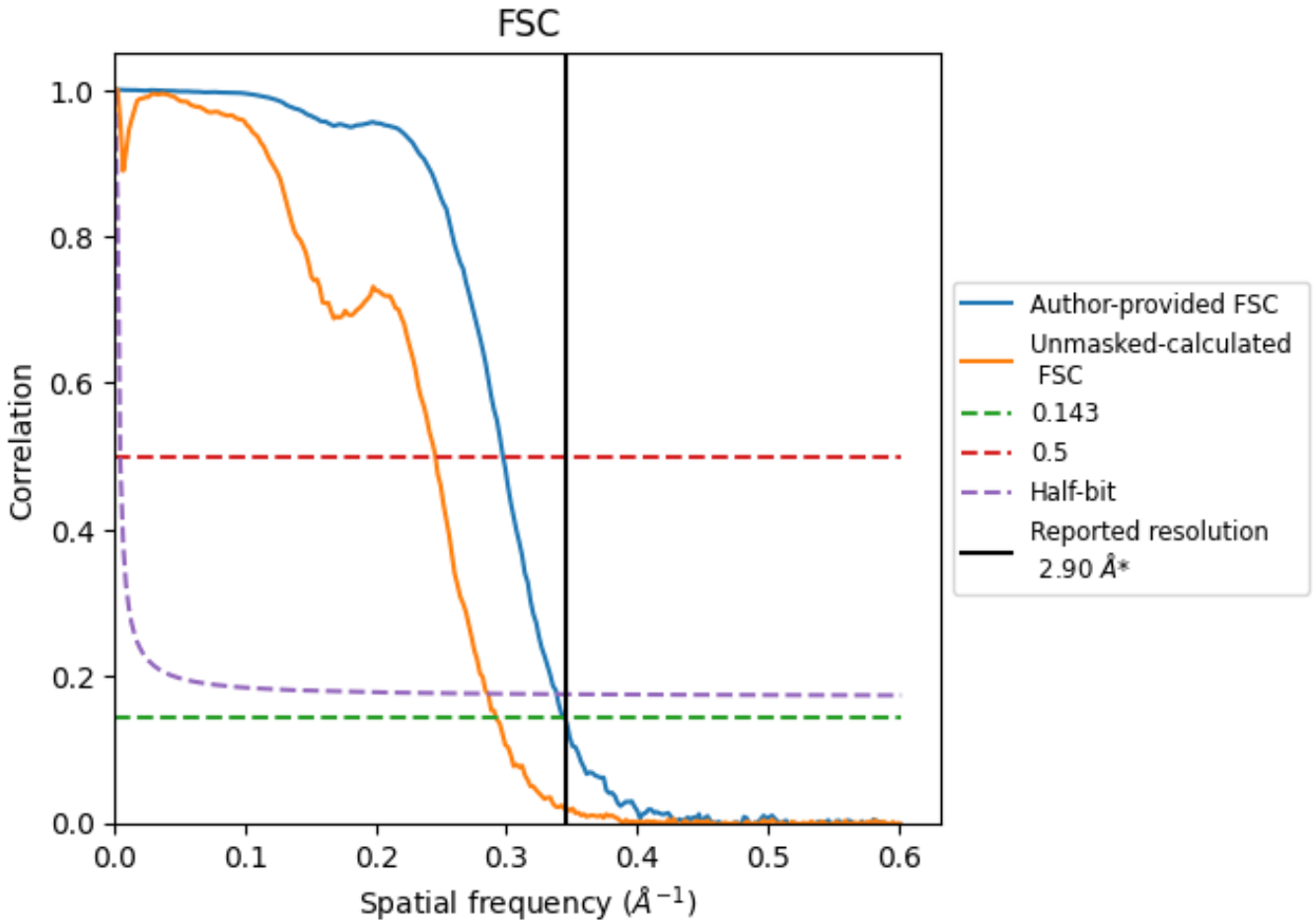


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

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)

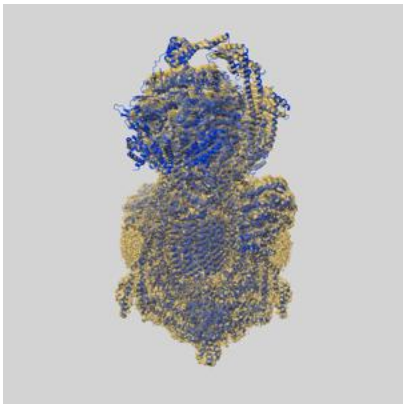
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.36	2.96
Unmasked-calculated*	3.42	4.07	3.50

