Full wwPDB EM Validation Report ⓘ

Oct 19, 2022 – 05:07 am BST

PDB ID	:	8APE
EMDB ID	:	EMD-15567
Title	:	rotational state 1e 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

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

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

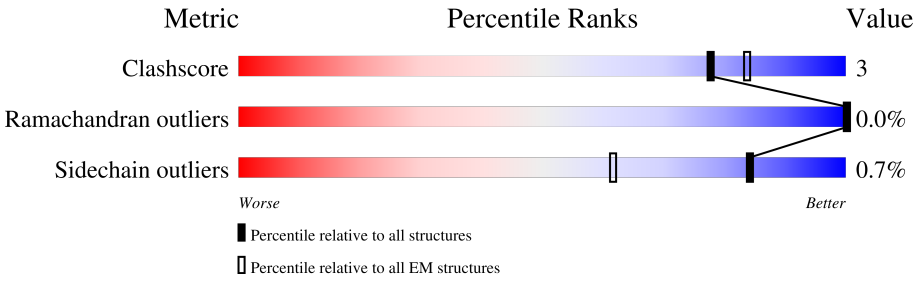
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

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)
Clashscore	158937	4297
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	A1	584	21% 84% 7% 9%
1	B1	584	23% 83% 7% 10%
1	C1	584	35% 84% 6% 10%
2	D1	519	34% 87% 7% 6%
2	E1	519	24% 86% 8% 6%
2	F1	519	28% 87% 8% 6%
3	G1	305	25% 81% 15%
4	H1	182	29% 76% 12% 12%

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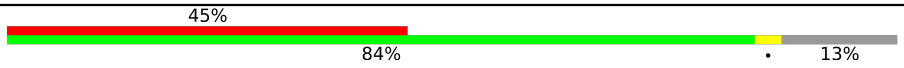
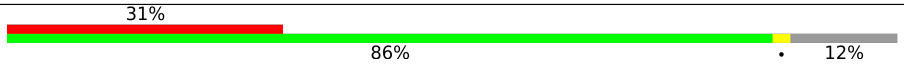
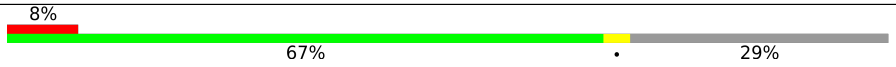
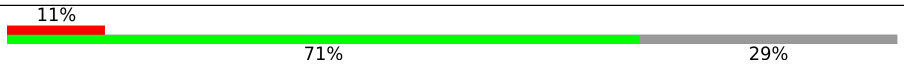
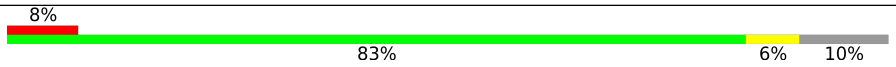
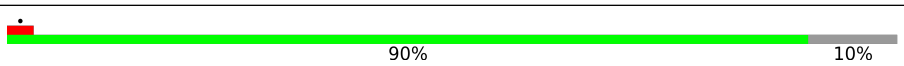
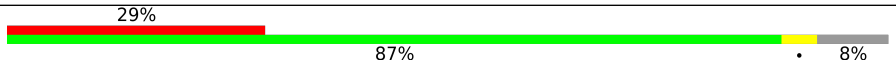
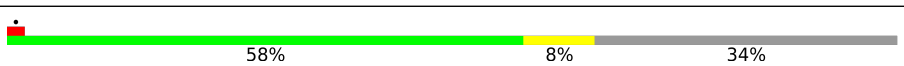
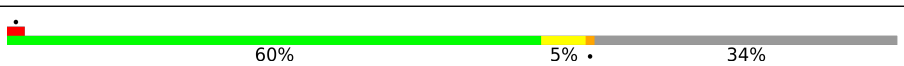
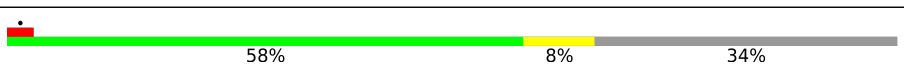
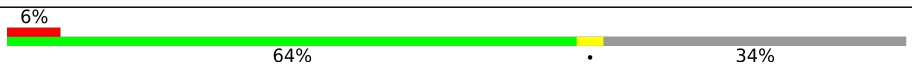
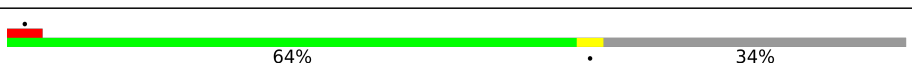
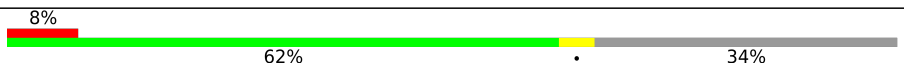
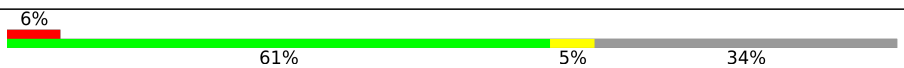
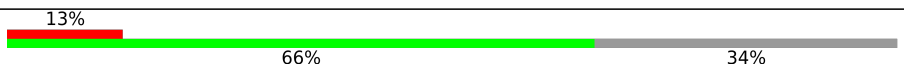
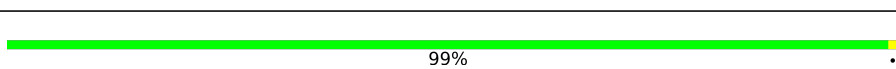
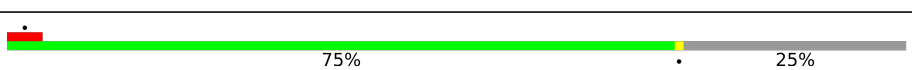
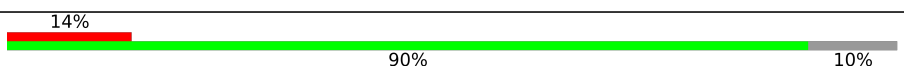
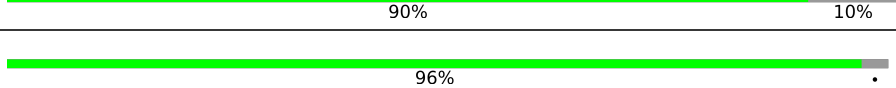
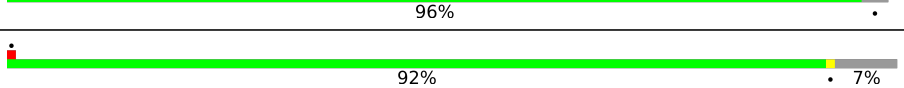
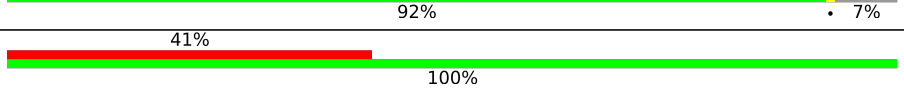
Mol	Chain	Length	Quality of chain
5	I1	75	
6	J1	188	
6	K1	188	
6	L1	188	
7	L	92	
7	l	92	
8	M	144	
8	m	144	
9	M1	255	
10	O1	118	
10	P1	118	
10	Q1	118	
10	R1	118	
10	S1	118	
10	T1	118	
10	U1	118	
10	V1	118	
10	W1	118	
10	X1	118	
11	a	231	
12	c	114	
13	d	370	
14	e	396	
15	f	145	
16	g	269	

