wwPDB EM Validation Summary Report

Oct 19, 2022 – 03:13 am BST

PDB ID	:	8APK
EMDB ID	:	EMD-15573
Title	:	rotational state 3 of the Trypanosoma brucei mitochondrial ATP synthase dimer
Authors	:	Muehleip, A.; Gahura, O.; Zikova, A.; Amunts, A.
Deposited on	:	2022-08-09
Resolution	:	3.70 Å(reported)

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

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

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

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

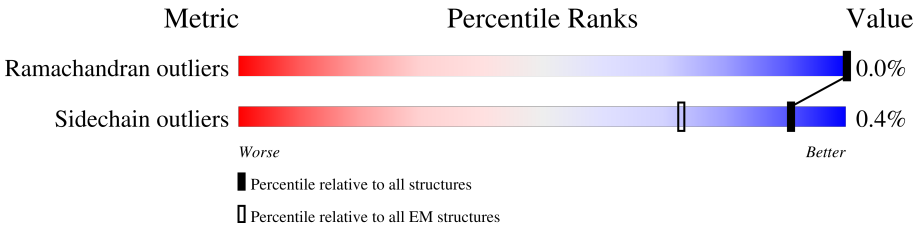
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	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	L	92	10% 71% 29%
1	l	92	10% 71% 29%
2	M	144	10% 89% 10%
2	m	144	90% 10%
3	a	231	99%
4	c	114	75% 25%
5	d	370	90% 10%
6	e	396	96%
7	f	145	92% 7%

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Mol	Chain	Length	Quality of chain
8	g	269	24% 100%
9	h	157	6% 87% 13%
10	i	104	99%
11	j	169	99%
12	k	124	85% 15%
13	n	156	88% 11%
14	o	101	94% 5%
15	p	105	76% 24%
16	q	98	87% 13%
17	r	62	100%
18	A1	584	90% 10%
18	B1	584	89% 11%
18	C1	584	91% 9%
19	D1	519	93% 6%
19	E1	519	93% 6%
19	F1	519	94% 6%
20	G1	305	98%
21	H1	182	88% 12%
22	I1	75	87% 13%
23	J1	188	88% 12%
23	K1	188	88% 12%
23	L1	188	88% 12%
24	M1	255	91% 8%
25	O1	118	65% 34%
25	P1	118	66% 34%

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Mol	Chain	Length	Quality of chain
25	Q1	118	66% 34%
25	R1	118	65% 34%
25	S1	118	66% 34%
25	T1	118	66% 34%
25	U1	118	66% 34%
25	V1	118	66% 34%
25	W1	118	65% 34%
25	X1	118	65% 34%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	Q7G	e	406	X	-	-	-
30	Q7G	n	201	X	-	-	-

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 129566 atoms, of which 65465 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called subunit-e.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	L	65	Total	C	H	N	O	S	0	0
			1082	340	545	104	92	1		
1	l	65	Total	C	H	N	O	S	0	0
			1082	340	545	104	92	1		

- Molecule 2 is a protein called subunit-g.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	M	129	Total	C	H	N	O	S	0	0
			2069	662	1042	177	186	2		
2	m	129	Total	C	H	N	O	S	0	0
			2069	662	1042	177	186	2		

- Molecule 3 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	a	231	Total	C	H	N	O	S	0	0
			4076	1459	2044	261	284	28		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	23	TRP	-	insertion	UNP P24499
a	180	TRP	-	insertion	UNP P24499

- Molecule 4 is a protein called subunit-8.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	c	86	Total	C	H	N	O	S	0	0
			1460	494	715	116	130	5		

- Molecule 5 is a protein called subunit-d.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	d	332	Total	C	H	N	O	S	0	0
			5499	1710	2762	505	514	8		

- Molecule 6 is a protein called ATPTB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	e	383	Total	C	H	N	O	S	0	0
			6270	2060	3050	558	585	17		

- Molecule 7 is a protein called subunit-f.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	f	135	Total	C	H	N	O	S	0	0
			2256	744	1111	201	195	5		

- Molecule 8 is a protein called ATPTB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	g	268	Total	C	H	N	O	S	0	0
			3953	1211	2020	343	378	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	176	ALA	VAL	conflict	UNP A0A3L6KRX7

- Molecule 9 is a protein called ATPTB4.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	h	137	Total	C	H	N	O	S	0	0
			2158	680	1088	184	203	3		

- Molecule 10 is a protein called subunit-i/j.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	i	103	Total	C	H	N	O	S	0	0
			1740	574	857	152	151	6		

- Molecule 11 is a protein called ATPTB6.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	j	168	Total	C	H	N	O	S	0	0
			2835	919	1411	249	249	7		

- Molecule 12 is a protein called subunit-k.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	k	105	Total	C	H	N	O	S	0	0
			1749	577	876	149	141	6		

- Molecule 13 is a protein called ATPTB11.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	n	139	Total	C	H	N	O	S	0	0
			2210	730	1082	183	208	7		

- Molecule 14 is a protein called ATPTB12.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	o	96	Total	C	H	N	O	S	0	0
			1556	506	767	140	140	3		

- Molecule 15 is a protein called subunit-b.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	p	80	Total	C	H	N	O	S	0	0
			1335	448	651	108	125	3		

- Molecule 16 is a protein called ATPEG3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	q	85	Total	C	H	N	O	0	0
			1486	499	720	142	125		

- Molecule 17 is a protein called ATPEG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	r	62	Total	C	H	N	O	S	0	0
			1040	358	498	94	85	5		

- Molecule 18 is a protein called ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	A1	524	Total	C	H	N	O	S	0	0
			8219	2594	4171	703	731	20		
18	B1	522	Total	C	H	N	O	S	0	0
			8174	2578	4146	700	730	20		
18	C1	530	Total	C	H	N	O	S	0	0
			8281	2612	4197	710	742	20		

- Molecule 19 is a protein called ATP synthase subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	D1	487	Total	C	H	N	O	S	0	0
			7431	2329	3742	631	710	19		
19	E1	487	Total	C	H	N	O	S	0	0
			7431	2329	3742	631	710	19		
19	F1	488	Total	C	H	N	O	S	0	0
			7446	2334	3750	632	711	19		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
20	G1	300	Total	C	H	N	O	S	0	0
			4774	1507	2387	423	448	9		

- Molecule 21 is a protein called ATP synthase, epsilon chain, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	H1	161	Total	C	H	N	O	S	0	0
			2483	788	1232	211	248	4		

- Molecule 22 is a protein called ATP synthase subunit epsilon, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	I1	65	Total	C	H	N	O	S	0	0
			1046	332	513	97	102	2		

- Molecule 23 is a protein called ATP synthase subunit p18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	J1	166	Total	C	H	N	O	S	0	0
			2590	822	1276	221	257	14		
23	K1	166	Total	C	H	N	O	S	0	0
			2591	822	1276	221	258	14		

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Mol	Chain	Residues	Atoms						AltConf	Trace
23	L1	165	Total	C	H	N	O	S	0	0
			2581	819	1271	220	257	14		

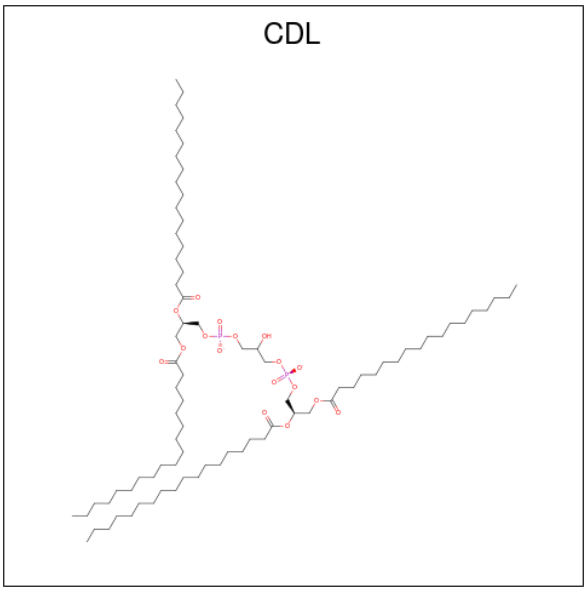
- Molecule 24 is a protein called OSCP.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	M1	234	Total	C	H	N	O	S	0	0
			3750	1212	1873	302	360	3		

- Molecule 25 is a protein called ATPase subunit 9, putative.

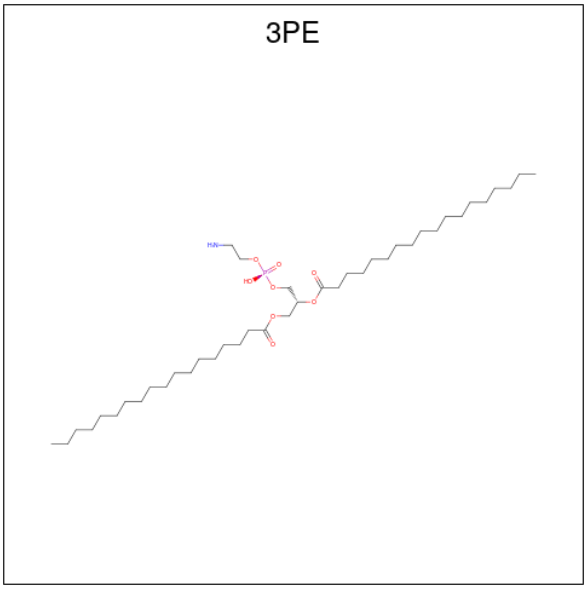
Mol	Chain	Residues	Atoms						AltConf	Trace
25	O1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
25	P1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
25	Q1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
25	R1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
25	S1	78	Total	C	H	N	O	S	0	0
			1166	376	601	89	96	4		
25	T1	78	Total	C	H	N	O	S	0	0
			1166	376	601	89	96	4		
25	U1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
25	V1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
25	W1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
25	X1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



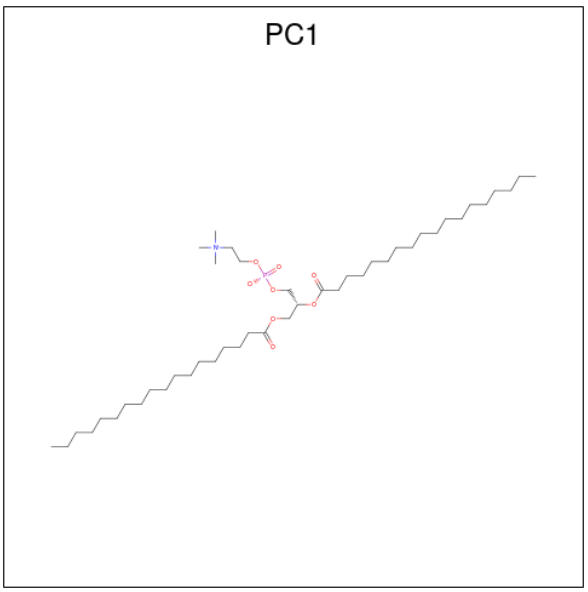
Mol	Chain	Residues	Atoms					AltConf
26	M	1	Total	C	H	O	P	0
			512	162	312	34	4	
26	M	1	Total	C	H	O	P	0
			512	162	312	34	4	
26	a	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	c	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	e	1	Total	C	H	O	P	0
			1024	324	624	68	8	
26	e	1	Total	C	H	O	P	0
			1024	324	624	68	8	
26	e	1	Total	C	H	O	P	0
			1024	324	624	68	8	
26	e	1	Total	C	H	O	P	0
			1024	324	624	68	8	
26	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	j	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	k	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	l	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	m	1	Total	C	H	O	P	0
			256	81	156	17	2	
26	q	1	Total	C	H	O	P	0
			256	81	156	17	2	

- Molecule 27 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



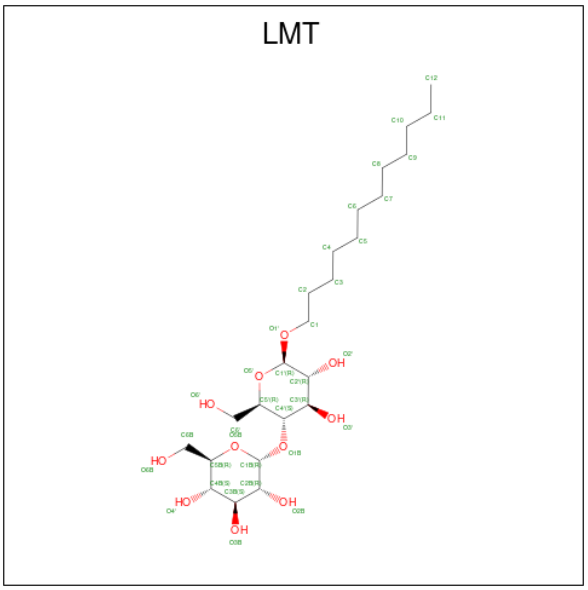
Mol	Chain	Residues	Atoms						AltConf
27	M	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
27	f	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
27	m	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

- Molecule 28 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).



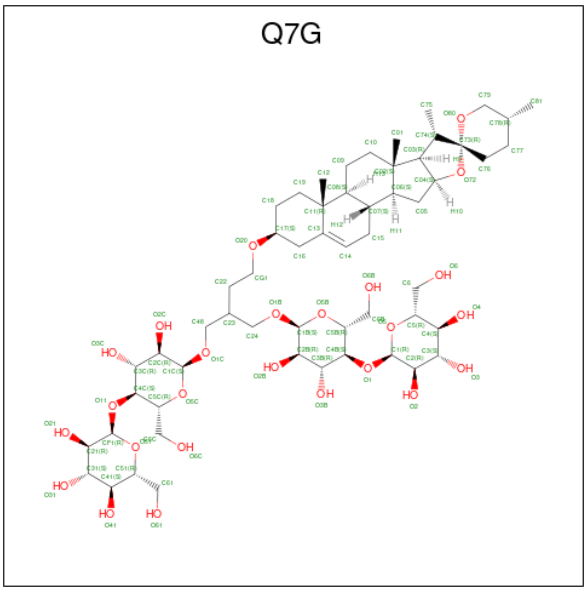
Mol	Chain	Residues	Atoms						AltConf
28	a	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
28	i	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
28	j	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
28	p	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



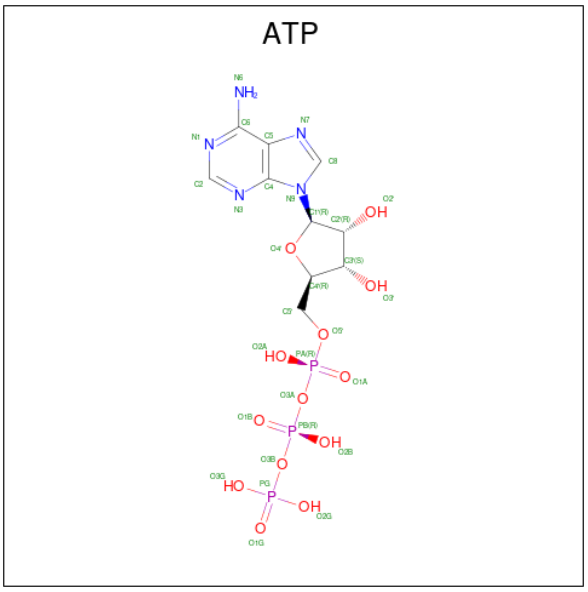
Mol	Chain	Residues	Atoms				AltConf
29	e	1	Total	C	H	O	0
			74	24	39	11	
29	j	1	Total	C	H	O	0
			74	24	39	11	

- Molecule 30 is 2-{[(4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranosyl)oxy]methyl}-4-{[(3beta,9beta,14beta,17beta,25R)-spirost-5-en-3-yl]oxy}butyl 4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranoside (three-letter code: Q7G) (formula: $C_{56}H_{92}O_{25}$).



Mol	Chain	Residues	Atoms				AltConf
30	e	1	Total	C	H	O	0
			108	38	60	10	
30	n	1	Total	C	H	O	0
			129	44	70	15	

- Molecule 31 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
31	A1	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

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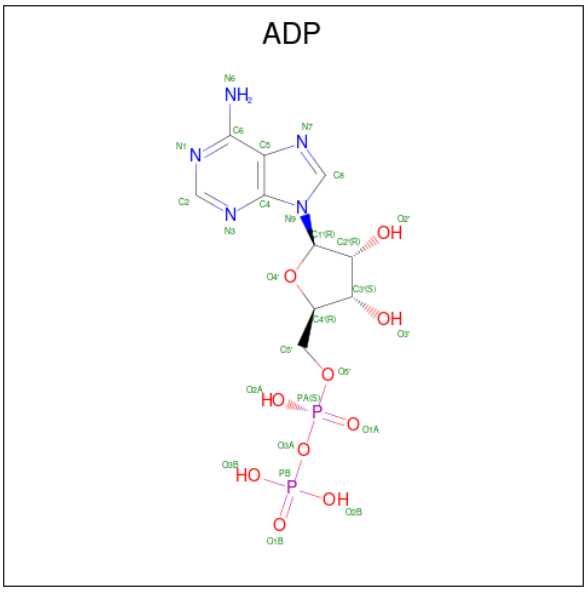
Mol	Chain	Residues	Atoms						AltConf
31	B1	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
31	C1	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
31	E1	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

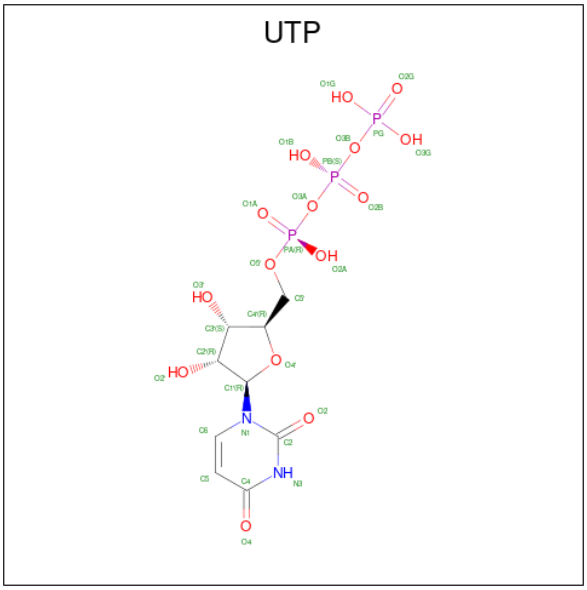
Mol	Chain	Residues	Atoms		AltConf
32	A1	1	Total	Mg	0
			1	1	
32	B1	1	Total	Mg	0
			1	1	
32	C1	1	Total	Mg	0
			1	1	
32	E1	1	Total	Mg	0
			1	1	
32	F1	1	Total	Mg	0
			1	1	

- Molecule 33 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
			Total	C	H	N	O	P	
33	F1	1	39	10	12	5	10	2	0

- Molecule 34 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$) (labeled as "Ligand of Interest" by depositor).