*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 %

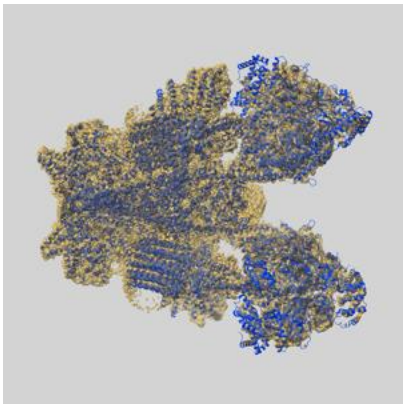
9 Map-model fit

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.

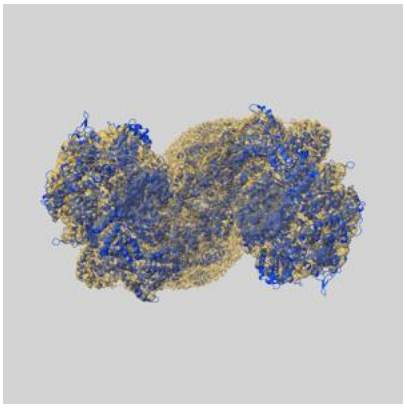
9.1 Map-model overlay



X



Y



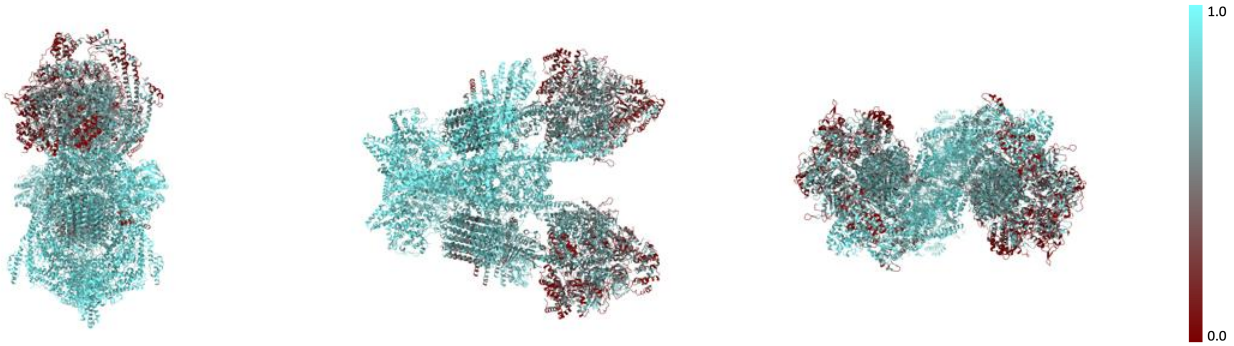
Z

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

This section was not generated.