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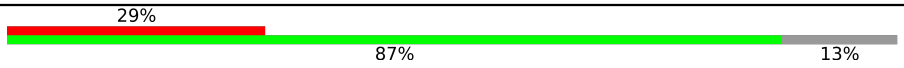
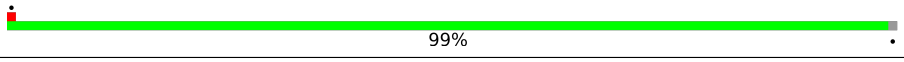
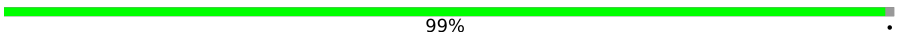
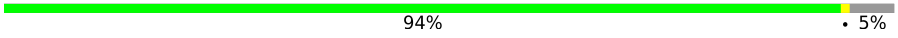
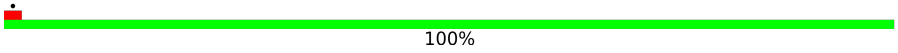
Mol	Chain	Length	Quality of chain
17	h	157	
18	i	104	
19	j	169	
20	k	124	
21	n	156	
22	o	101	
23	p	105	
24	q	98	
25	r	62	

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
34	Q7G	e	407	X	-	-	-
34	Q7G	n	201	X	-	-	-

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 129568 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 ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A1	530	Total	C	H	N	O	S	0	0
			8281	2612	4197	710	742	20		
1	B1	523	Total	C	H	N	O	S	0	0
			8200	2585	4162	702	731	20		
1	C1	523	Total	C	H	N	O	S	0	0
			8194	2587	4155	701	731	20		

- Molecule 2 is a protein called ATP synthase subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D1	487	Total	C	H	N	O	S	0	0
			7431	2329	3742	631	710	19		
2	E1	486	Total	C	H	N	O	S	0	0
			7415	2324	3733	630	709	19		
2	F1	489	Total	C	H	N	O	S	0	0
			7462	2339	3759	633	712	19		

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

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

- Molecule 4 is a protein called ATP synthase, epsilon chain, putative.

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

- Molecule 5 is a protein called ATP synthase subunit epsilon, mitochondrial.

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

- Molecule 6 is a protein called ATP synthase subunit p18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	J1	166	Total	C	H	N	O	S	0	0
			2591	822	1276	221	258	14		
6	K1	166	Total	C	H	N	O	S	0	0
			2591	822	1276	221	258	14		
6	L1	165	Total	C	H	N	O	S	0	0
			2581	819	1271	220	257	14		

- Molecule 7 is a protein called subunit-e.

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

- Molecule 8 is a protein called subunit-g.

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

- Molecule 9 is a protein called OSCP.

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

- Molecule 10 is a protein called ATPase subunit 9, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	O1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		
10	P1	78	Total	C	H	N	O	S	0	0
			1165	376	600	89	96	4		

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

- Molecule 11 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	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 12 is a protein called subunit-8.

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

- Molecule 13 is a protein called subunit-d.

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

- Molecule 14 is a protein called ATPTB1.

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

- Molecule 15 is a protein called subunit-f.

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

- Molecule 16 is a protein called ATPTB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	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 17 is a protein called ATPTB4.

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

- Molecule 18 is a protein called subunit-i/j.

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

- Molecule 19 is a protein called ATPTB6.

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

- Molecule 20 is a protein called subunit-k.

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

- Molecule 21 is a protein called ATPTB11.

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

- Molecule 22 is a protein called ATPTB12.

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

- Molecule 23 is a protein called subunit-b.

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

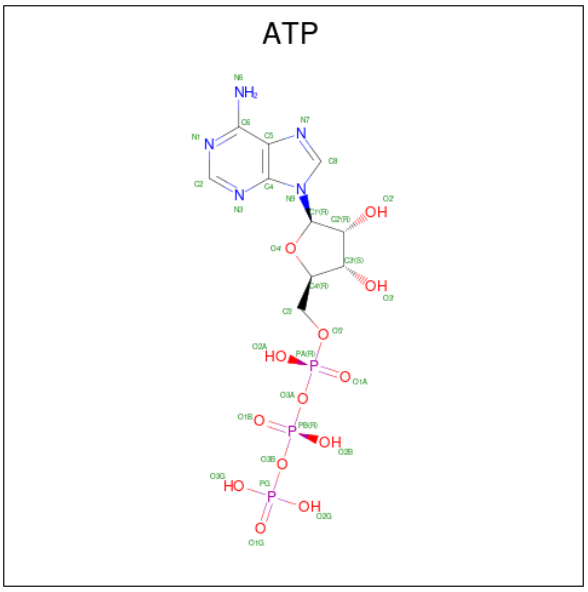
- Molecule 24 is a protein called ATPEG3.

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

- Molecule 25 is a protein called ATPEG4.

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

- Molecule 26 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).

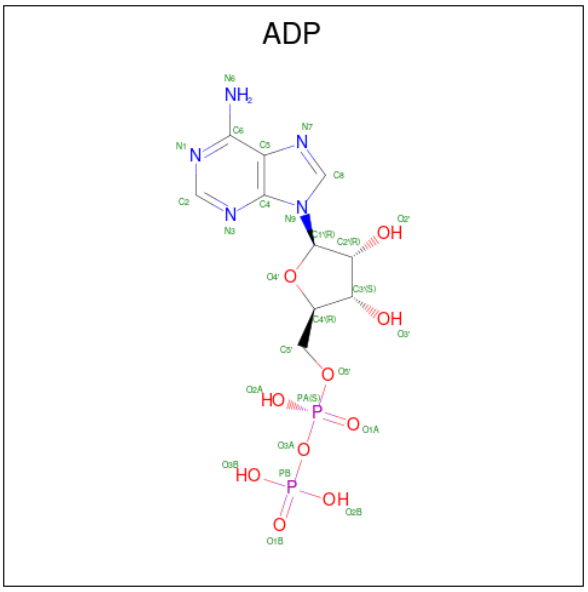


Mol	Chain	Residues	Atoms						AltConf
26	A1	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
26	B1	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
26	C1	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
26	F1	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