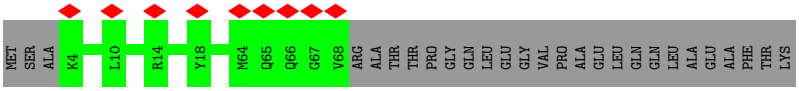
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
34	H1	1	40	9	11	2	15	3	0

3 Residue-property plots (i)

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

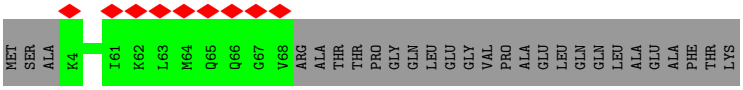
- Molecule 1: subunit-e

Chain L:



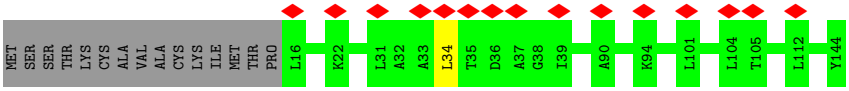
- Molecule 1: subunit-e

Chain l:



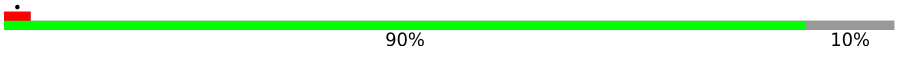
- Molecule 2: subunit-g

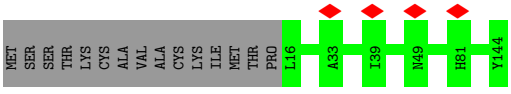
Chain M:



- Molecule 2: subunit-g

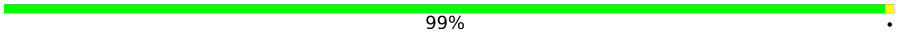
Chain m:

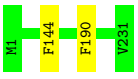




- Molecule 3: ATP synthase subunit a

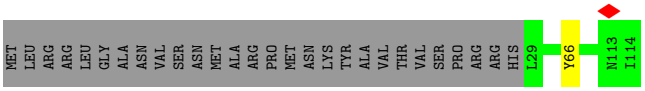
Chain a:





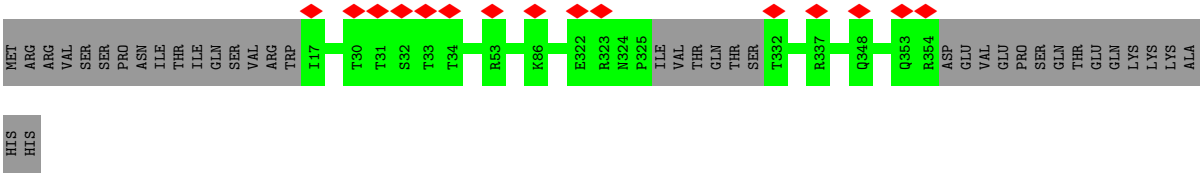
- Molecule 4: subunit-8

Chain c:



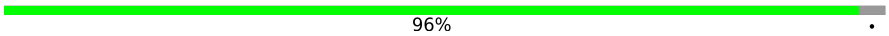
• Molecule 5: subunit-d

Chain d:



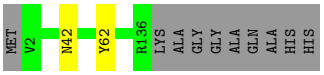
• Molecule 6: ATPTB1

Chain e:



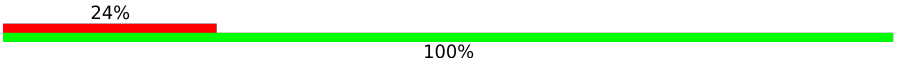
• Molecule 7: subunit-f

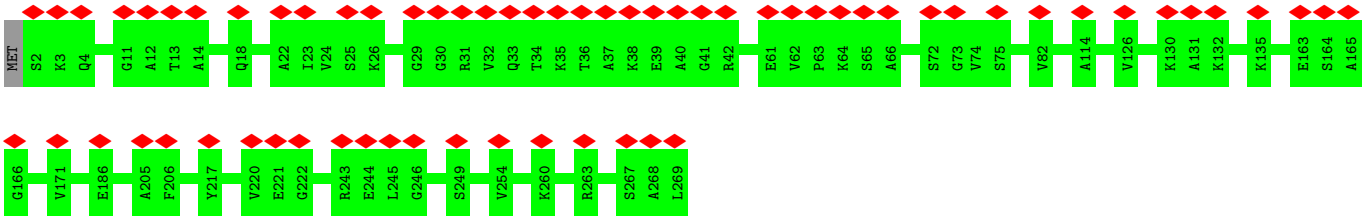
Chain f:



• Molecule 8: ATPTB3

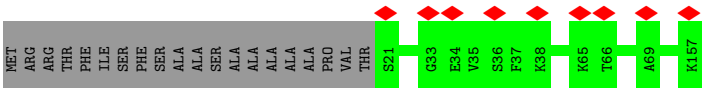
Chain g:





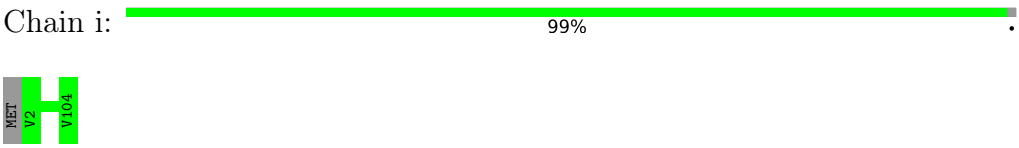
• Molecule 9: ATPTB4

Chain h:



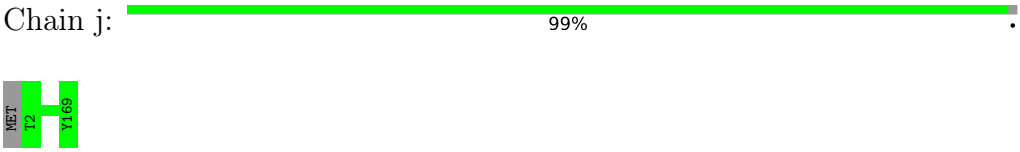
• Molecule 10: subunit-i/j

Chain i:



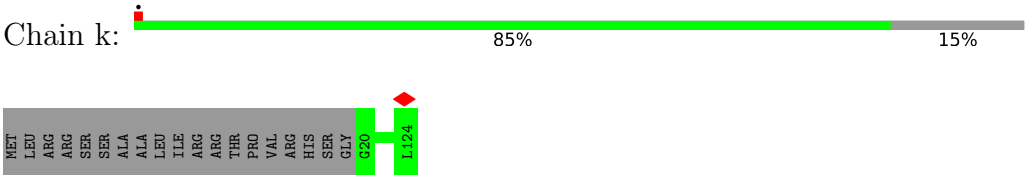
• Molecule 11: ATPTB6

Chain j:



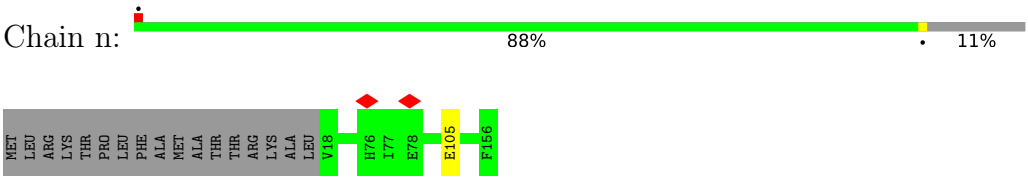
• Molecule 12: subunit-k

Chain k:



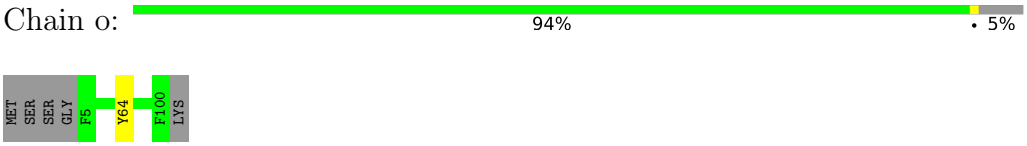
• Molecule 13: ATPTB11

Chain n:



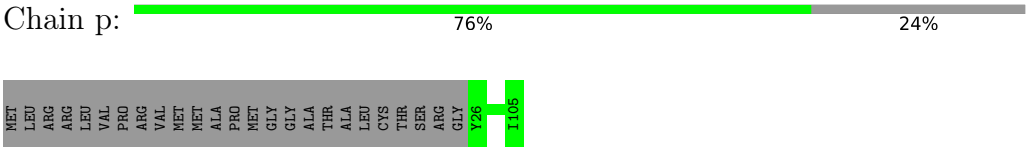
• Molecule 14: ATPTB12

Chain o:



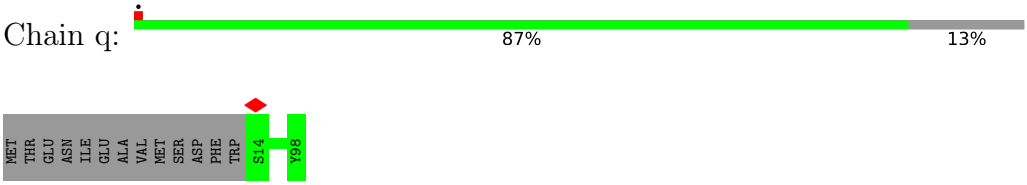
• Molecule 15: subunit-b

Chain p:



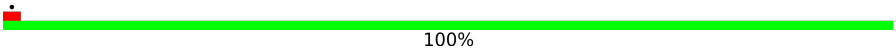
• Molecule 16: ATPEG3

Chain q:



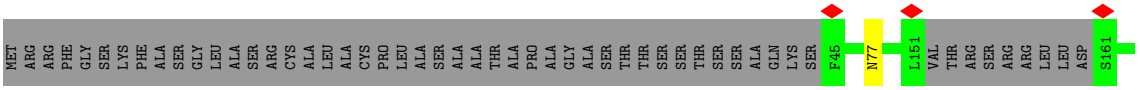
• Molecule 17: ATPEG4

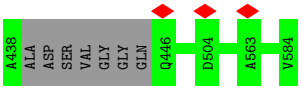
Chain r:



• Molecule 18: ATP synthase subunit alpha, mitochondrial

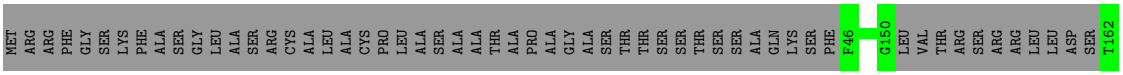
Chain A1:

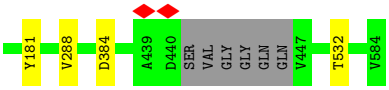




• Molecule 18: ATP synthase subunit alpha, mitochondrial

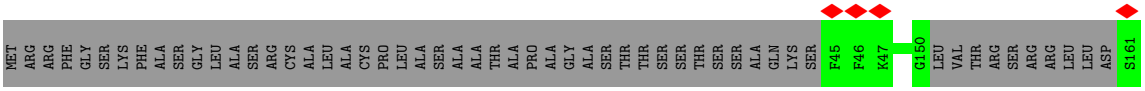
Chain B1:

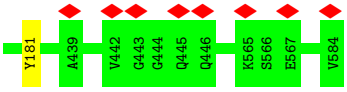




• Molecule 18: ATP synthase subunit alpha, mitochondrial

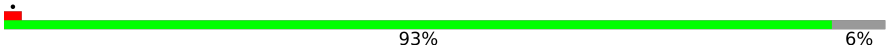
Chain C1:

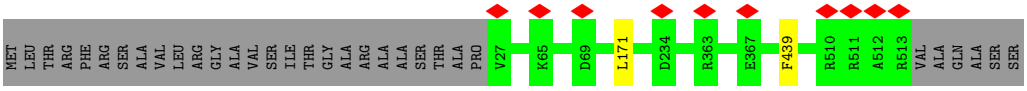




• Molecule 19: ATP synthase subunit beta, mitochondrial

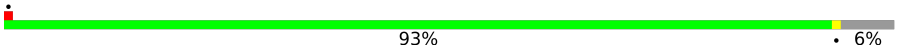
Chain D1:

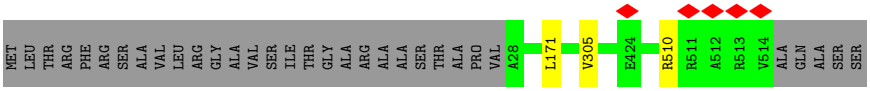




• Molecule 19: ATP synthase subunit beta, mitochondrial

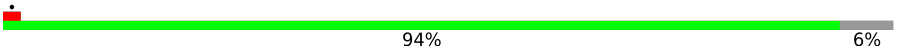
Chain E1:

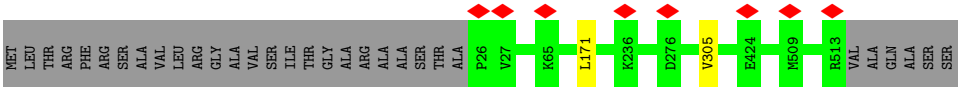




• Molecule 19: ATP synthase subunit beta, mitochondrial

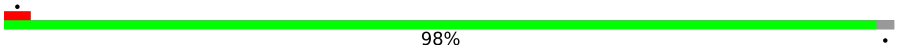
Chain F1:

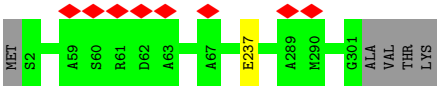




• Molecule 20: ATP synthase gamma subunit

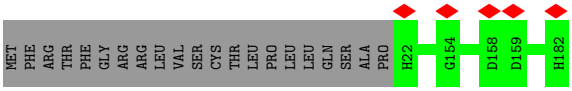
Chain G1:





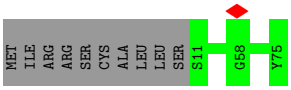
• Molecule 21: ATP synthase, epsilon chain, putative

Chain H1:



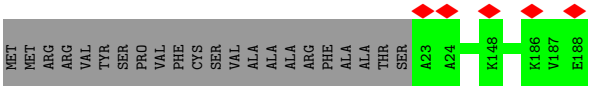
• Molecule 22: ATP synthase subunit epsilon, mitochondrial

Chain I1:



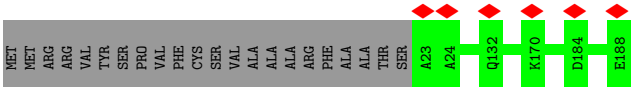
• Molecule 23: ATP synthase subunit p18, mitochondrial

Chain J1:



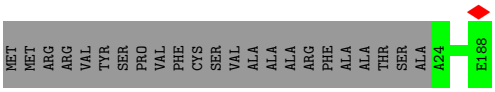
• Molecule 23: ATP synthase subunit p18, mitochondrial

Chain K1:



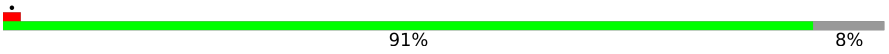
• Molecule 23: ATP synthase subunit p18, mitochondrial

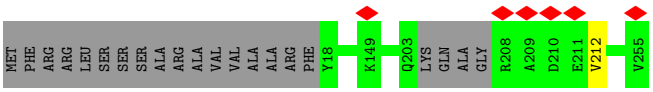
Chain L1:



• Molecule 24: OSCP

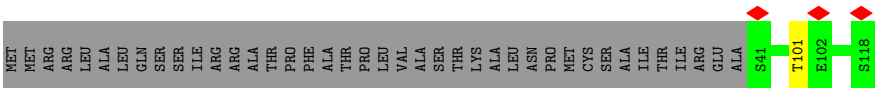
Chain M1:





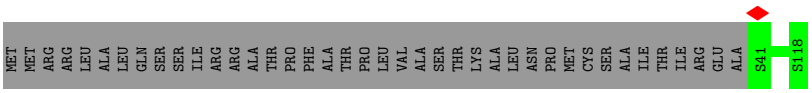
• Molecule 25: ATPase subunit 9, putative

Chain O1:



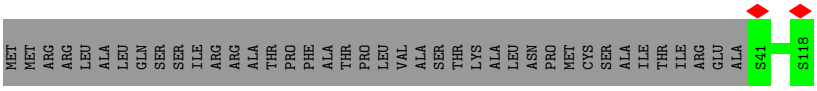
• Molecule 25: ATPase subunit 9, putative

Chain P1:



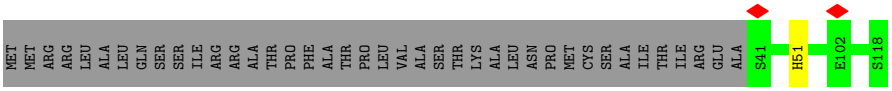
• Molecule 25: ATPase subunit 9, putative

Chain Q1:



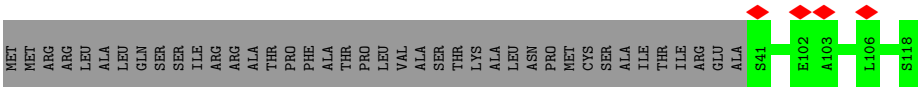
• Molecule 25: ATPase subunit 9, putative

Chain R1:



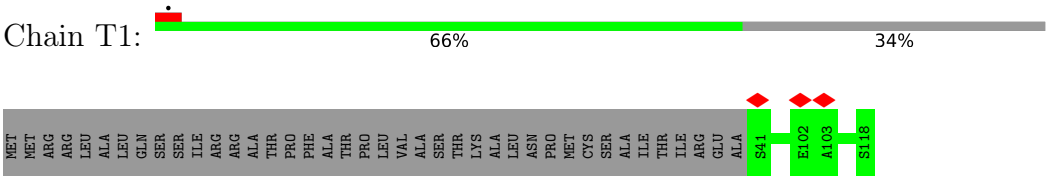
• Molecule 25: ATPase subunit 9, putative

Chain S1:



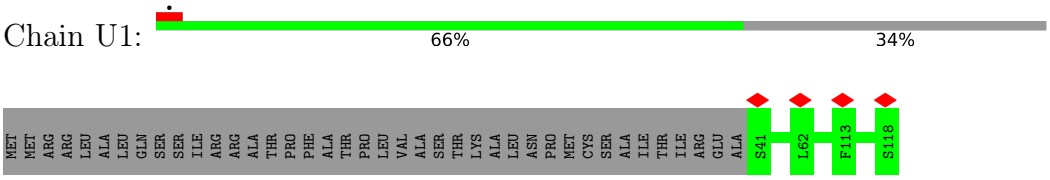
• Molecule 25: ATPase subunit 9, putative

Chain T1:



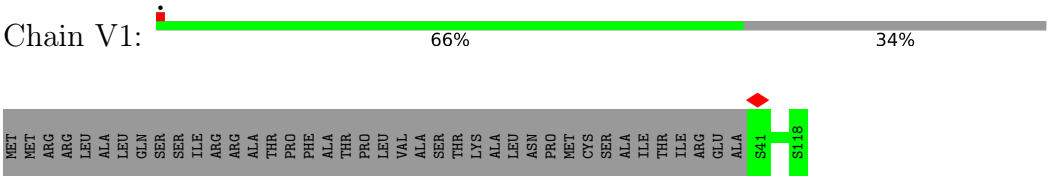
• Molecule 25: ATPase subunit 9, putative

Chain U1:



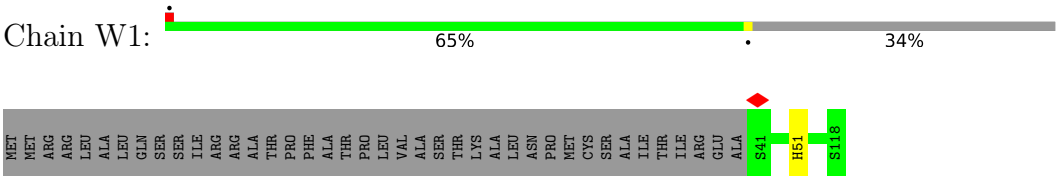
• Molecule 25: ATPase subunit 9, putative

Chain V1:



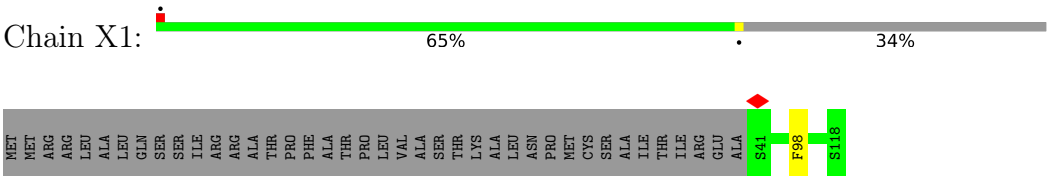
• Molecule 25: ATPase subunit 9, putative

Chain W1:



• Molecule 25: ATPase subunit 9, putative

Chain X1:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17312	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 ($e^-/Å^2$)	33	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	-0.083	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	464.8, 464.8, 464.8	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, UTP, PC1, 3PE, ADP, ATP, Q7G, AME, CDL, LMT