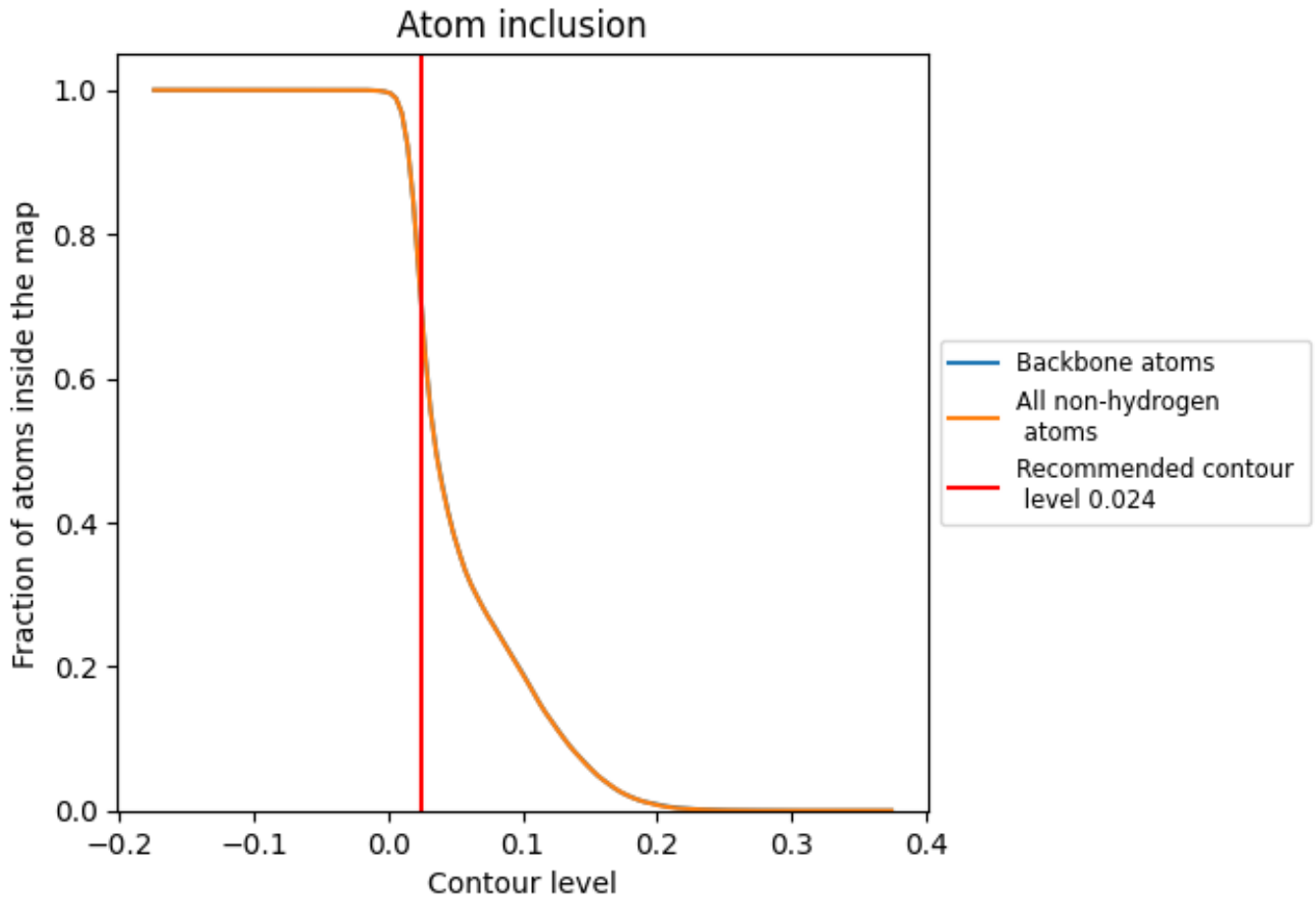
9.3 Atom inclusion mapped to coordinate model



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
All	0.7151
A	0.8470
A1	0.4344
A2	0.3703
B	0.7263
B1	0.6197
B2	0.5914
C	0.8435
C1	0.6151
C2	0.6099
D	0.9319
D1	0.5764
D2	0.5552
E	0.9328
E1	0.4687
E2	0.4098
F	0.9182
F1	0.3654
F2	0.3170
G	0.9404
G1	0.3517
G2	0.2880
H	0.9411
H1	0.7042
H2	0.7445
I	0.9048
I1	0.6660
I2	0.7123
J	0.9651
J1	0.6559
J2	0.7143
K	0.8898
K1	0.6901
K2	0.7203
L	0.9445

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Chain	Atom inclusion
L1	0.7123
L2	0.6761
M	0.9561
M1	0.7525
M2	0.6841
N	0.9059
N1	0.7505
N2	0.7304
O	0.8925
O1	0.8068
O2	0.7787
P	0.9444
P1	0.8008
P2	0.7887
Q	0.8813
Q1	0.7867
Q2	0.7827
R	0.8224
S	0.9242
T	0.9237
U	0.8829
V	0.9486
W	0.9518
X	0.9424
a	0.8357
b	0.7519
c	0.8336
d	0.9328
d1	0.6059
d2	0.6999
e	0.9320
e1	0.7471
e2	0.7605
f	0.9196
g	0.9380
g1	0.7295
g2	0.7305
h	0.9417
i	0.9034
i1	0.7204
i2	0.7295
j	0.9651

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Chain	Atom inclusion
k	0.8930
l	0.9439
m	0.9601
n	0.9067
o	0.8925
p	0.9456
q	0.8622
r	0.8300
s	0.9229
t	0.9181
u	0.8853
v	0.9467
w	0.9558
x	0.9409