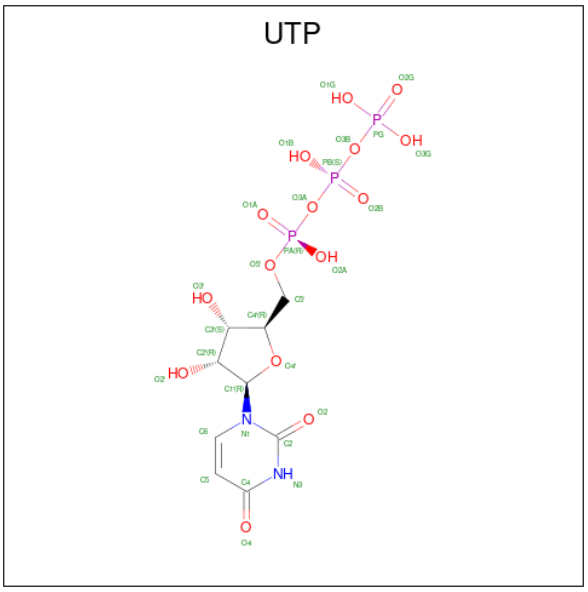
Mol	Chain	Residues	Atoms		AltConf
27	A1	1	Total	Mg	0
			1	1	
27	B1	1	Total	Mg	0
			1	1	
27	C1	1	Total	Mg	0
			1	1	
27	D1	1	Total	Mg	0
			1	1	
27	F1	1	Total	Mg	0
			1	1	

- Molecule 28 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).



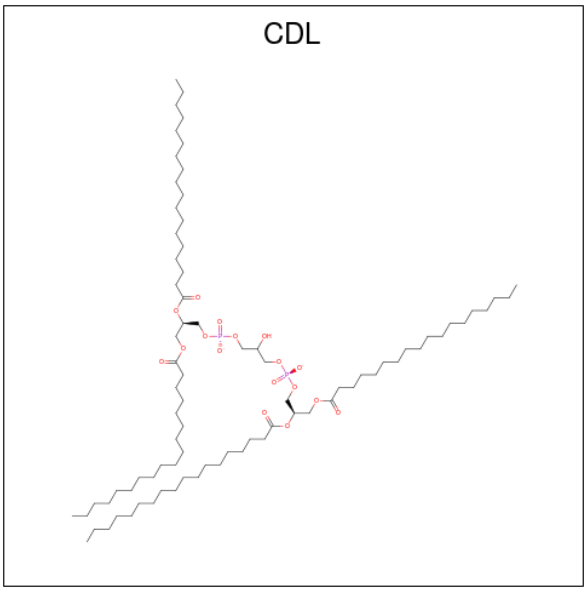
Mol	Chain	Residues	Atoms						AltConf
28	D1	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

- Molecule 29 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$) (labeled as "Ligand of Interest" by depositor).



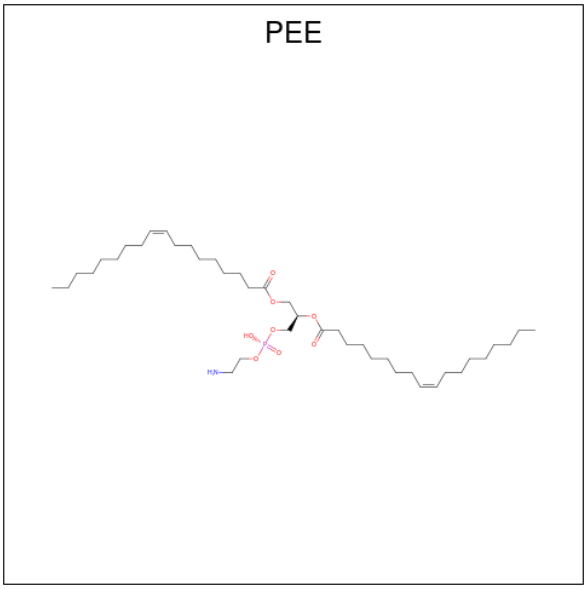
Mol	Chain	Residues	Atoms						AltConf
29	H1	1	Total	C	H	N	O	P	0
			40	9	11	2	15	3	

- Molecule 30 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



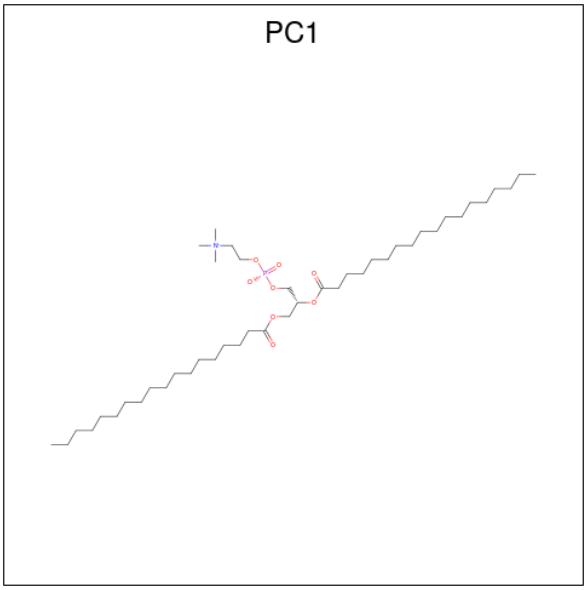
Mol	Chain	Residues	Atoms					AltConf
30	L	1	Total	C	H	O	P	0
			256	81	156	17	2	
30	M	1	Total	C	H	O	P	0
			256	81	156	17	2	
30	c	1	Total	C	H	O	P	0
			256	81	156	17	2	
30	e	1	Total	C	H	O	P	0
			1280	405	780	85	10	
30	e	1	Total	C	H	O	P	0
			1280	405	780	85	10	
30	e	1	Total	C	H	O	P	0
			1280	405	780	85	10	
30	e	1	Total	C	H	O	P	0
			1280	405	780	85	10	
30	e	1	Total	C	H	O	P	0
			1280	405	780	85	10	
30	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
30	j	1	Total	C	H	O	P	0
			512	162	312	34	4	
30	j	1	Total	C	H	O	P	0
			512	162	312	34	4	
30	l	1	Total	C	H	O	P	0
			256	81	156	17	2	
30	m	1	Total	C	H	O	P	0
			256	81	156	17	2	
30	q	1	Total	C	H	O	P	0
			256	81	156	17	2	

- Molecule 31 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



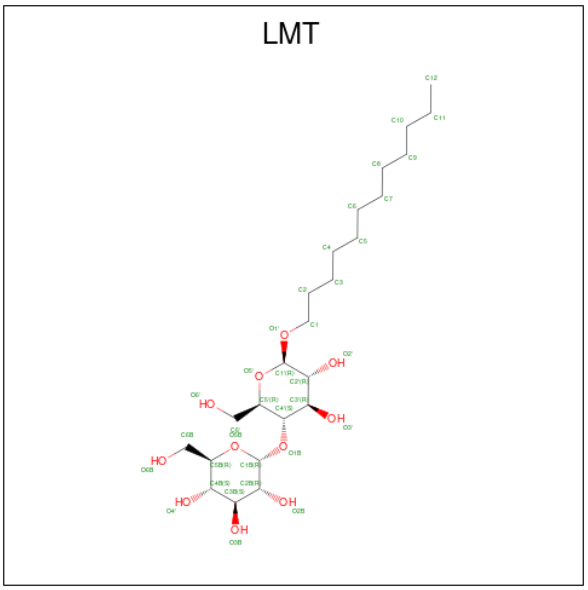
Mol	Chain	Residues	Atoms						AltConf
31	M	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
31	f	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
31	m	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

- Molecule 32 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).