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	L	0.24	0/547	0.43	0/735
1	l	0.24	0/547	0.43	0/735
2	M	0.25	0/1049	0.42	0/1423
2	m	0.26	0/1049	0.42	0/1423
3	a	0.34	0/2111	0.41	0/2861
4	c	0.33	0/772	0.46	0/1054
5	d	0.25	0/2786	0.49	0/3760
6	e	0.28	0/3305	0.46	0/4482
7	f	0.30	0/1183	0.51	0/1601
8	g	0.24	0/1953	0.44	0/2650
9	h	0.24	0/1088	0.38	0/1466
10	i	0.30	0/913	0.47	0/1240
11	j	0.26	0/1462	0.48	0/1973
12	k	0.27	0/904	0.49	0/1228
13	n	0.31	0/1166	0.45	0/1581
14	o	0.26	0/814	0.39	0/1100
15	p	0.27	0/707	0.43	0/957
16	q	0.28	0/799	0.50	0/1091
17	r	0.30	0/567	0.46	0/767
18	A1	0.28	0/4122	0.47	0/5582
18	B1	0.27	0/4101	0.47	0/5553
18	C1	0.28	0/4159	0.47	0/5632
19	D1	0.27	0/3745	0.47	0/5077
19	E1	0.27	0/3745	0.47	0/5077
19	F1	0.27	0/3753	0.47	0/5088
20	G1	0.27	0/2427	0.48	0/3268
21	H1	0.27	0/1274	0.45	0/1728
22	I1	0.25	0/547	0.49	0/738
23	J1	0.24	0/1341	0.39	0/1810
23	K1	0.24	0/1342	0.39	0/1810
23	L1	0.24	0/1337	0.39	0/1803
24	M1	0.25	0/1916	0.40	0/2591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
25	O1	0.27	0/574	0.43	0/777
25	P1	0.26	0/574	0.42	0/777
25	Q1	0.26	0/574	0.41	0/777
25	R1	0.26	0/574	0.42	0/777
25	S1	0.27	0/574	0.42	0/777
25	T1	0.26	0/574	0.42	0/777
25	U1	0.26	0/574	0.42	0/777
25	V1	0.27	0/574	0.44	0/777
25	W1	0.28	0/574	0.44	0/777
25	X1	0.28	0/574	0.41	0/777
All	All	0.27	0/63271	0.45	0/85654

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	63/92 (68%)	63 (100%)	0	0	100	100
1	l	63/92 (68%)	63 (100%)	0	0	100	100
2	M	127/144 (88%)	126 (99%)	1 (1%)	0	100	100
2	m	127/144 (88%)	127 (100%)	0	0	100	100
3	a	229/231 (99%)	227 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	c	84/114 (74%)	80 (95%)	4 (5%)	0	100	100
5	d	328/370 (89%)	325 (99%)	3 (1%)	0	100	100
6	e	381/396 (96%)	373 (98%)	8 (2%)	0	100	100
7	f	133/145 (92%)	129 (97%)	4 (3%)	0	100	100
8	g	266/269 (99%)	262 (98%)	4 (2%)	0	100	100
9	h	135/157 (86%)	133 (98%)	2 (2%)	0	100	100
10	i	101/104 (97%)	100 (99%)	1 (1%)	0	100	100
11	j	166/169 (98%)	160 (96%)	6 (4%)	0	100	100
12	k	103/124 (83%)	101 (98%)	2 (2%)	0	100	100
13	n	137/156 (88%)	130 (95%)	7 (5%)	0	100	100
14	o	94/101 (93%)	94 (100%)	0	0	100	100
15	p	78/105 (74%)	76 (97%)	2 (3%)	0	100	100
16	q	83/98 (85%)	81 (98%)	2 (2%)	0	100	100
17	r	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
18	A1	518/584 (89%)	502 (97%)	16 (3%)	0	100	100
18	B1	516/584 (88%)	506 (98%)	9 (2%)	1 (0%)	47	78
18	C1	526/584 (90%)	513 (98%)	13 (2%)	0	100	100
19	D1	485/519 (93%)	476 (98%)	9 (2%)	0	100	100
19	E1	485/519 (93%)	477 (98%)	7 (1%)	1 (0%)	47	78
19	F1	486/519 (94%)	476 (98%)	9 (2%)	1 (0%)	47	78
20	G1	298/305 (98%)	297 (100%)	1 (0%)	0	100	100
21	H1	159/182 (87%)	156 (98%)	3 (2%)	0	100	100
22	I1	63/75 (84%)	62 (98%)	1 (2%)	0	100	100
23	J1	164/188 (87%)	161 (98%)	3 (2%)	0	100	100
23	K1	164/188 (87%)	157 (96%)	7 (4%)	0	100	100
23	L1	163/188 (87%)	160 (98%)	3 (2%)	0	100	100
24	M1	230/255 (90%)	224 (97%)	6 (3%)	0	100	100
25	O1	76/118 (64%)	76 (100%)	0	0	100	100
25	P1	76/118 (64%)	76 (100%)	0	0	100	100
25	Q1	76/118 (64%)	76 (100%)	0	0	100	100
25	R1	76/118 (64%)	76 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	S1	76/118 (64%)	75 (99%)	1 (1%)	0	100	100
25	T1	76/118 (64%)	76 (100%)	0	0	100	100
25	U1	76/118 (64%)	74 (97%)	2 (3%)	0	100	100
25	V1	76/118 (64%)	76 (100%)	0	0	100	100
25	W1	76/118 (64%)	76 (100%)	0	0	100	100
25	X1	76/118 (64%)	76 (100%)	0	0	100	100
All	All	7775/8943 (87%)	7633 (98%)	139 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	E1	305	VAL
19	F1	305	VAL
18	B1	532	THR

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	L	55/75 (73%)	55 (100%)	0	100	100
1	l	55/75 (73%)	55 (100%)	0	100	100
2	M	111/124 (90%)	110 (99%)	1 (1%)	78	88
2	m	111/124 (90%)	111 (100%)	0	100	100
3	a	225/225 (100%)	223 (99%)	2 (1%)	78	88
4	c	80/104 (77%)	79 (99%)	1 (1%)	69	83
5	d	297/334 (89%)	297 (100%)	0	100	100
6	e	334/341 (98%)	333 (100%)	1 (0%)	92	96
7	f	119/124 (96%)	117 (98%)	2 (2%)	60	79
8	g	205/206 (100%)	205 (100%)	0	100	100
9	h	110/123 (89%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	i	95/96 (99%)	95 (100%)	0	100	100
11	j	149/150 (99%)	149 (100%)	0	100	100
12	k	91/107 (85%)	91 (100%)	0	100	100
13	n	123/137 (90%)	122 (99%)	1 (1%)	81	89
14	o	82/86 (95%)	81 (99%)	1 (1%)	71	84
15	p	75/94 (80%)	75 (100%)	0	100	100
16	q	80/92 (87%)	80 (100%)	0	100	100
17	r	56/56 (100%)	56 (100%)	0	100	100
18	A1	436/479 (91%)	435 (100%)	1 (0%)	93	97
18	B1	433/479 (90%)	430 (99%)	3 (1%)	84	91
18	C1	439/479 (92%)	438 (100%)	1 (0%)	93	97
19	D1	398/420 (95%)	396 (100%)	2 (0%)	88	94
19	E1	398/420 (95%)	396 (100%)	2 (0%)	88	94
19	F1	399/420 (95%)	398 (100%)	1 (0%)	92	96
20	G1	253/257 (98%)	252 (100%)	1 (0%)	91	95
21	H1	137/156 (88%)	137 (100%)	0	100	100
22	I1	58/67 (87%)	58 (100%)	0	100	100
23	J1	145/162 (90%)	145 (100%)	0	100	100
23	K1	145/162 (90%)	145 (100%)	0	100	100
23	L1	145/162 (90%)	145 (100%)	0	100	100
24	M1	200/215 (93%)	199 (100%)	1 (0%)	88	94
25	O1	56/89 (63%)	55 (98%)	1 (2%)	59	77
25	P1	56/89 (63%)	56 (100%)	0	100	100
25	Q1	56/89 (63%)	56 (100%)	0	100	100
25	R1	56/89 (63%)	55 (98%)	1 (2%)	59	77
25	S1	56/89 (63%)	56 (100%)	0	100	100
25	T1	56/89 (63%)	56 (100%)	0	100	100
25	U1	56/89 (63%)	56 (100%)	0	100	100
25	V1	56/89 (63%)	56 (100%)	0	100	100
25	W1	56/89 (63%)	55 (98%)	1 (2%)	59	77
25	X1	56/89 (63%)	55 (98%)	1 (2%)	59	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6599/7441 (89%)	6574 (100%)	25 (0%)	91 95

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	D1	171	LEU
19	E1	510	ARG
25	X1	98	PHE
19	E1	171	LEU
19	F1	171	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
20	G1	207	GLN
25	O1	48	GLN
23	J1	93	ASN
23	L1	111	ASN
25	O1	83	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
6	AME	e	1	6	9,10,11	0.26	0	9,11,13	0.48	0

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
6	AME	e	1	6	-	4/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	e	1	AME	CT2-CT1-N-CA
6	e	1	AME	OT-CT1-N-CA
6	e	1	AME	CA-CB-CG-SD
6	e	1	AME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 5 are monoatomic - leaving 31 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
26	CDL	e	401	-	99,99,99	0.29	0	105,111,111	0.26	0
28	PC1	i	201	-	53,53,53	0.29	0	59,61,61	0.28	0
34	UTP	H1	201	-	22,30,30	0.92	1 (4%)	27,47,47	0.86	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CDL	c	201	-	99,99,99	0.29	0	105,111,111	0.27	0
30	Q7G	e	406	-	54,54,90	0.14	0	82,84,138	0.30	0
26	CDL	f	201	-	99,99,99	0.30	0	105,111,111	0.27	0
26	CDL	q	101	-	99,99,99	0.29	0	105,111,111	0.29	0
30	Q7G	n	201	-	66,66,90	0.13	0	100,102,138	0.28	0
26	CDL	m	201	-	99,99,99	0.29	0	105,111,111	0.25	0
29	LMT	j	203	-	36,36,36	0.12	0	47,47,47	0.18	0
26	CDL	M	201	-	99,99,99	0.29	0	105,111,111	0.25	0
26	CDL	k	201	-	99,99,99	0.29	0	105,111,111	0.25	0
31	ATP	E1	601	32	26,33,33	0.63	0	31,52,52	0.62	1 (3%)
28	PC1	j	202	-	53,53,53	0.28	0	59,61,61	0.27	0
33	ADP	F1	601	32	24,29,29	0.75	0	29,45,45	0.80	1 (3%)
26	CDL	a	301	-	99,99,99	0.29	0	105,111,111	0.26	0
26	CDL	l	101	-	99,99,99	0.30	0	105,111,111	0.26	0
26	CDL	M	202	-	99,99,99	0.30	0	105,111,111	0.25	0
26	CDL	e	403	-	99,99,99	0.29	0	105,111,111	0.26	0
31	ATP	B1	601	32	26,33,33	0.63	0	31,52,52	0.62	1 (3%)
31	ATP	C1	601	32	26,33,33	0.63	0	31,52,52	0.64	1 (3%)
26	CDL	j	201	-	99,99,99	0.29	0	105,111,111	0.26	0
27	3PE	f	202	-	50,50,50	0.27	0	53,55,55	0.22	0
27	3PE	M	203	-	50,50,50	0.26	0	53,55,55	0.23	0
28	PC1	a	302	-	53,53,53	0.28	0	59,61,61	0.27	0
29	LMT	e	405	-	36,36,36	0.11	0	47,47,47	0.15	0
26	CDL	e	404	-	99,99,99	0.30	0	105,111,111	0.26	0
28	PC1	p	201	-	53,53,53	0.29	0	59,61,61	0.28	0
27	3PE	m	202	-	50,50,50	0.25	0	53,55,55	0.23	0
31	ATP	A1	601	32	26,33,33	0.63	0	31,52,52	0.62	1 (3%)
26	CDL	e	402	-	99,99,99	0.29	0	105,111,111	0.26	0

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
26	CDL	e	401	-	-	18/110/110/110	-
28	PC1	i	201	-	-	8/57/57/57	-
34	UTP	H1	201	-	-	4/20/38/38	0/2/2/2
30	Q7G	e	406	-	1/1/19/34	5/15/123/200	0/7/7/10
26	CDL	c	201	-	-	22/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CDL	f	201	-	-	25/110/110/110	-
30	Q7G	n	201	-	2/2/24/34	5/20/148/200	0/8/8/10
26	CDL	q	101	-	-	34/110/110/110	-
26	CDL	m	201	-	-	25/110/110/110	-
29	LMT	j	203	-	-	5/21/61/61	0/2/2/2
26	CDL	M	201	-	-	16/110/110/110	-
26	CDL	k	201	-	-	26/110/110/110	-
31	ATP	E1	601	32	-	6/18/38/38	0/3/3/3
28	PC1	j	202	-	-	10/57/57/57	-
33	ADP	F1	601	32	-	2/12/32/32	0/3/3/3
26	CDL	a	301	-	-	26/110/110/110	-
26	CDL	l	101	-	-	13/110/110/110	-
26	CDL	M	202	-	-	30/110/110/110	-
26	CDL	e	403	-	-	27/110/110/110	-
31	ATP	B1	601	32	-	3/18/38/38	0/3/3/3
31	ATP	C1	601	32	-	4/18/38/38	0/3/3/3
26	CDL	j	201	-	-	24/110/110/110	-
27	3PE	f	202	-	-	12/54/54/54	-
27	3PE	M	203	-	-	16/54/54/54	-
28	PC1	a	302	-	-	9/57/57/57	-
29	LMT	e	405	-	-	1/21/61/61	0/2/2/2
26	CDL	e	404	-	-	17/110/110/110	-
28	PC1	p	201	-	-	5/57/57/57	-
27	3PE	m	202	-	-	9/54/54/54	-
31	ATP	A1	601	32	-	5/18/38/38	0/3/3/3
26	CDL	e	402	-	-	24/110/110/110	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	H1	201	UTP	C4-N3	3.07	1.38	1.33

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	H1	201	UTP	C5-C4-N3	-3.90	114.72	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C1	601	ATP	C5-C6-N6	2.33	123.89	120.35
31	A1	601	ATP	C5-C6-N6	2.31	123.87	120.35
31	E1	601	ATP	C5-C6-N6	2.29	123.83	120.35
31	B1	601	ATP	C5-C6-N6	2.29	123.83	120.35

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
30	e	406	Q7G	C1B
30	n	201	Q7G	C1C
30	n	201	Q7G	C1B

5 of 436 torsion outliers are listed below:

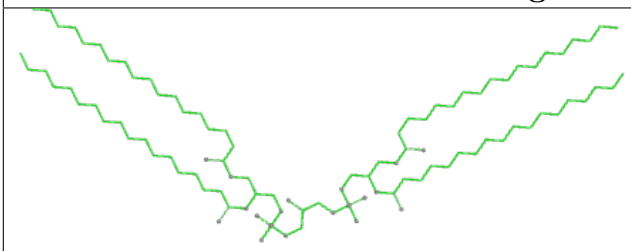
Mol	Chain	Res	Type	Atoms
26	M	202	CDL	CA3-OA5-PA1-OA3
26	M	202	CDL	CB2-OB2-PB2-OB3
26	M	202	CDL	CB2-OB2-PB2-OB5
26	M	202	CDL	C51-CB5-OB6-CB4
26	a	301	CDL	CA3-OA5-PA1-OA3

There are no ring outliers.

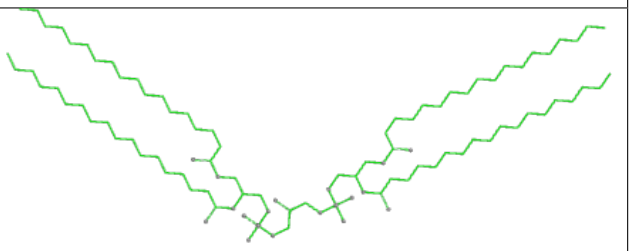
No monomer is involved in short contacts.

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.

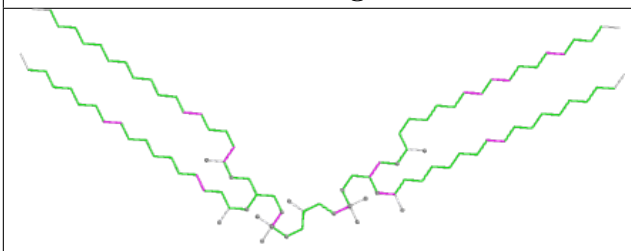
Ligand CDL e 401



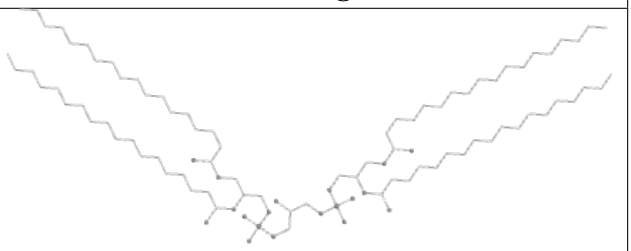
Bond lengths



Bond angles

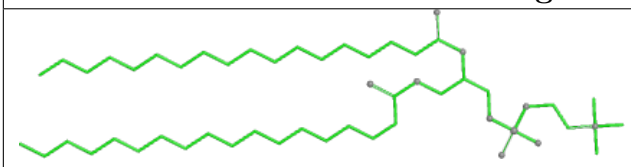


Torsions

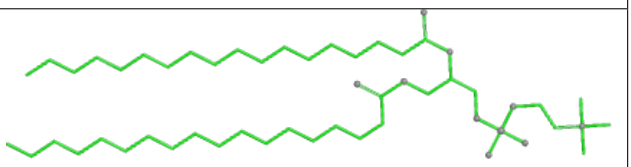


Rings

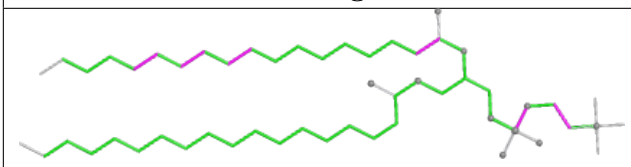
Ligand PC1 i 201



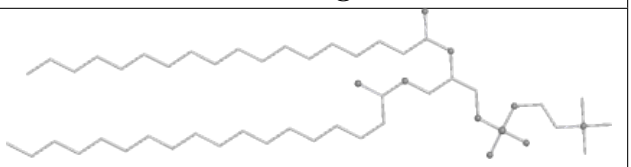
Bond lengths



Bond angles

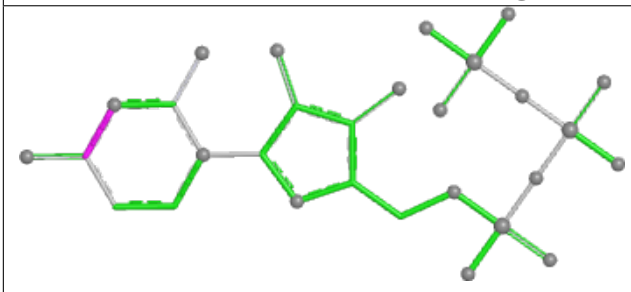


Torsions



Rings

Ligand UTP H1 201



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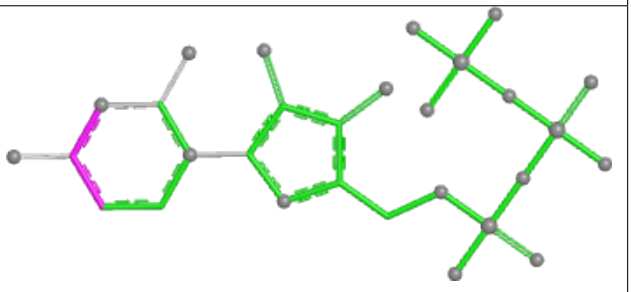

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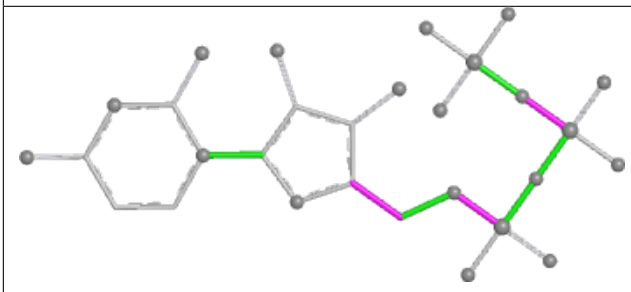

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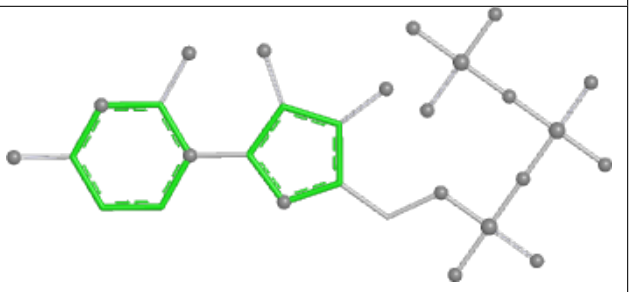
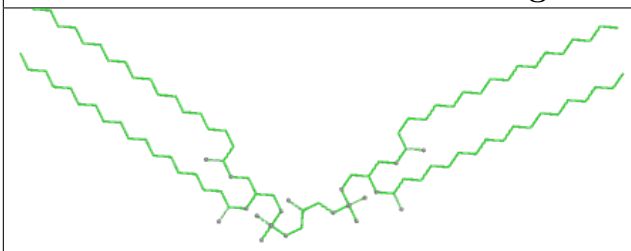


Rings

Ligand CDL c 201



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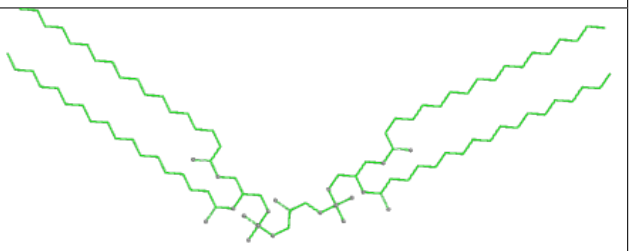

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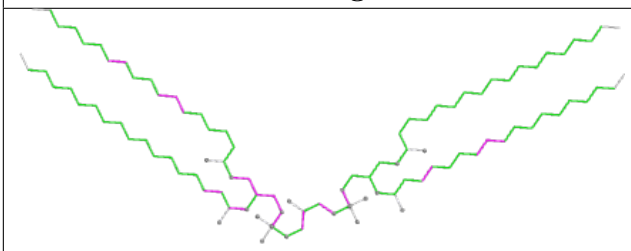

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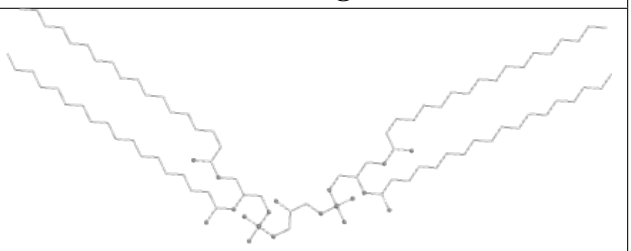
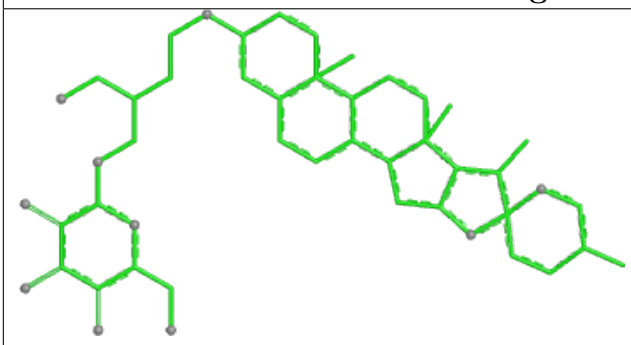


Rings

Ligand Q7G e 406



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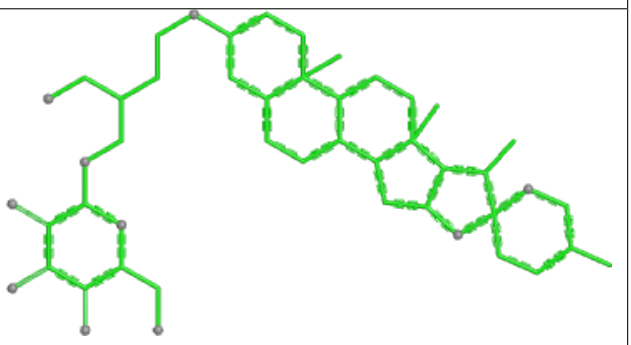

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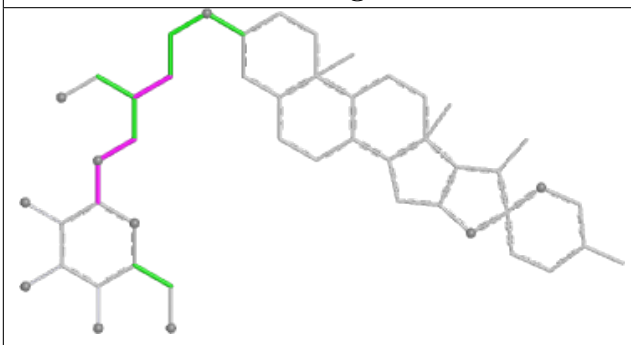

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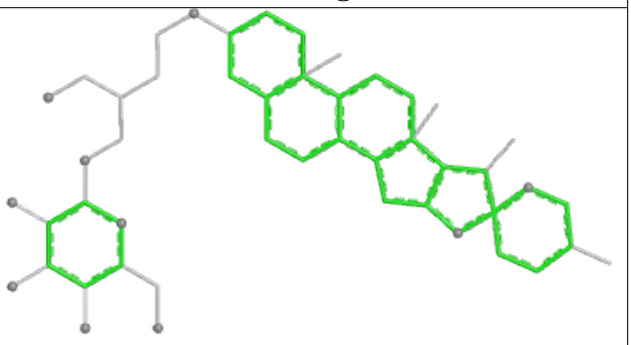
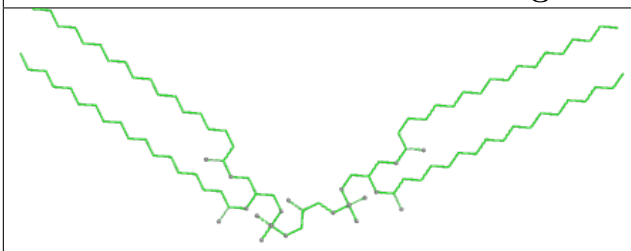


Rings

Ligand CDL f 201



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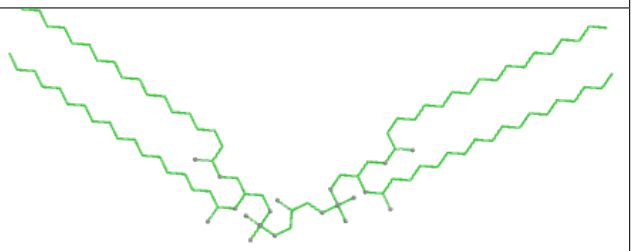

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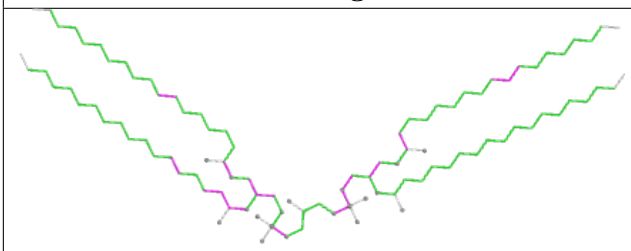

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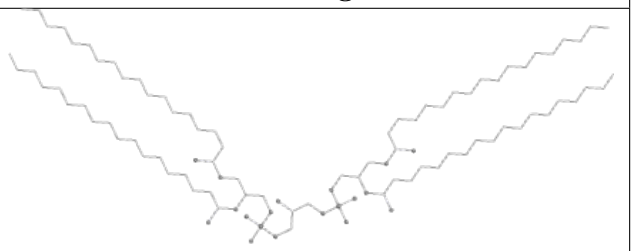
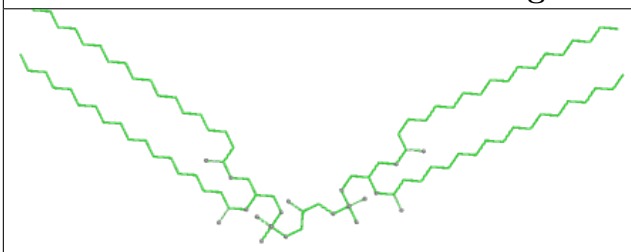


Rings

Ligand CDL q 101



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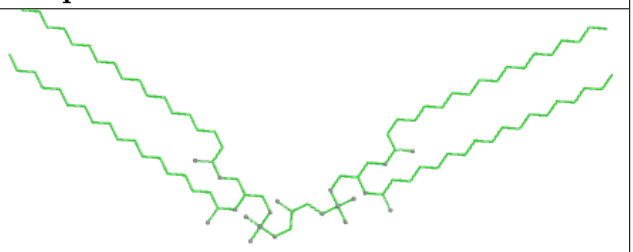

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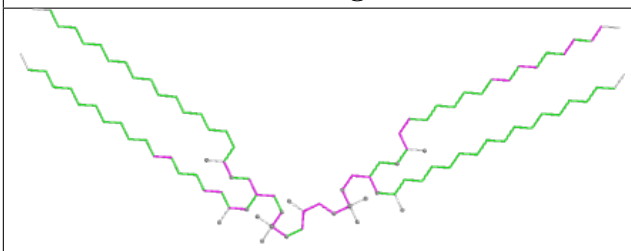

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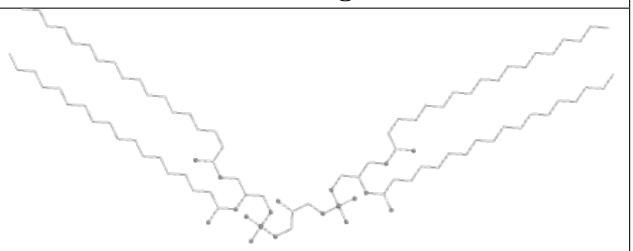
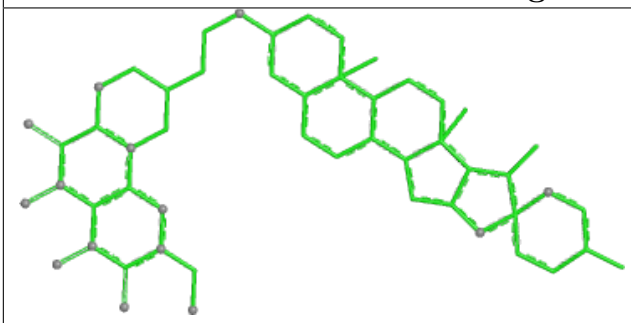


Rings

Ligand Q7G n 201



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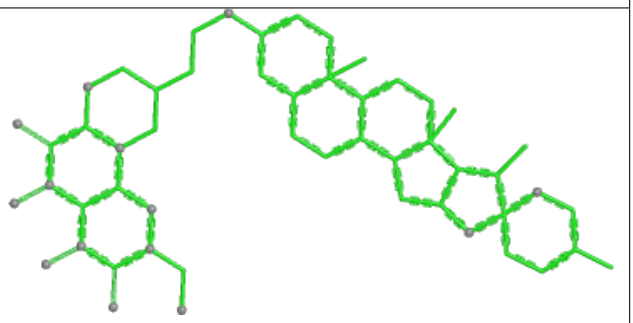

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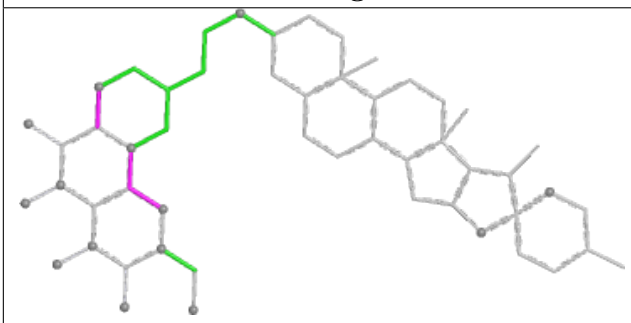

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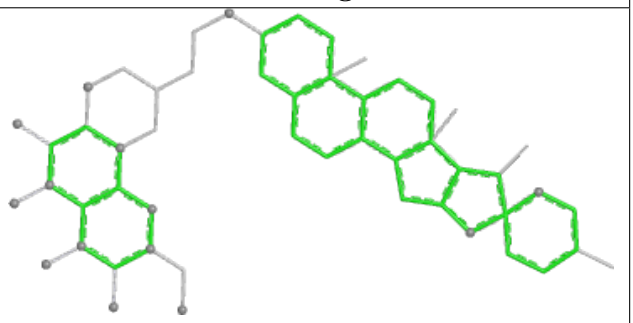
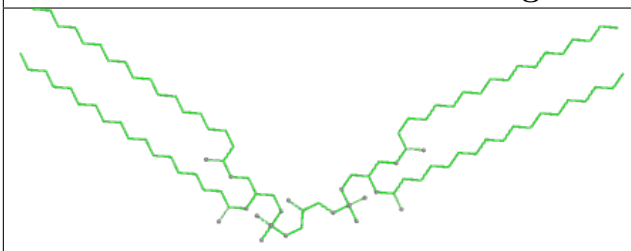


Rings

Ligand CDL m 201



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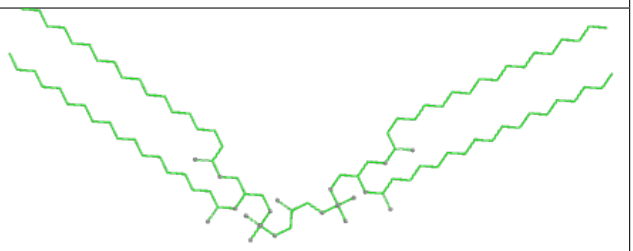
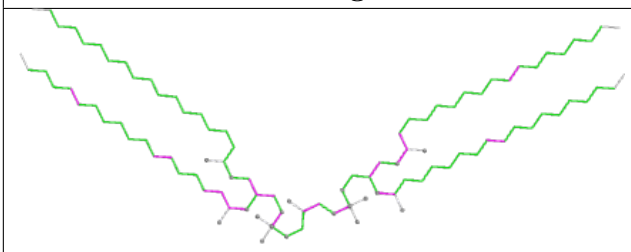


Bond angles



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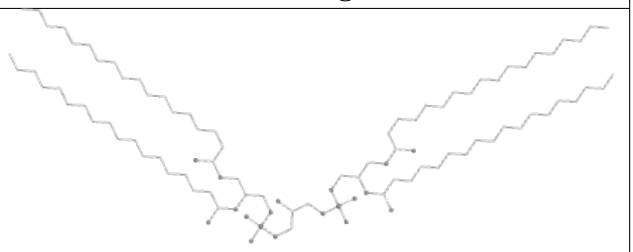
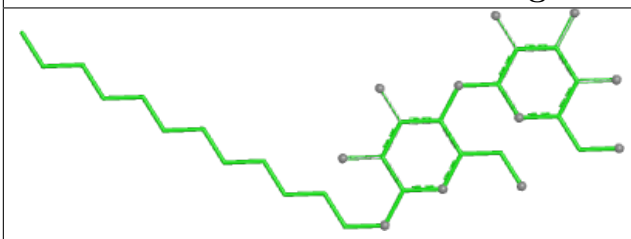


Rings

Ligand LMT j 203



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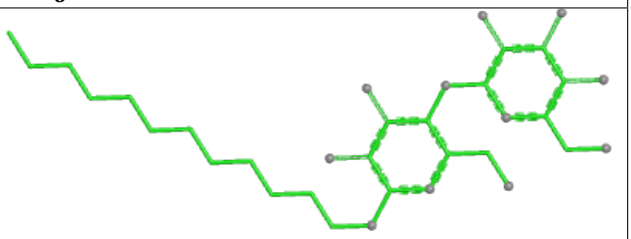

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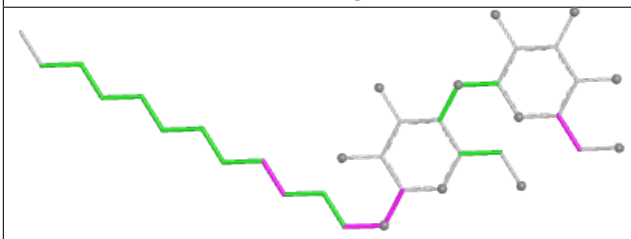

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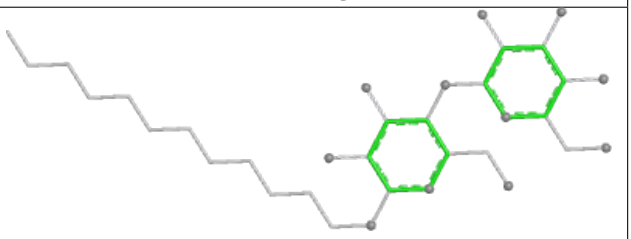
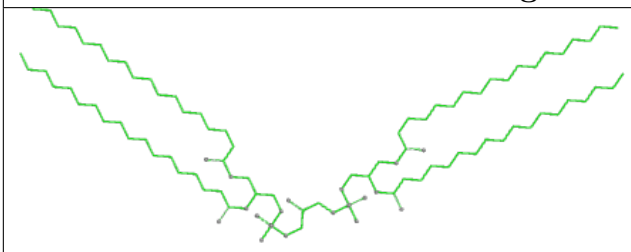


Rings

Ligand CDL M 201



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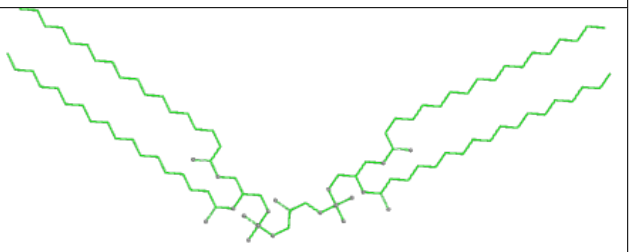

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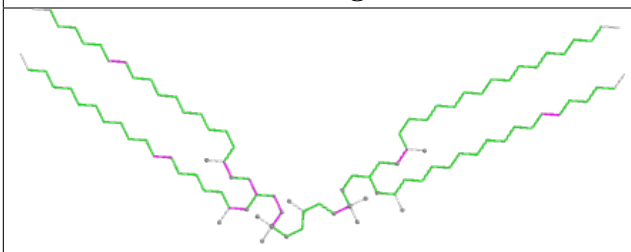

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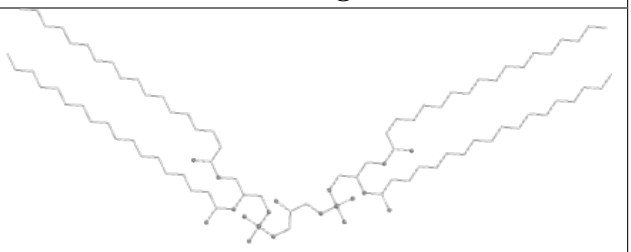
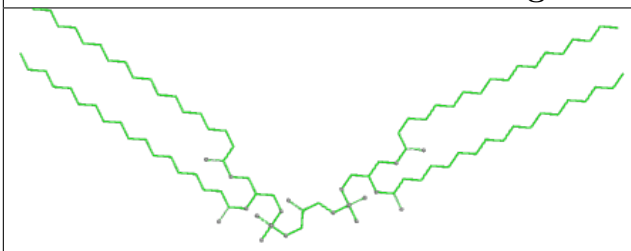


Rings

Ligand CDL k 201



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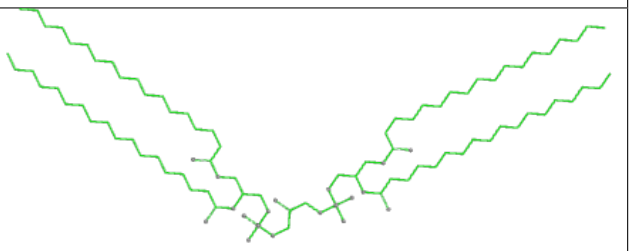

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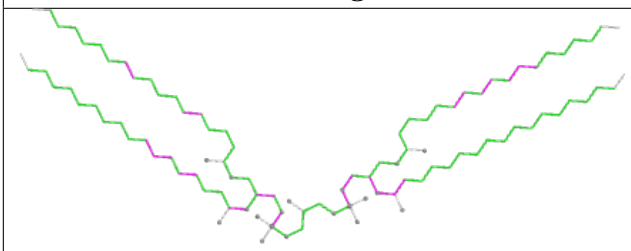

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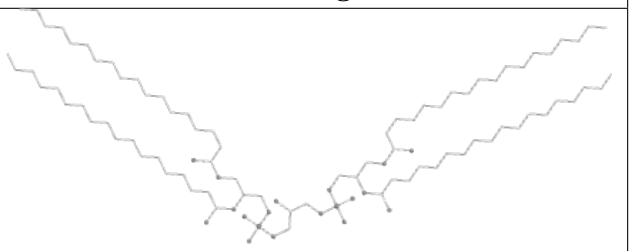
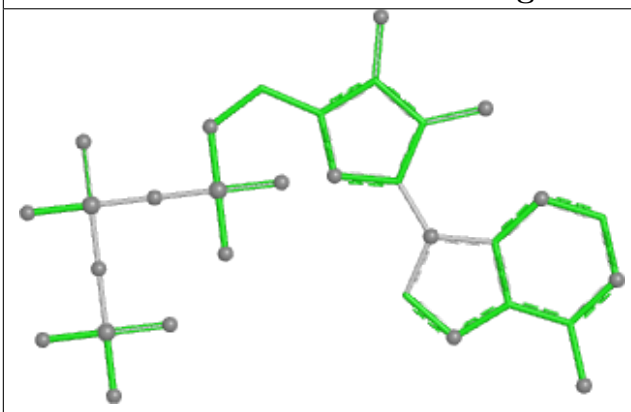


Rings

Ligand ATP E1 601



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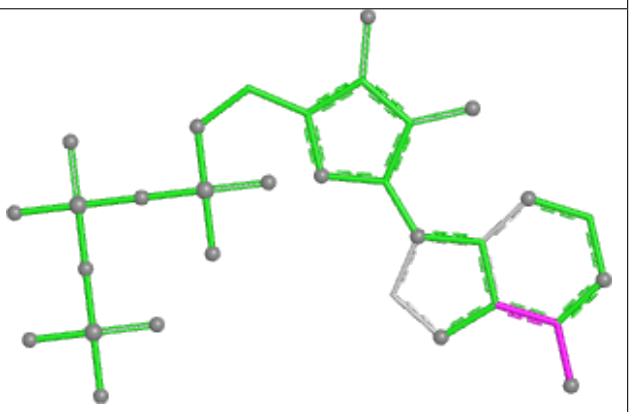
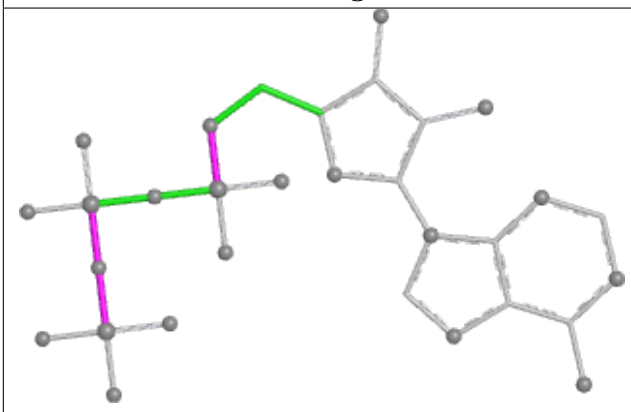


Bond angles



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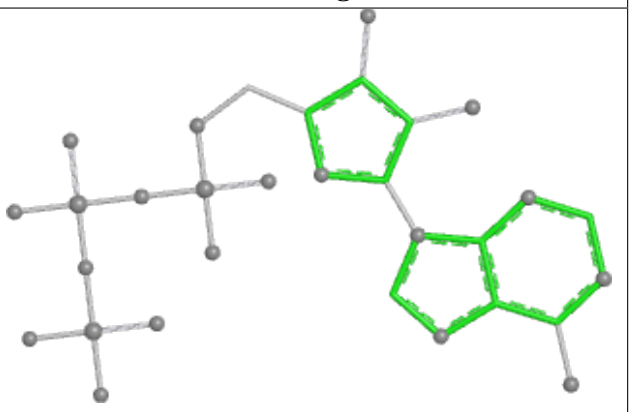
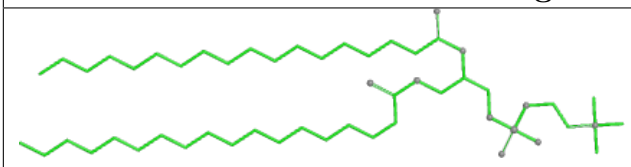
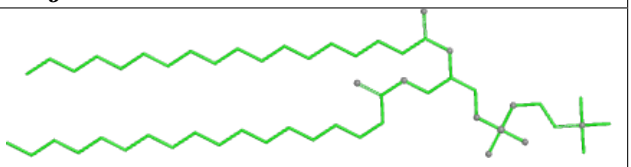
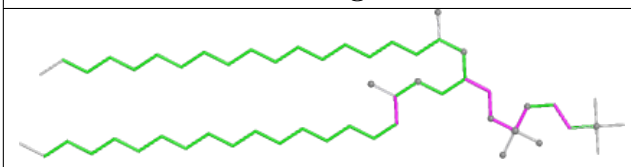
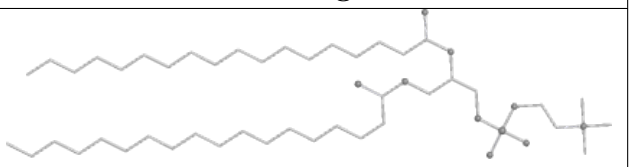
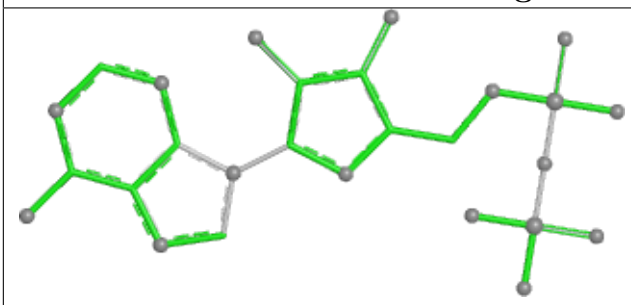
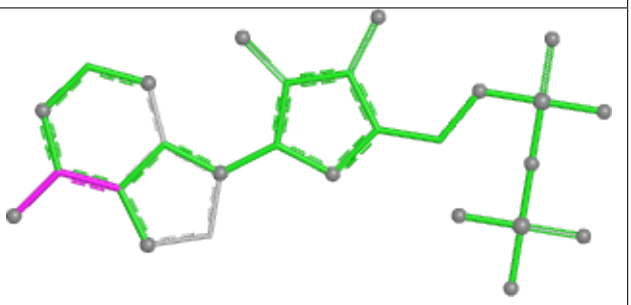
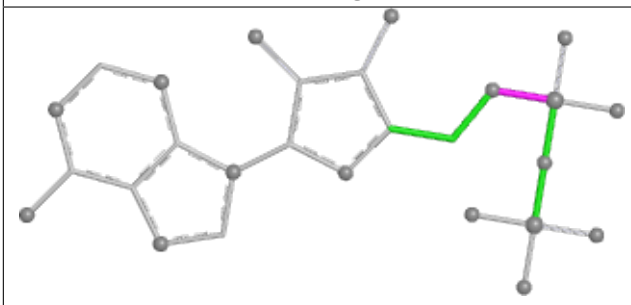
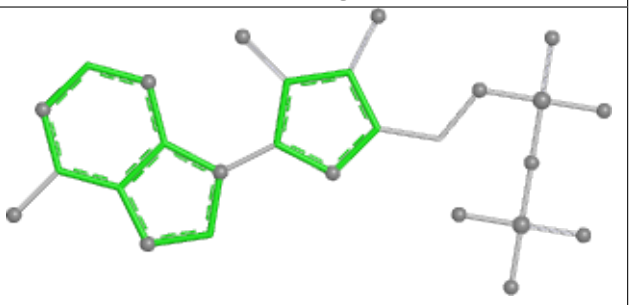
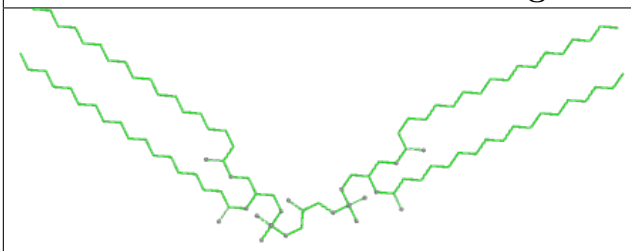


Rings

Ligand PC1 j 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP F1 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL a 301



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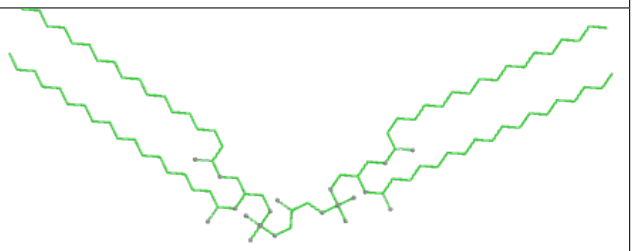
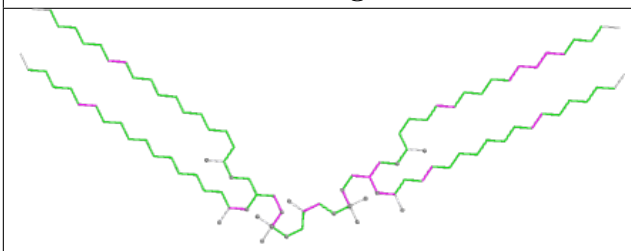
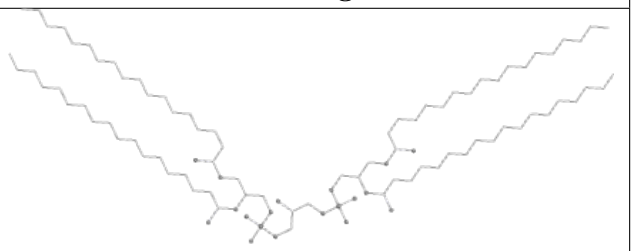


Bond angles

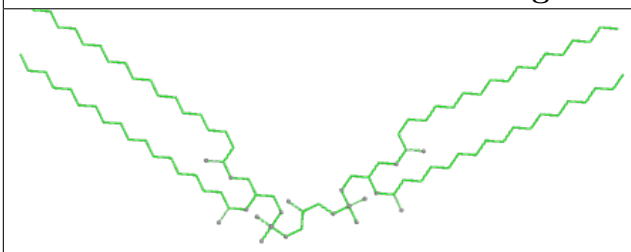


Torsions



Rings

Ligand CDL l 101



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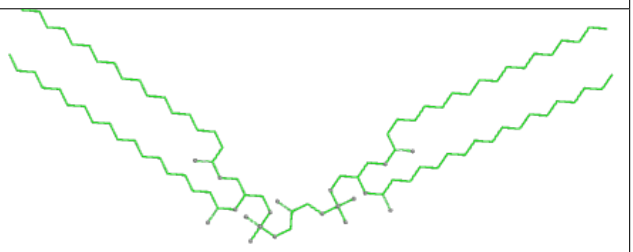

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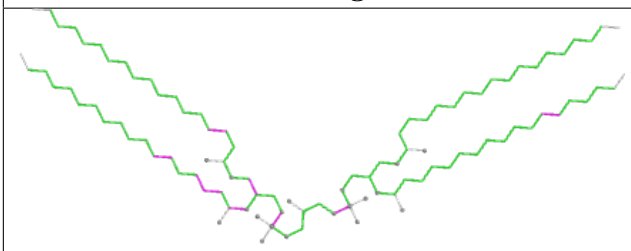

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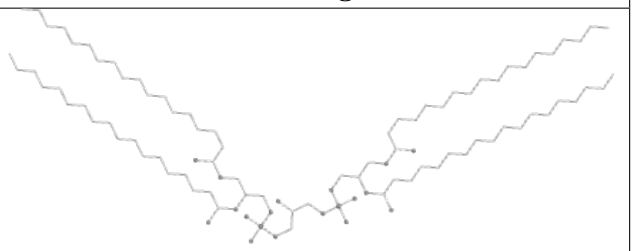
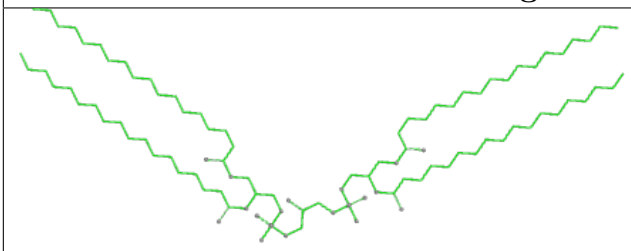


Rings

Ligand CDL M 202



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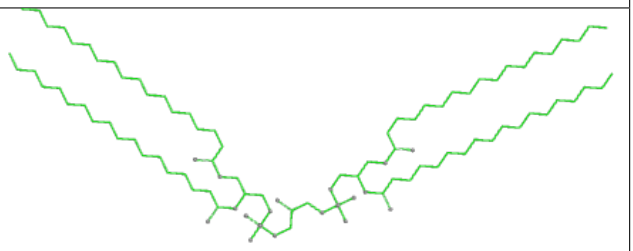

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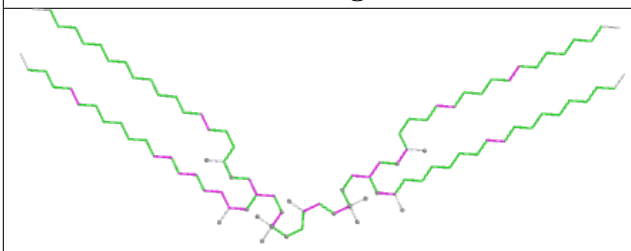

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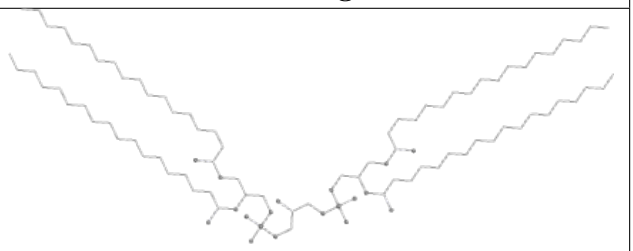
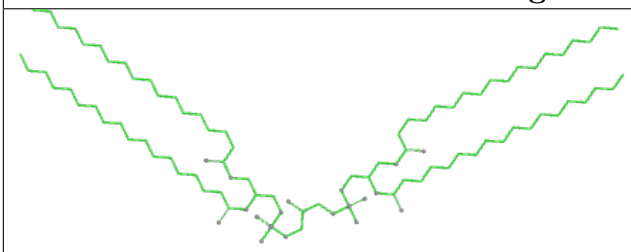


Rings

Ligand CDL e 403



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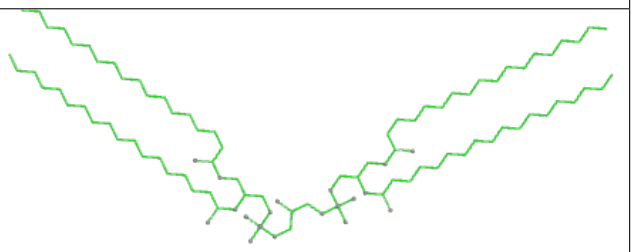

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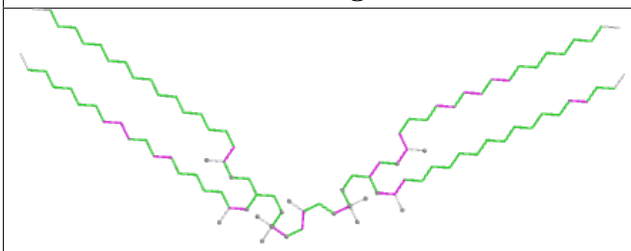

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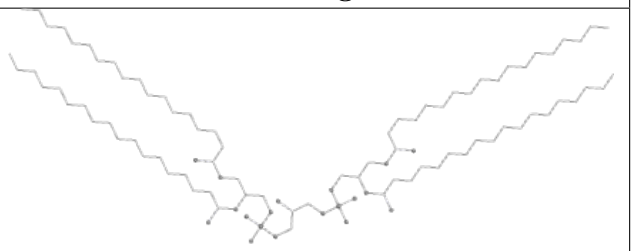
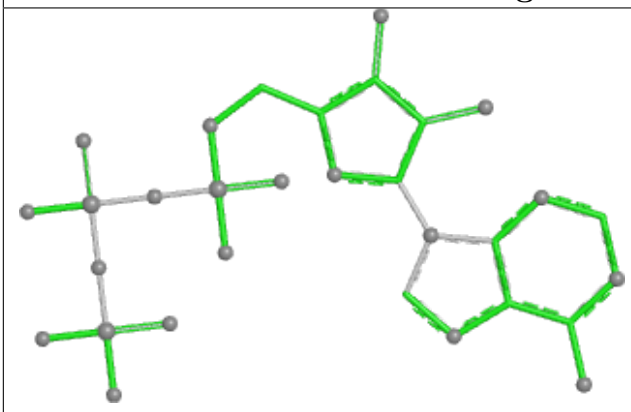


Rings

Ligand ATP B1 601



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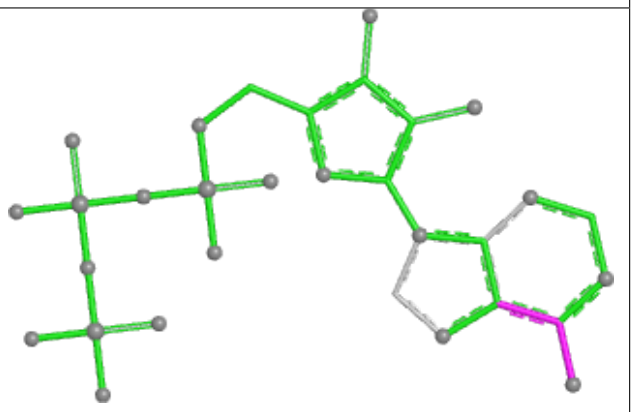

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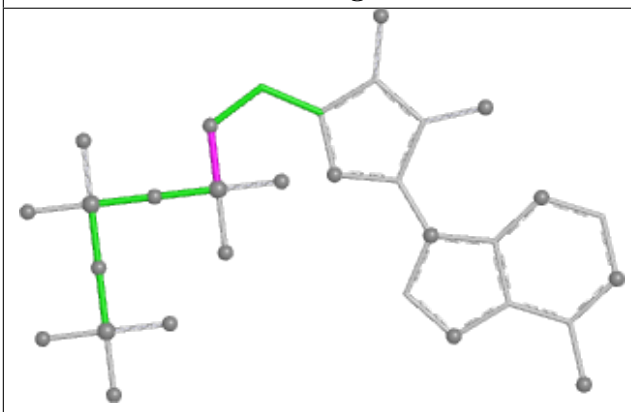

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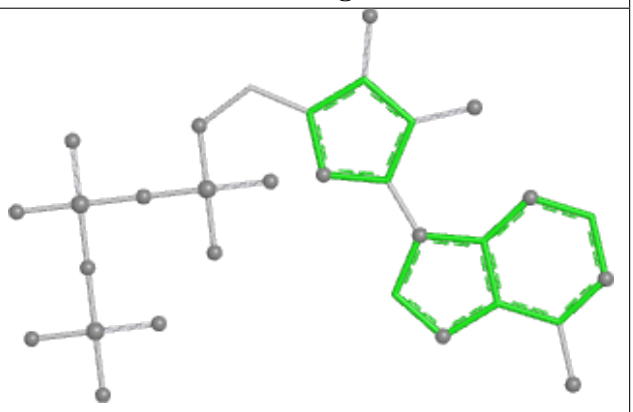
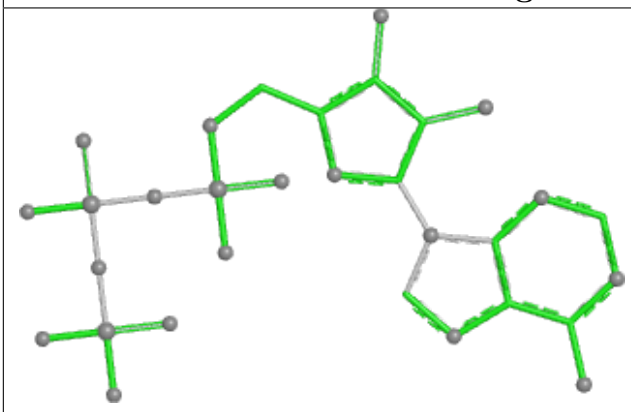


Rings

Ligand ATP C1 601



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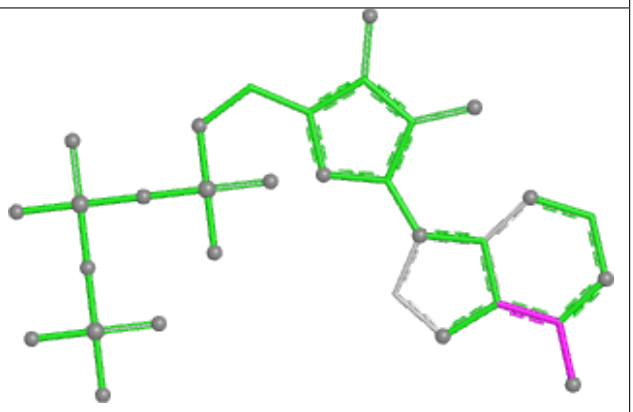

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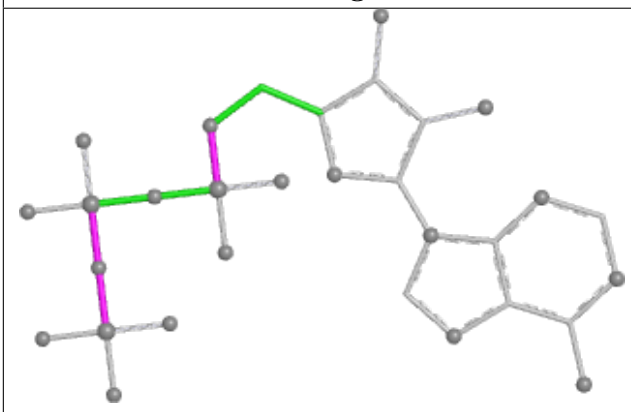

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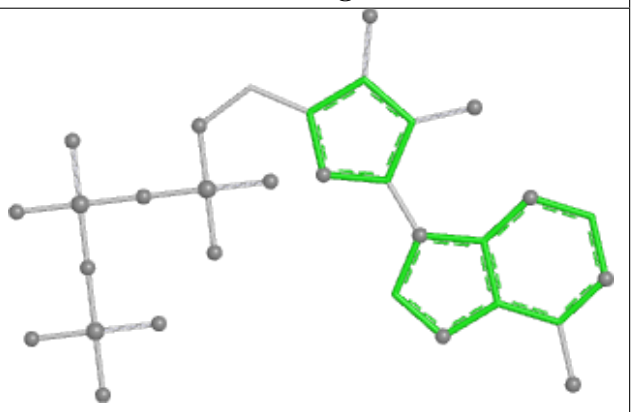
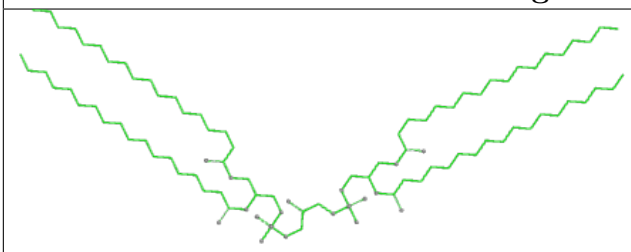


Rings

Ligand CDL j 201



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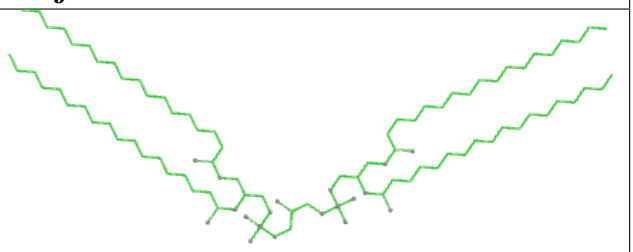

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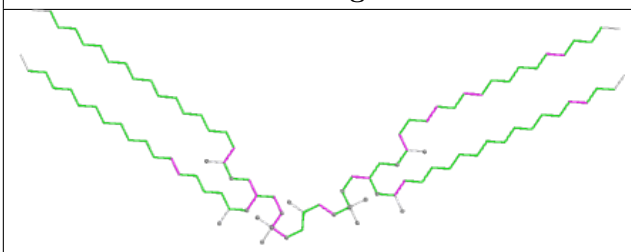

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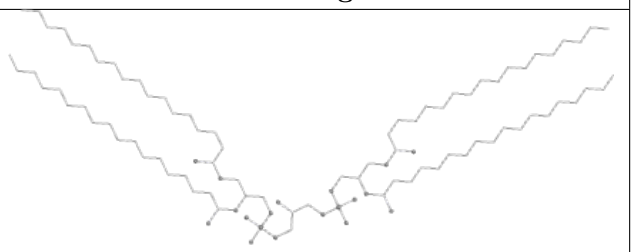
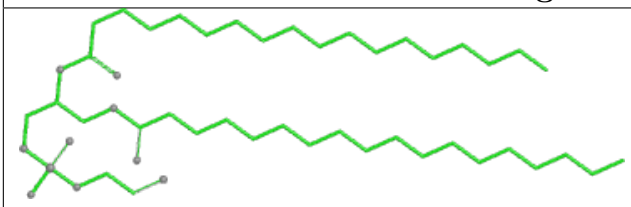


Rings

Ligand 3PE f 202



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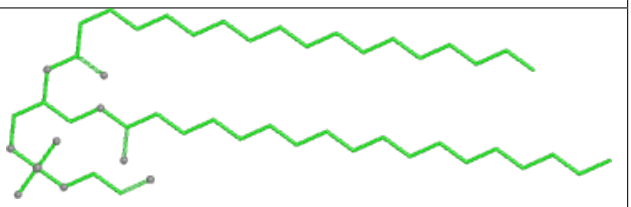

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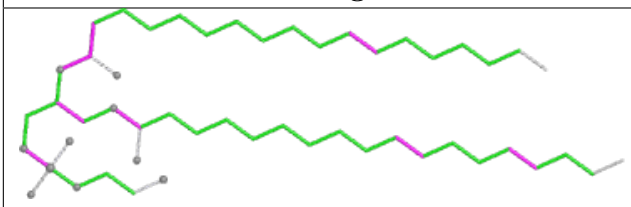

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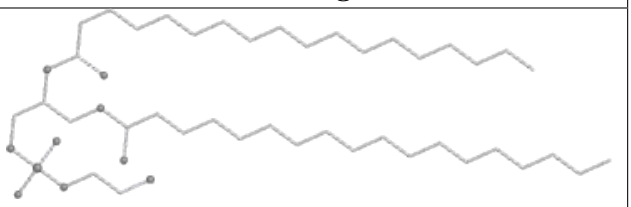
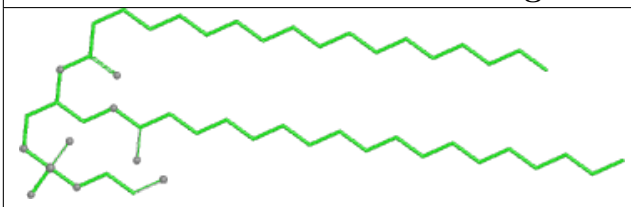


Rings

Ligand 3PE M 203



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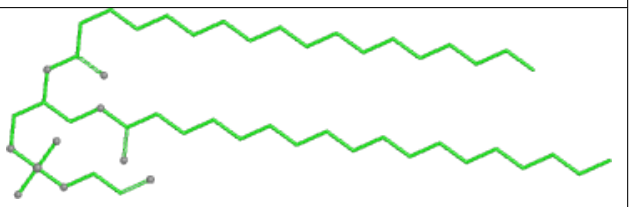

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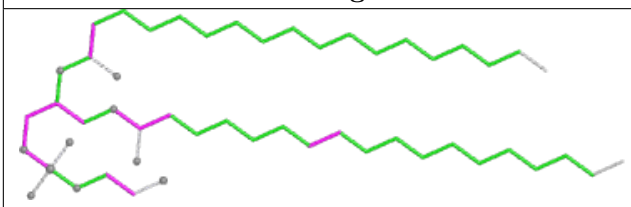

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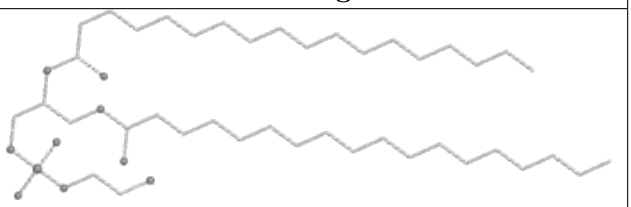
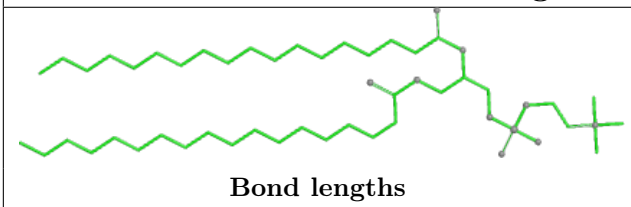


Rings

Ligand PC1 a 302



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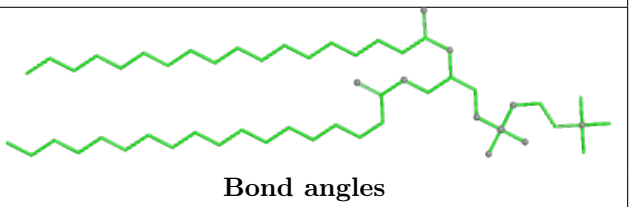
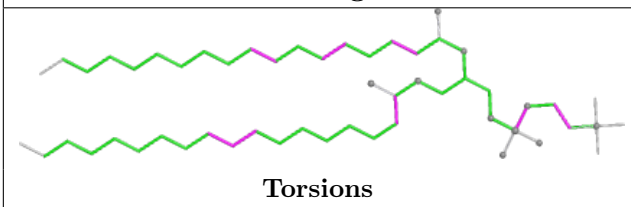


Bond angles



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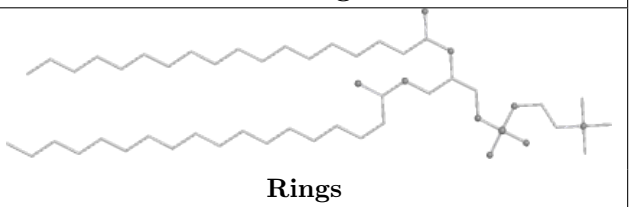
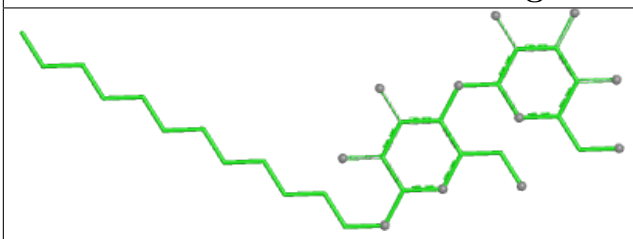


Rings

Ligand LMT e 405



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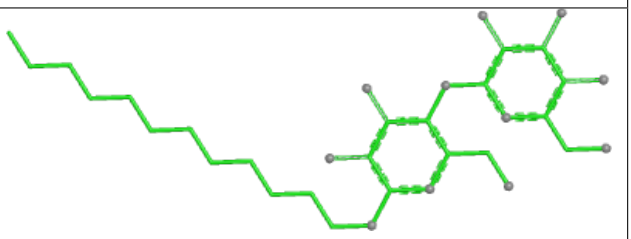
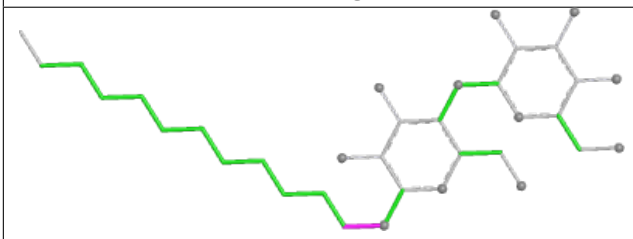


Bond angles



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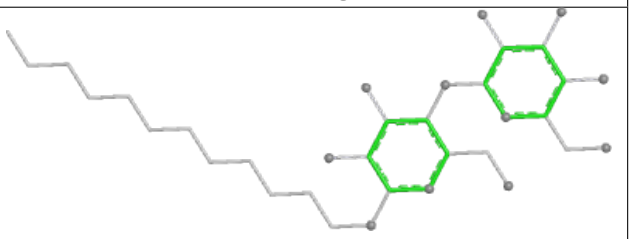
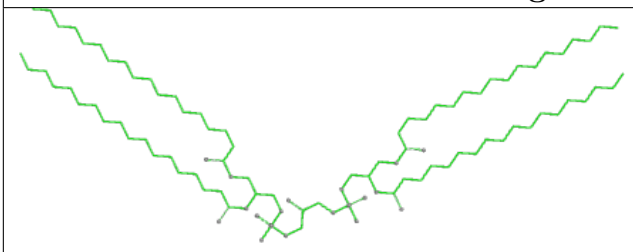


Rings

Ligand CDL e 404



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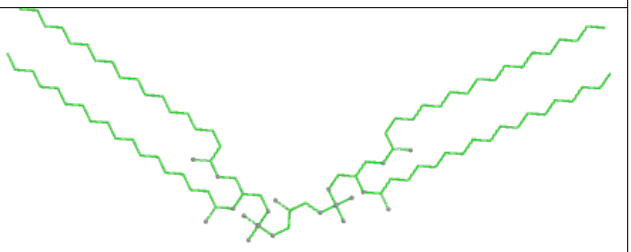
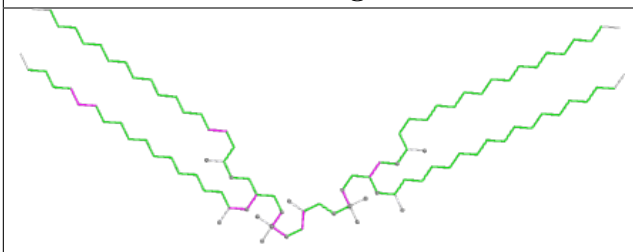


Bond angles



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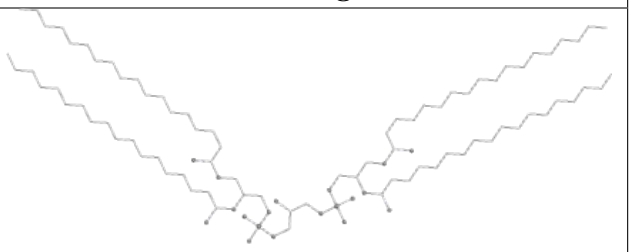
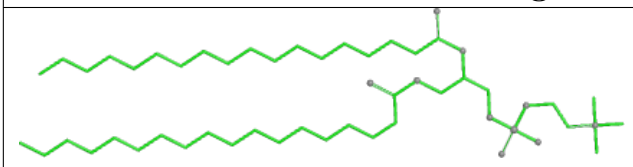


Rings

Ligand PC1 p 201



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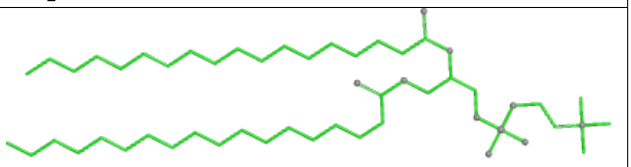

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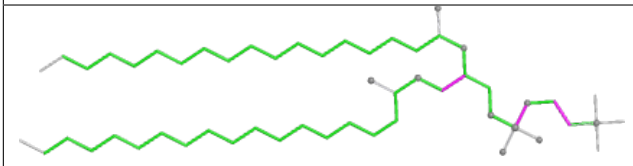

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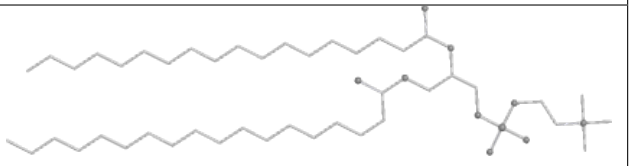
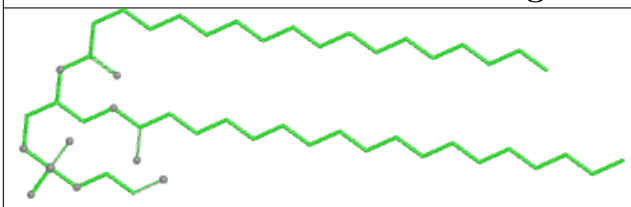


Rings

Ligand 3PE m 202



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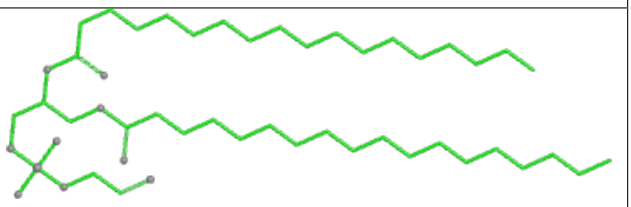
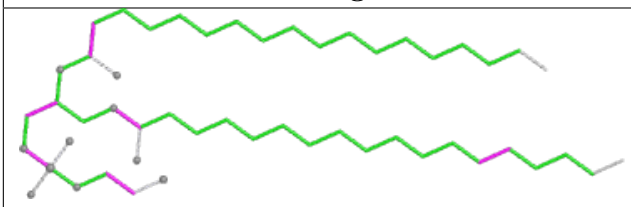


Bond angles



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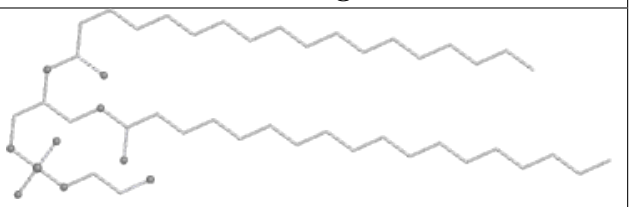
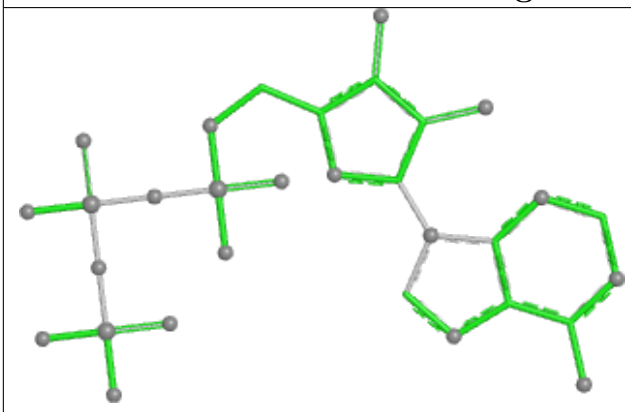


Rings

Ligand ATP A1 601



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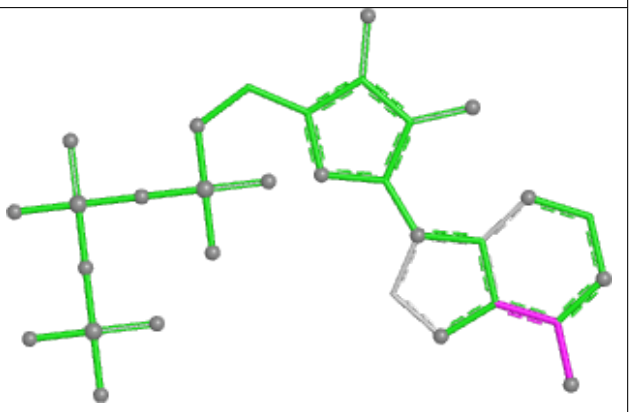
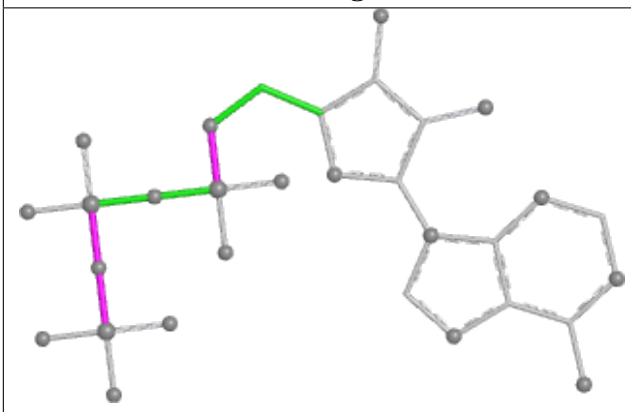


Bond angles



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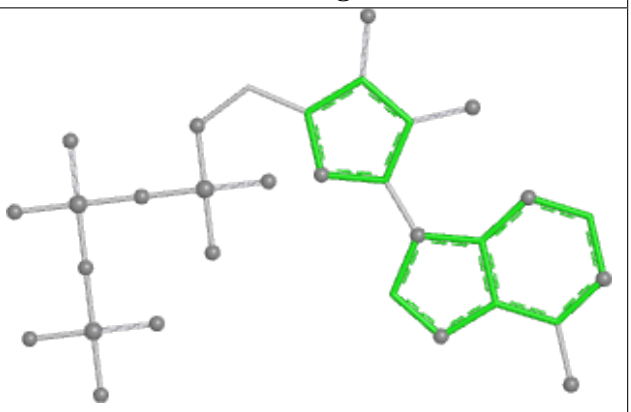
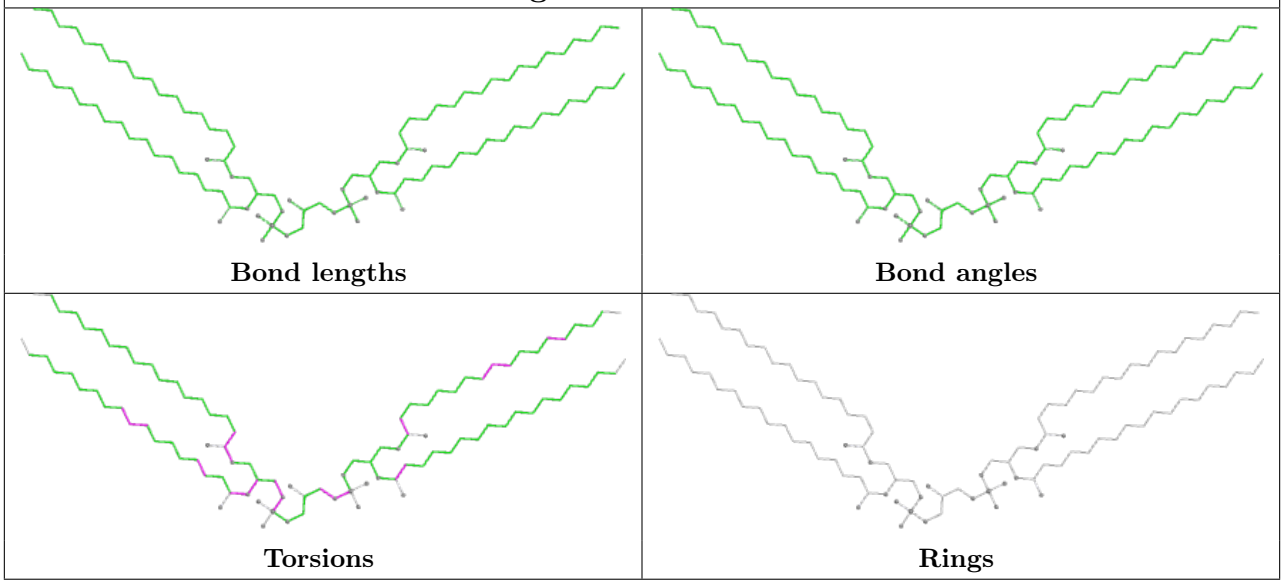


Rings

Ligand CDL e 402



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

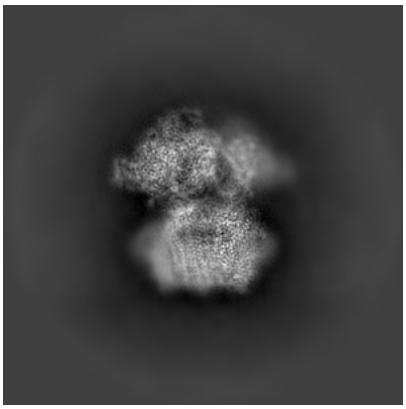
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15573. These allow visual inspection of the internal detail of the map and identification of artifacts.

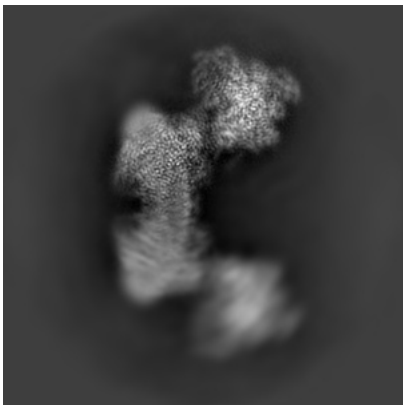
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

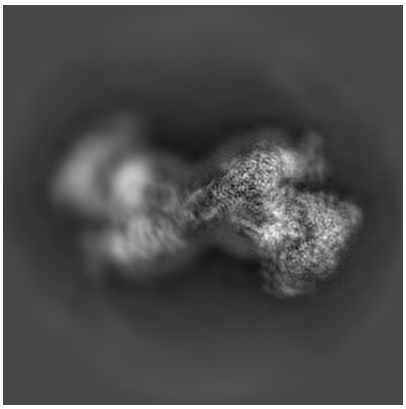
6.1.1 Primary map



X

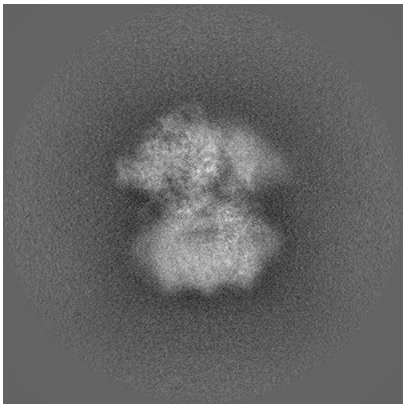


Y

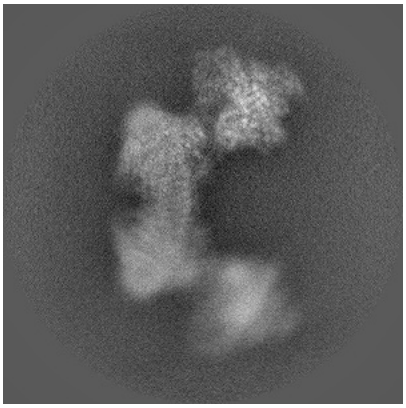


Z

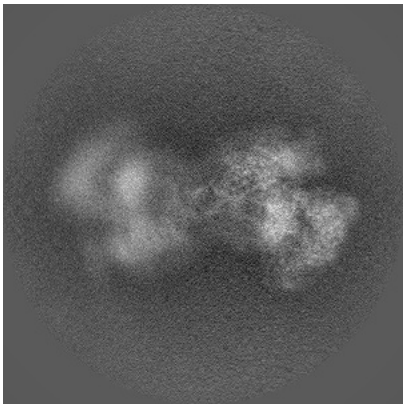
6.1.2 Raw map



X



Y

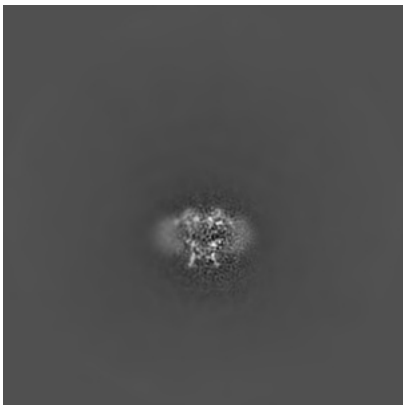


Z

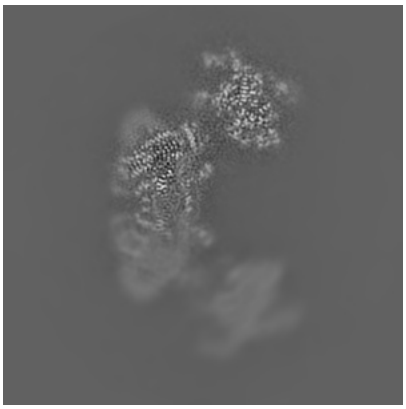
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

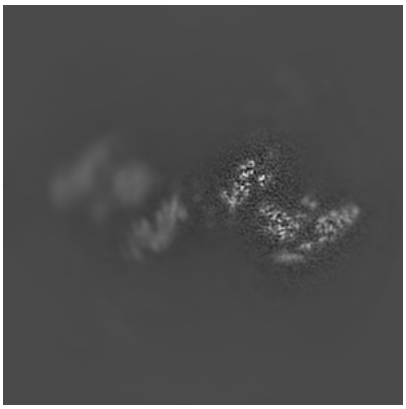
6.2.1 Primary map



X Index: 280

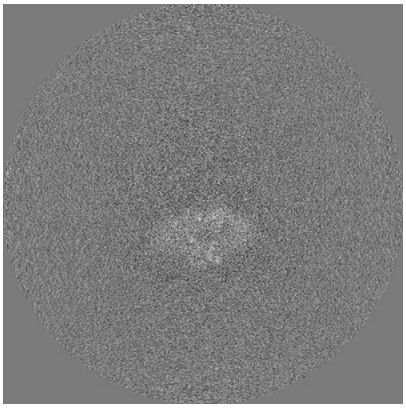


Y Index: 280

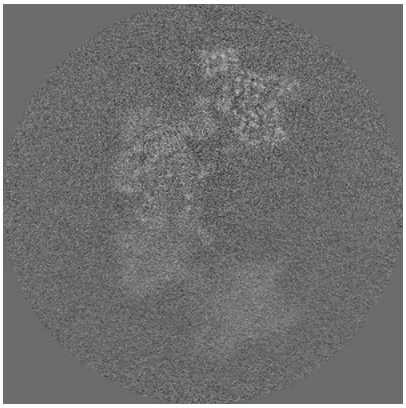


Z Index: 280

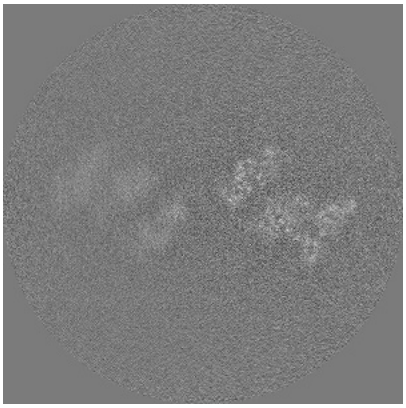
6.2.2 Raw map



X Index: 280



Y Index: 280

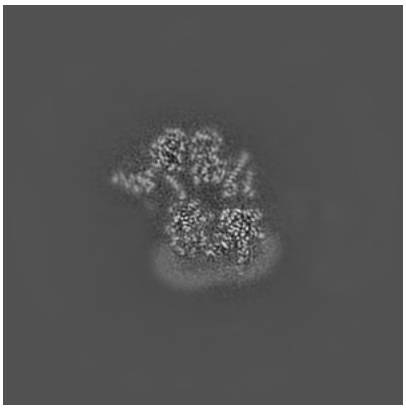


Z Index: 280

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

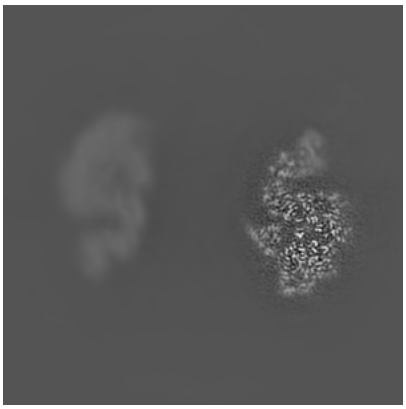
6.3 Largest variance slices (i)

6.3.1 Primary map



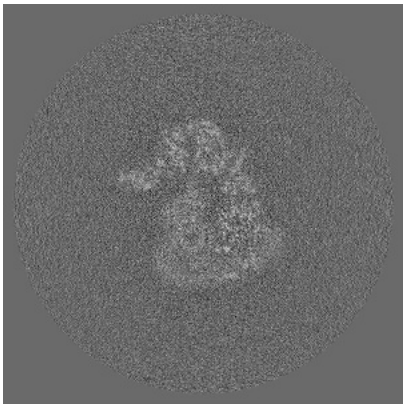
X Index: 380

Y Index: 319

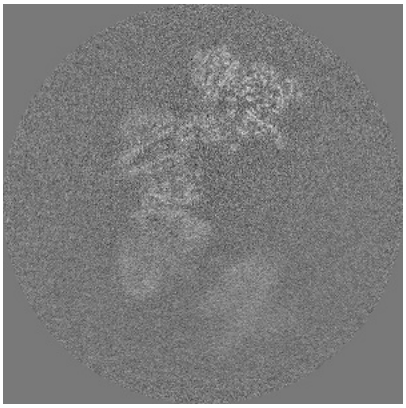


Z Index: 332

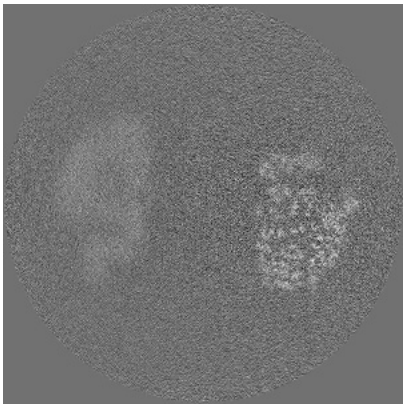
6.3.2 Raw map



X Index: 372



Y Index: 266



Z Index: 321

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 0.012. 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.

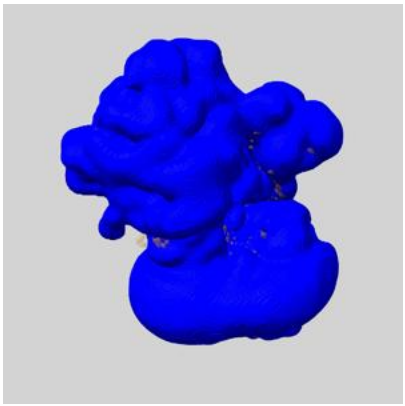
6.5 Mask visualisation

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

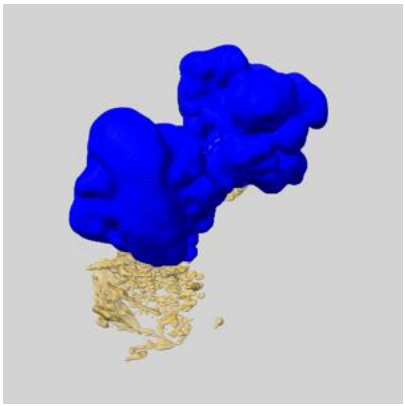
A mask typically either:

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

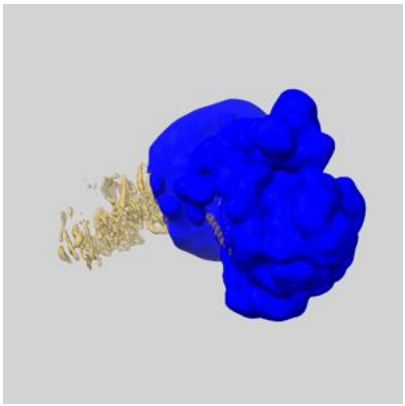
6.5.1 emd_15573_msk_1.map



X



Y

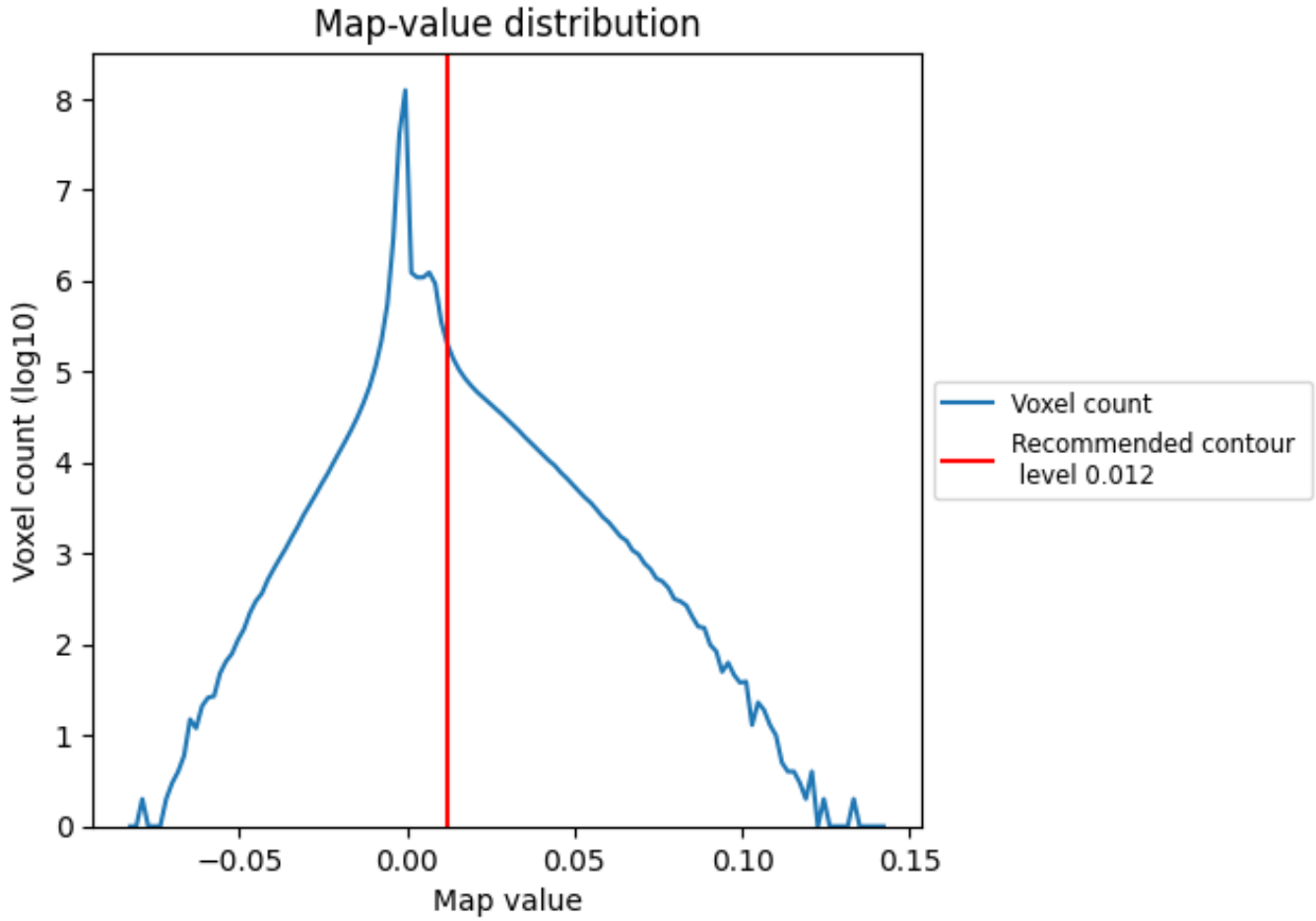


Z

7 Map analysis

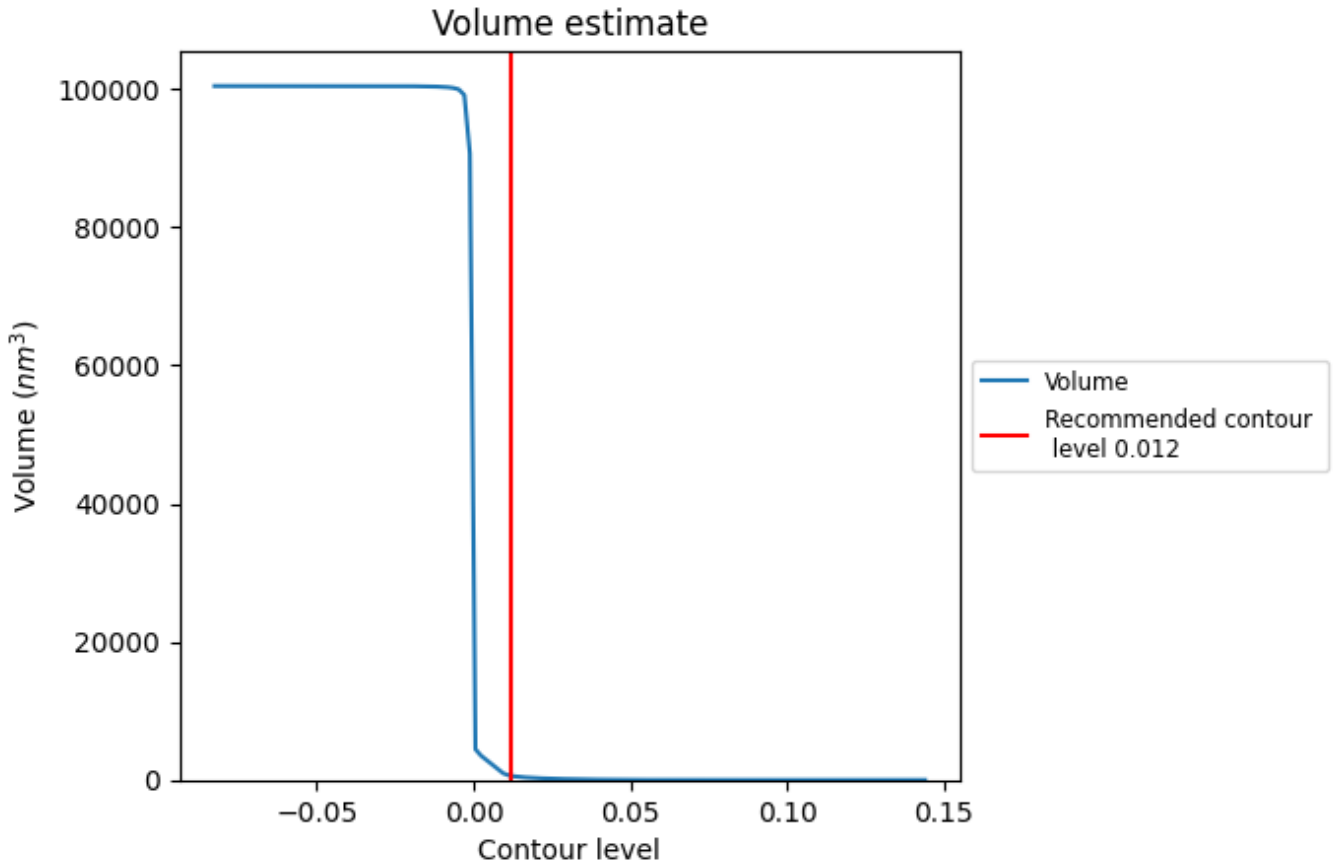
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

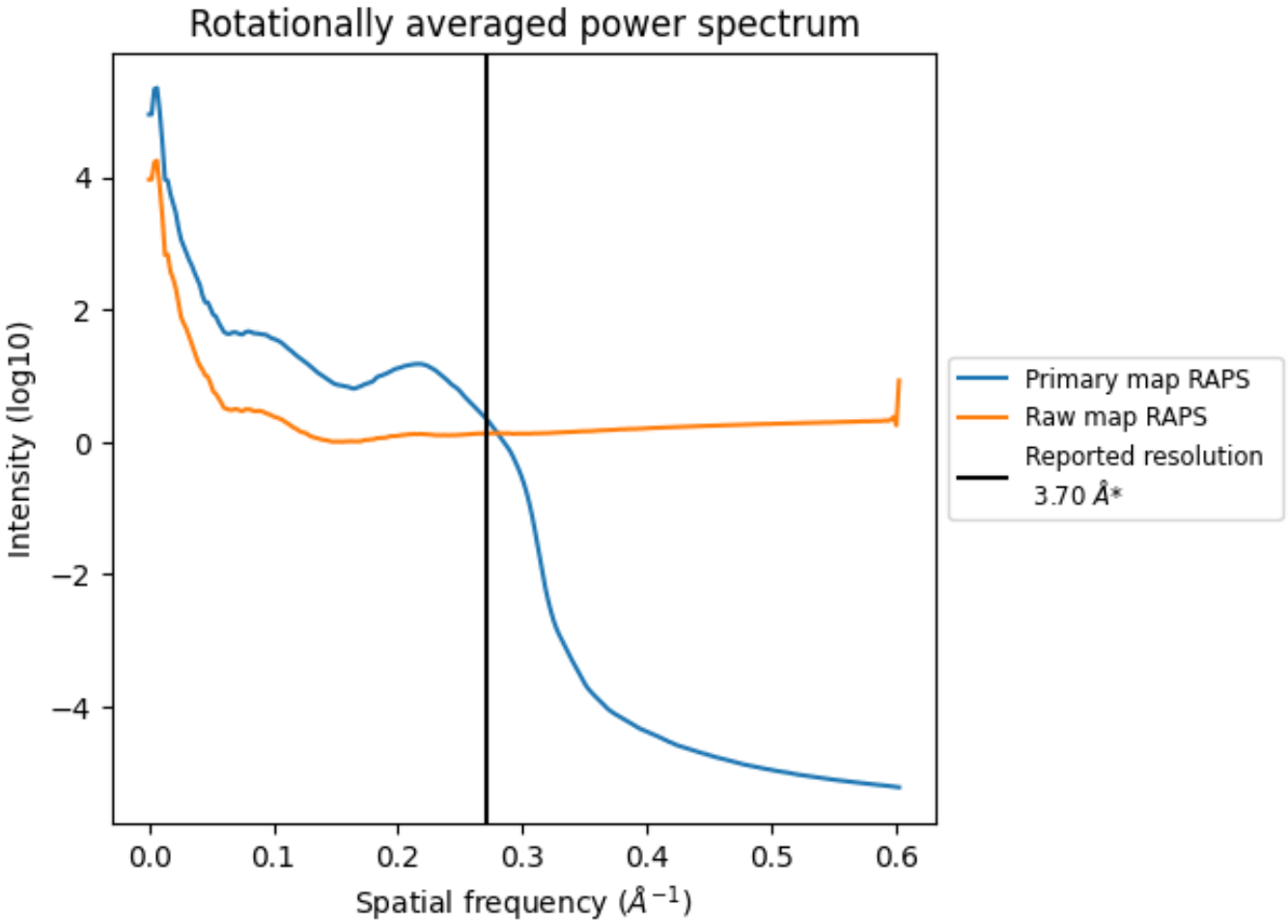
7.2 Volume estimate (i)



The volume at the recommended contour level is 607 nm^3; this corresponds to an approximate mass of 548 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)

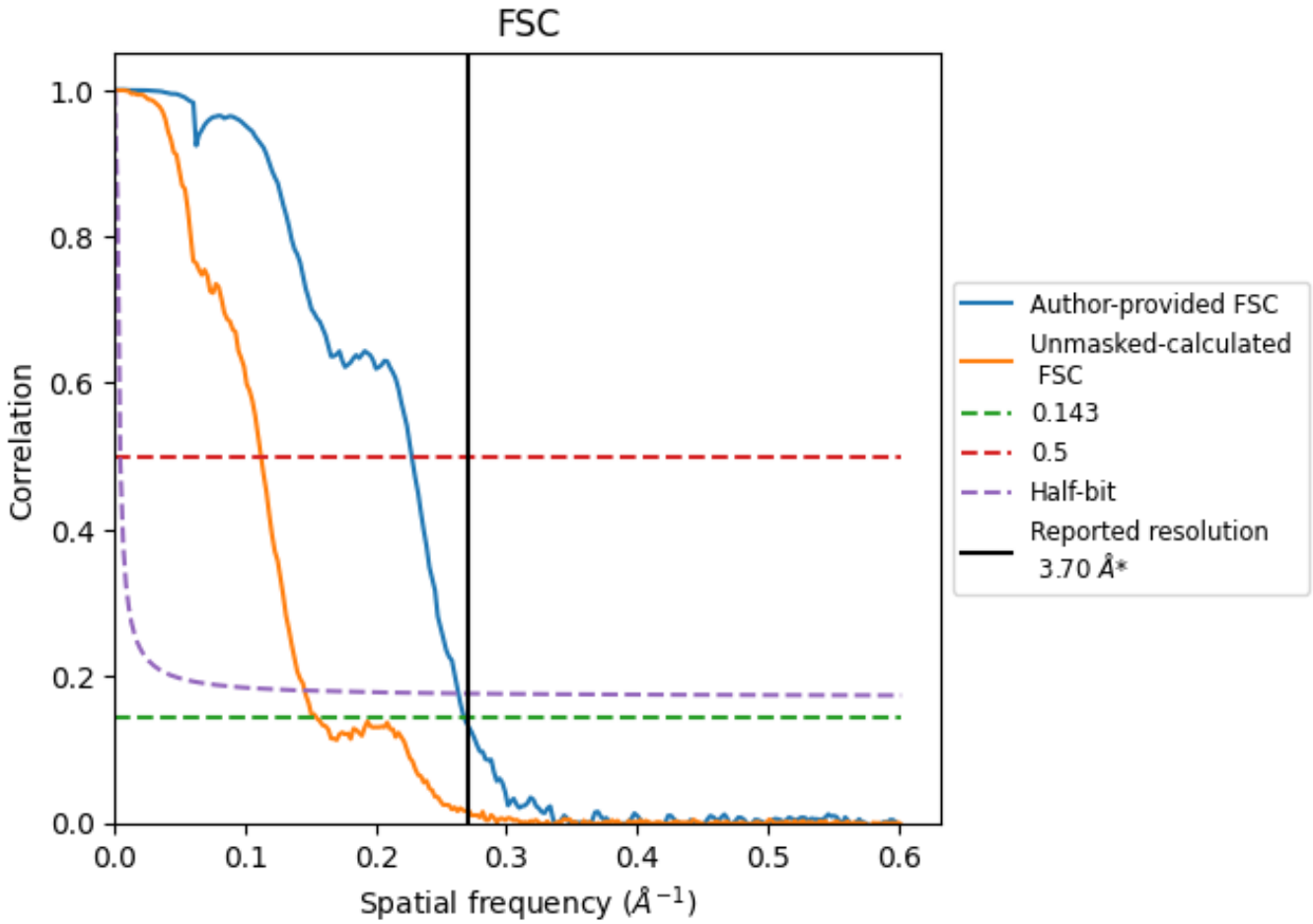


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

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 0.270 Å^{-1}

8.2 Resolution estimates (i)

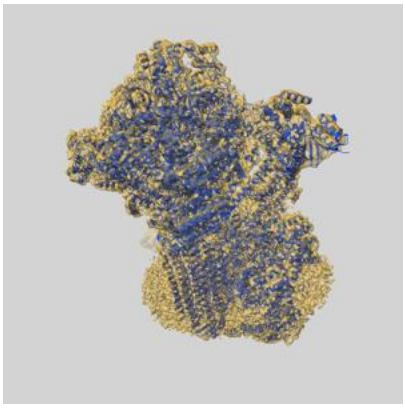
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.73	4.40	3.80
Unmasked-calculated*	6.47	8.92	6.87

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.47 differs from the reported value 3.7 by more than 10 %

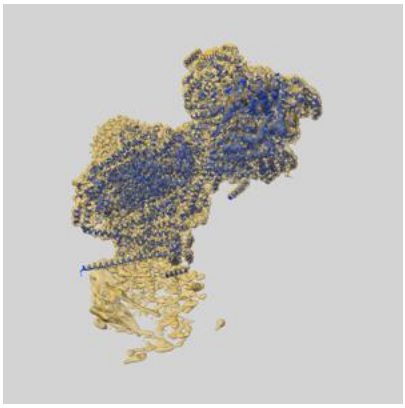
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15573 and PDB model 8APK. Per-residue inclusion information can be found in section 3 on page 16.

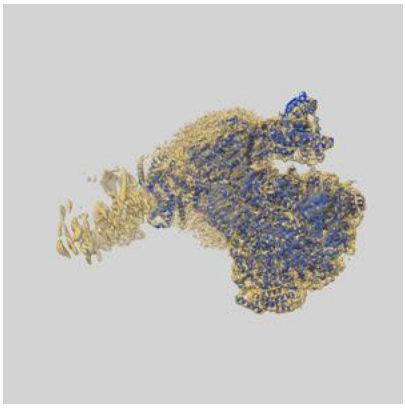
9.1 Map-model overlay



X



Y



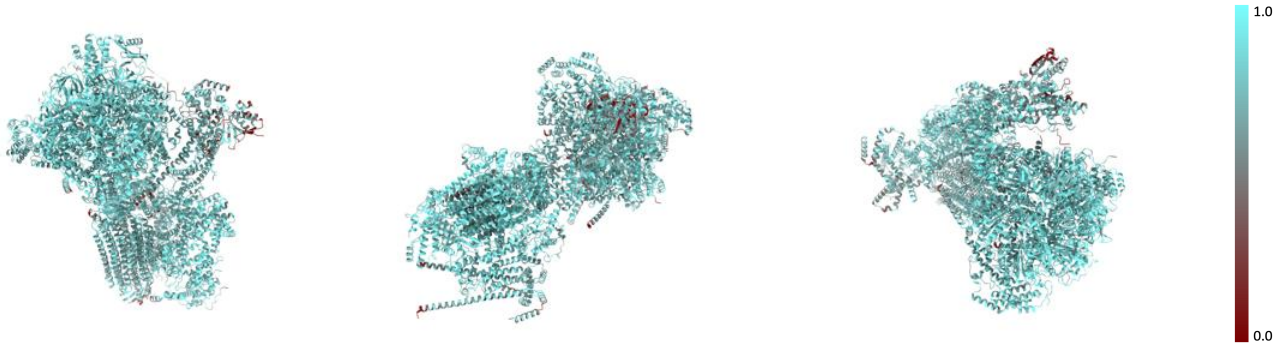
Z

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

9.2 Q-score mapped to coordinate model (i)

This section was not generated.

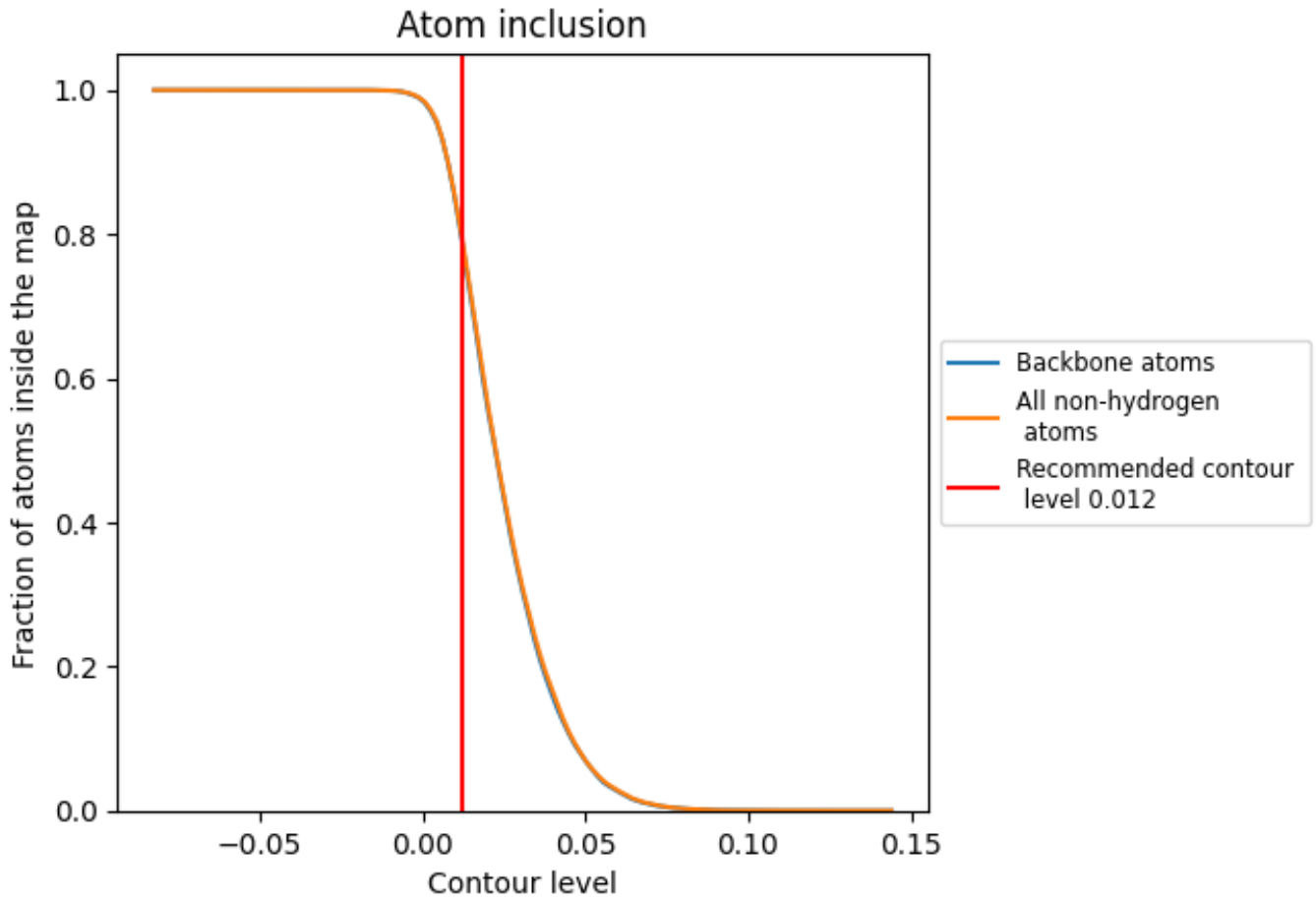
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.7967
A1	0.8500
B1	0.8621
C1	0.8409
D1	0.8133
E1	0.8619
F1	0.8303
G1	0.8074
H1	0.8074
I1	0.8275
J1	0.7881
K1	0.7829
L	0.6501
L1	0.7960
M	0.5801
M1	0.7742
O1	0.7504
P1	0.7433
Q1	0.7540
R1	0.7469
S1	0.7362
T1	0.7148
U1	0.7380
V1	0.7754
W1	0.7950
X1	0.7950
a	0.8622
c	0.8257
d	0.7718
e	0.8441
f	0.8244
g	0.5720
h	0.6847
i	0.8746
j	0.8228

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Chain	Atom inclusion
k	0.8076
l	0.5827
m	0.6667
n	0.8893
o	0.8566
p	0.7989
q	0.8535
r	0.8876