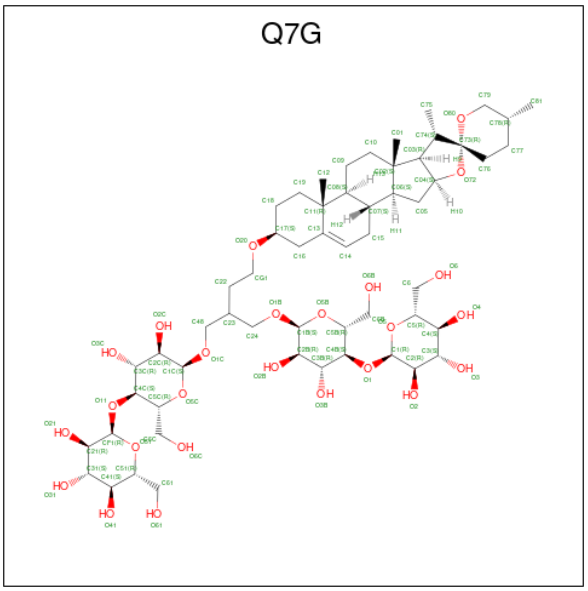
Mol	Chain	Residues	Atoms						AltConf
32	a	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
32	f	1	Total	C	H	N	O	P	0
			284	88	176	2	16	2	
32	f	1	Total	C	H	N	O	P	0
			284	88	176	2	16	2	
32	i	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

- Molecule 33 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

- Molecule 34 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: $C_{56}H_{92}O_{25}$).



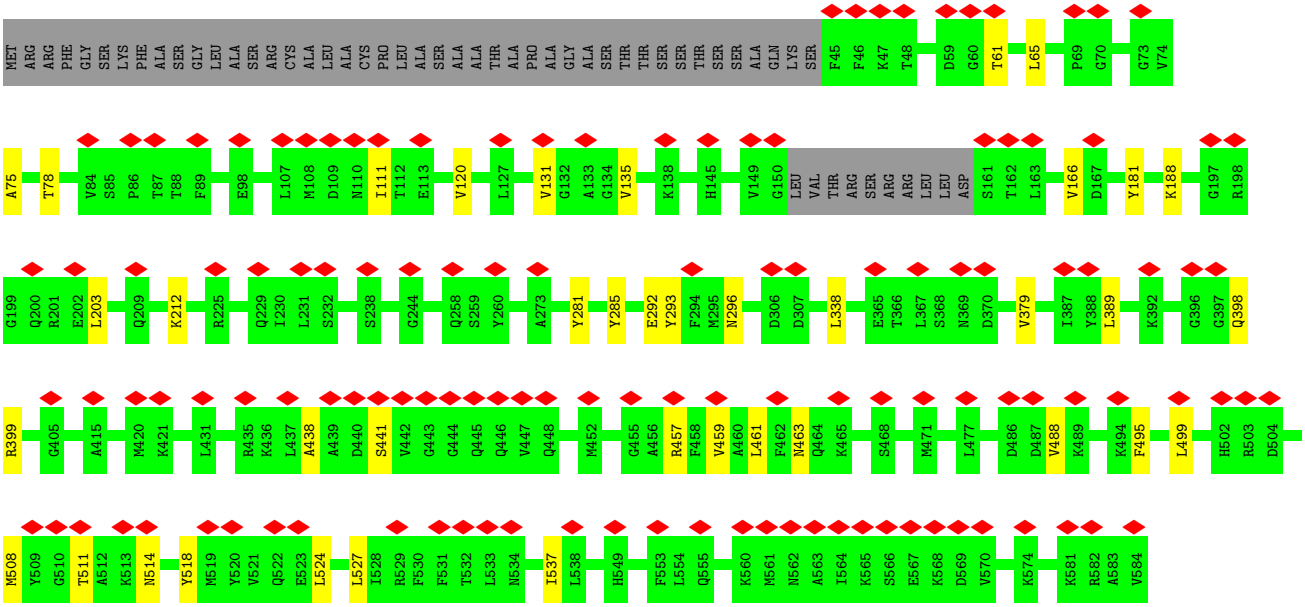
Mol	Chain	Residues	Atoms				AltConf
34	e	1	Total	C	H	O	0
			108	38	60	10	
34	n	1	Total	C	H	O	0
			129	44	70	15	

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.

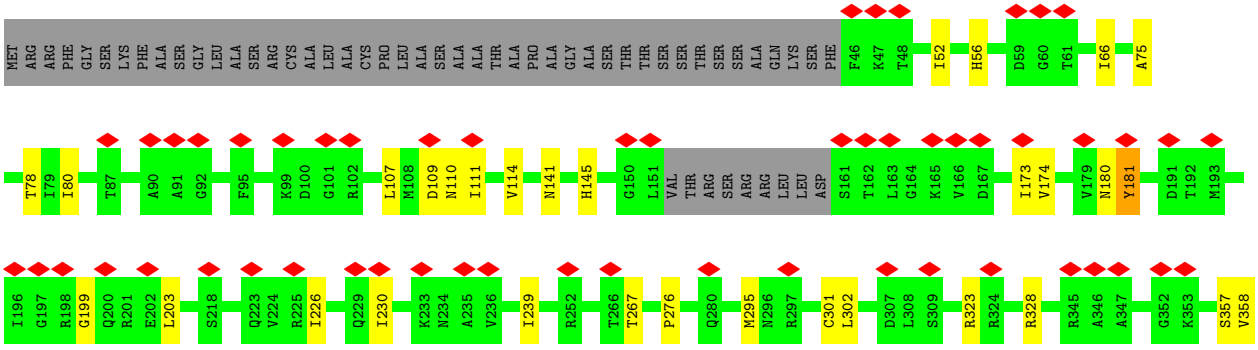
• Molecule 1: ATP synthase subunit alpha, mitochondrial

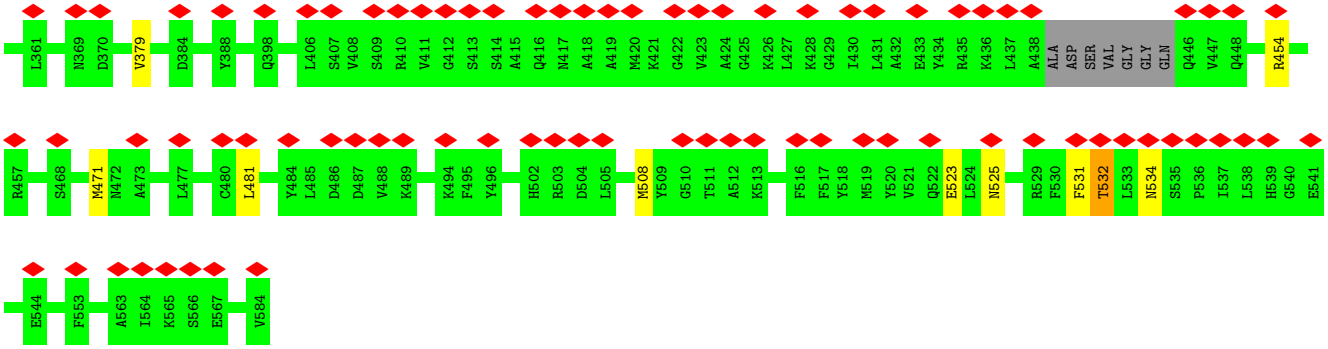
Chain A1:



• Molecule 1: ATP synthase subunit alpha, mitochondrial

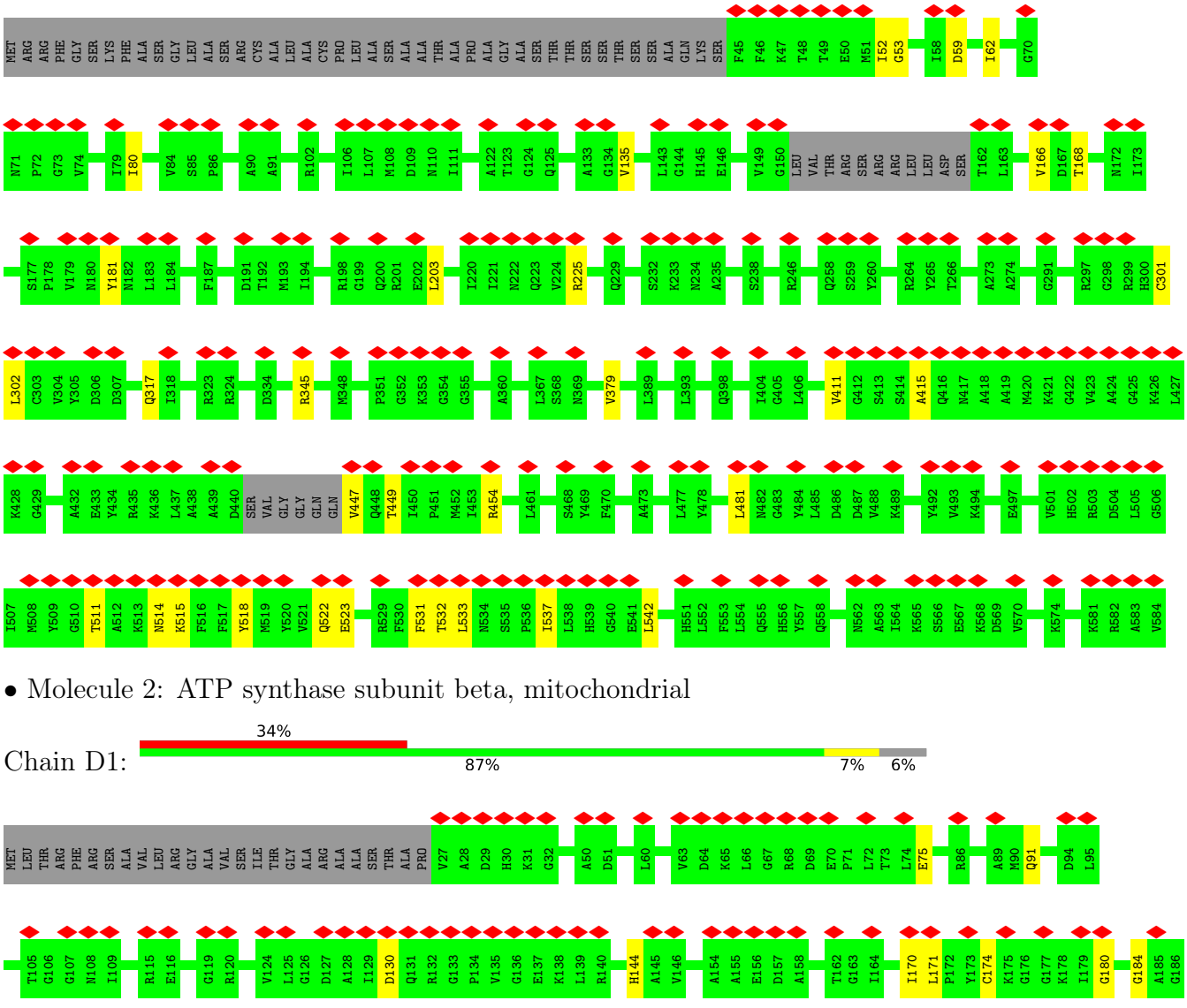
Chain B1:





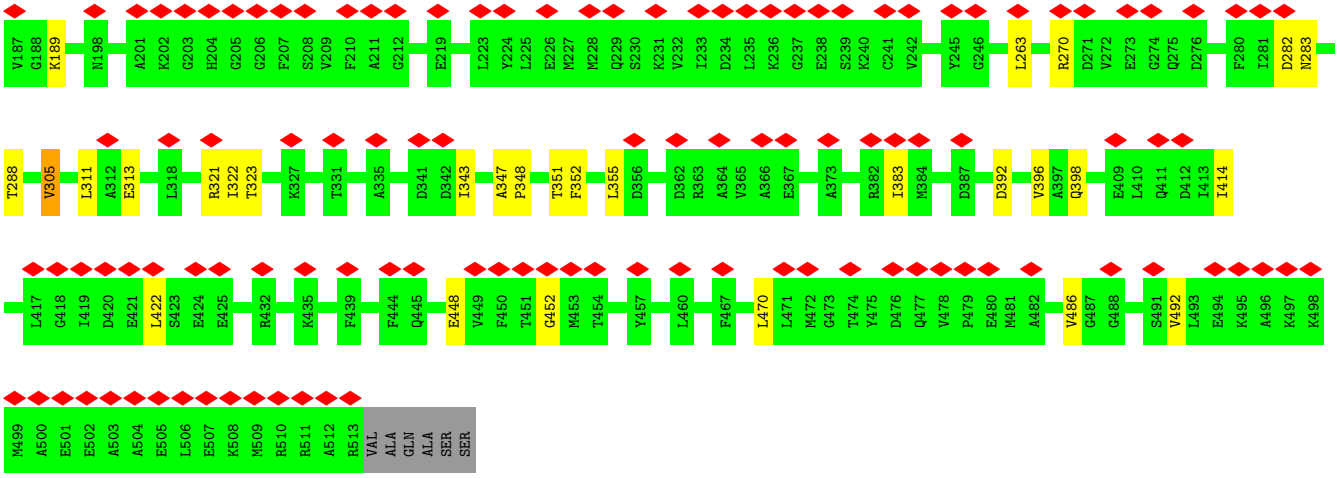
• Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain C1:



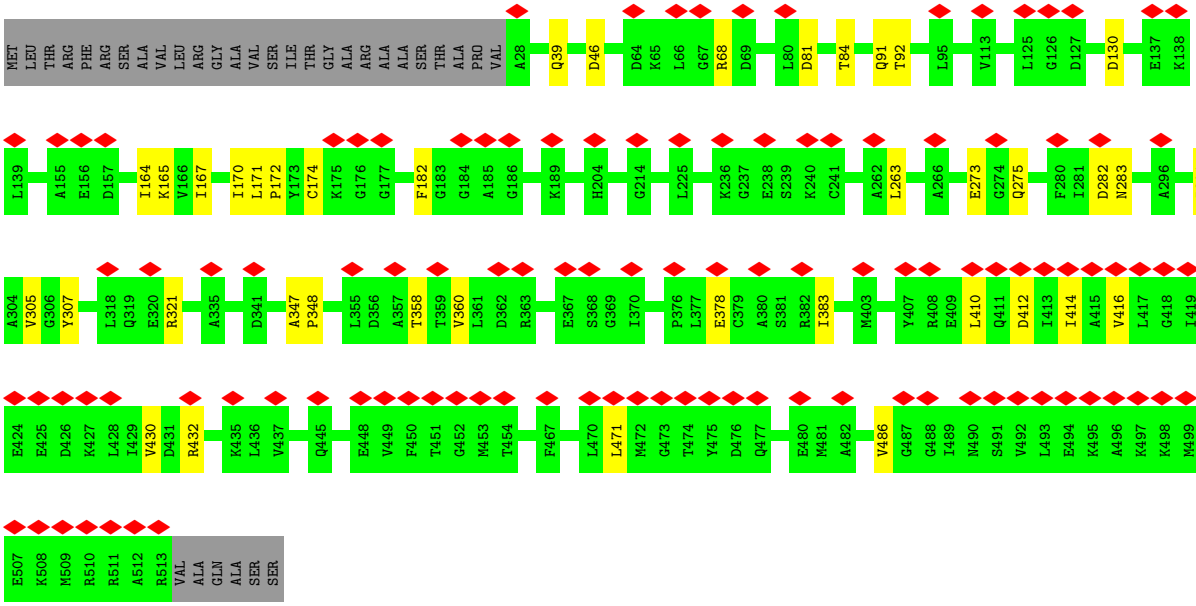
• Molecule 2: ATP synthase subunit beta, mitochondrial

Chain D1:



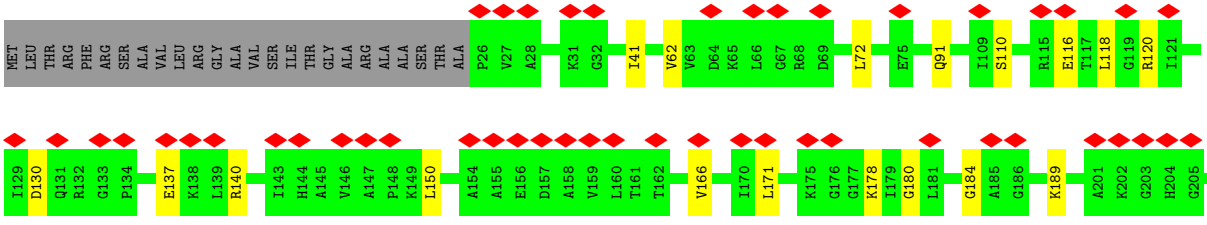
• Molecule 2: ATP synthase subunit beta, mitochondrial

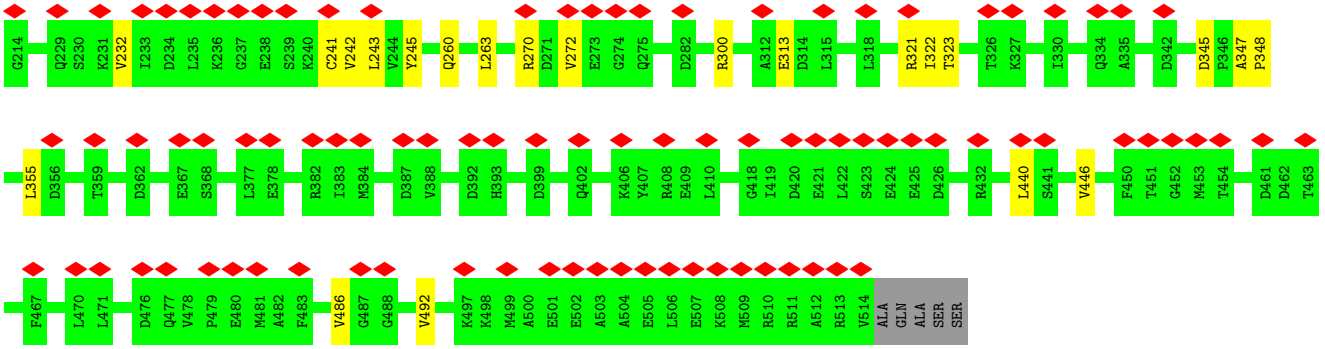
Chain E1:



• Molecule 2: ATP synthase subunit beta, mitochondrial

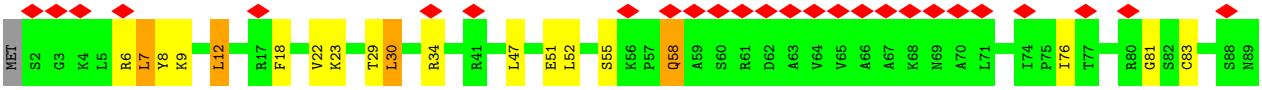
Chain F1:

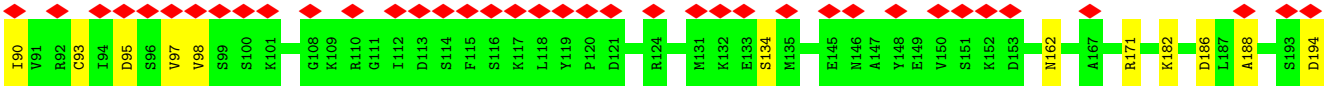


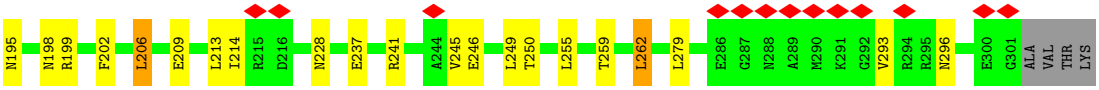


• Molecule 3: ATP synthase gamma subunit

Chain G1:

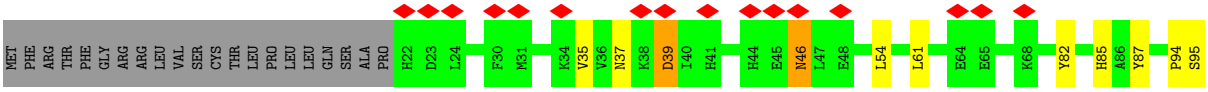


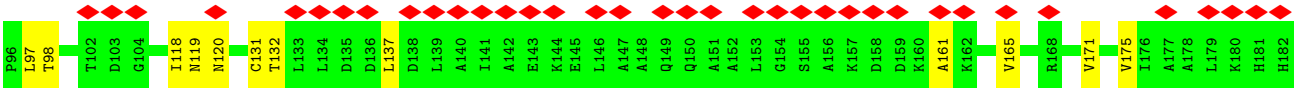




• Molecule 4: ATP synthase, epsilon chain, putative

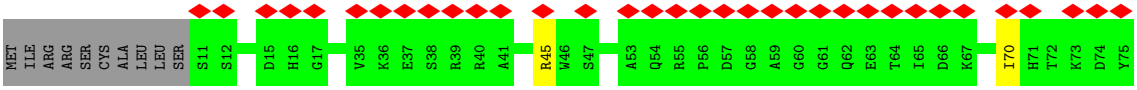
Chain H1:





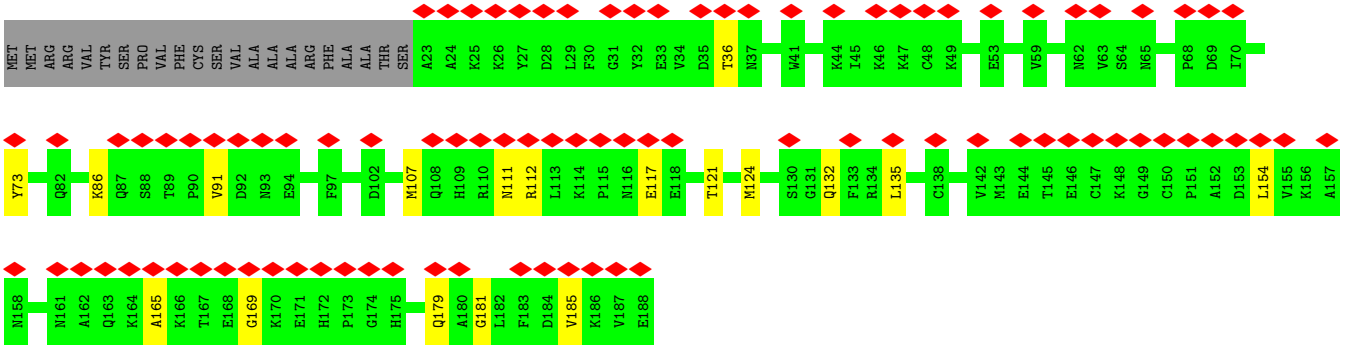
• Molecule 5: ATP synthase subunit epsilon, mitochondrial

Chain I1:



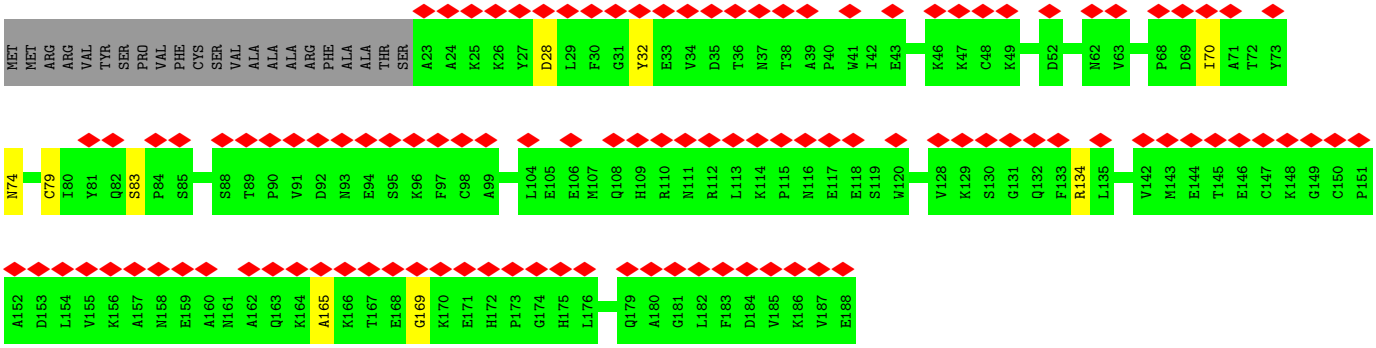
• Molecule 6: ATP synthase subunit p18, mitochondrial

Chain J1:



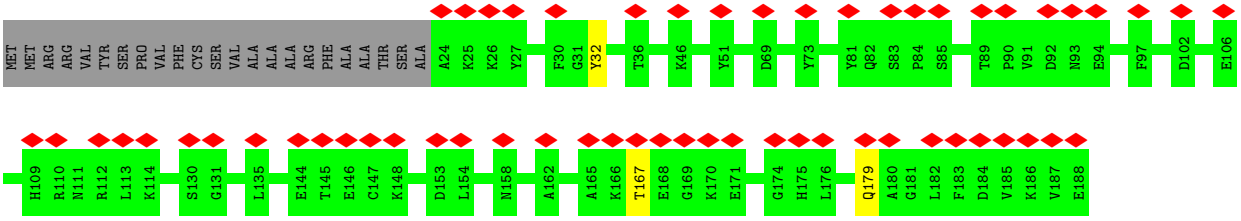
• Molecule 6: ATP synthase subunit p18, mitochondrial

Chain K1:



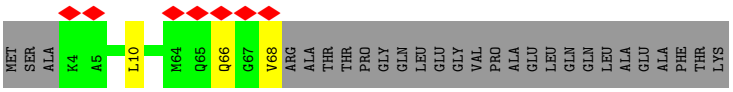
• Molecule 6: ATP synthase subunit p18, mitochondrial

Chain L1:



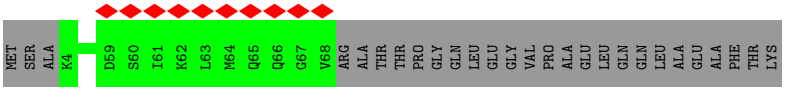
• Molecule 7: subunit-e

Chain L:

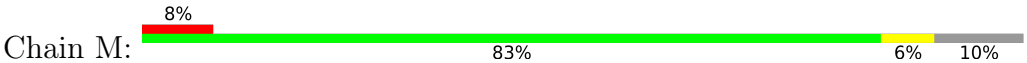


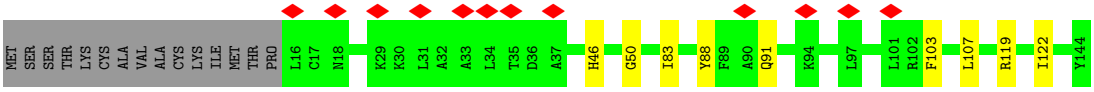
• Molecule 7: subunit-e

Chain l:

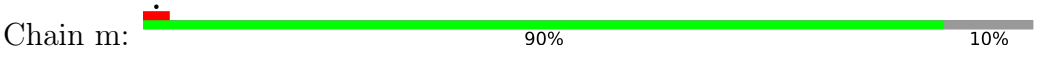


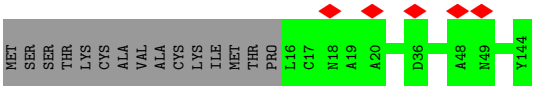
• Molecule 8: subunit-g



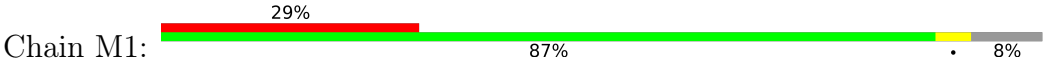


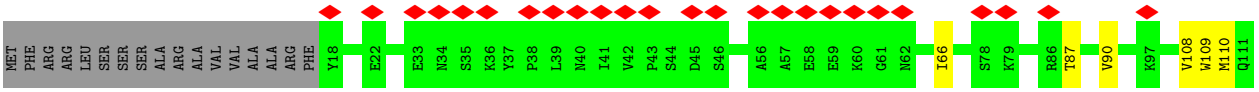
• Molecule 8: subunit-g

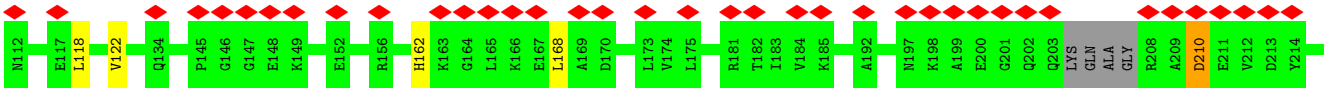


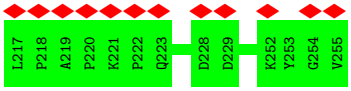


• Molecule 9: OSCP

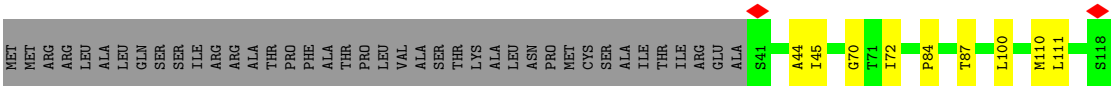




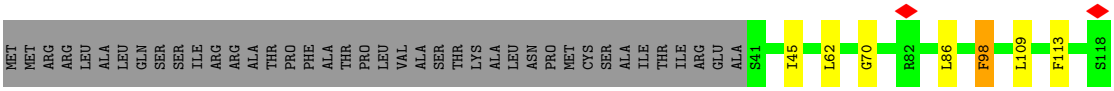




• Molecule 10: ATPase subunit 9, putative

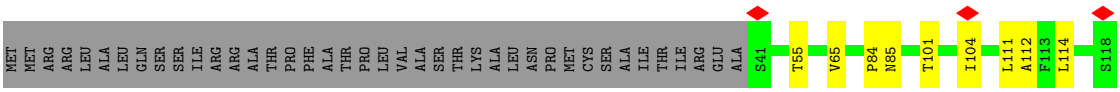


• Molecule 10: ATPase subunit 9, putative



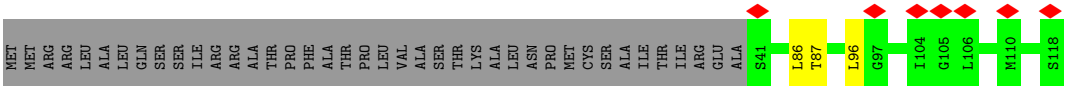
• Molecule 10: ATPase subunit 9, putative

Chain Q1:



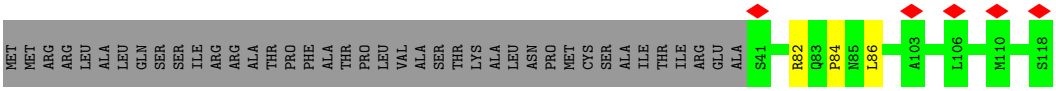
• Molecule 10: ATPase subunit 9, putative

Chain R1:



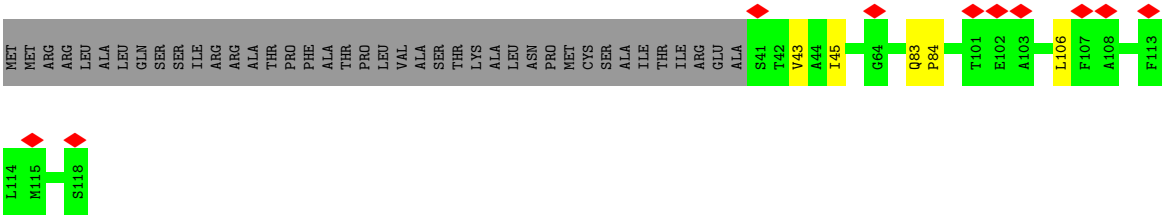
• Molecule 10: ATPase subunit 9, putative

Chain S1:



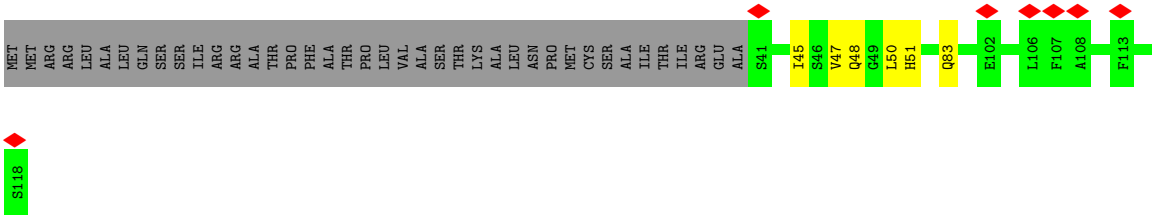
• Molecule 10: ATPase subunit 9, putative

Chain T1:



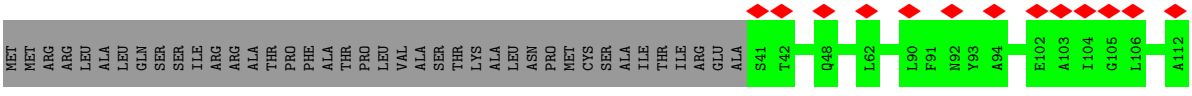
• Molecule 10: ATPase subunit 9, putative

Chain U1:



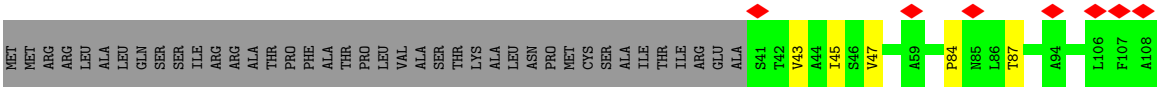
• Molecule 10: ATPase subunit 9, putative

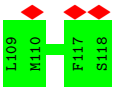
Chain V1:



• Molecule 10: ATPase subunit 9, putative

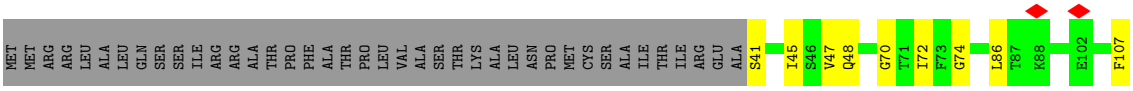
Chain W1:





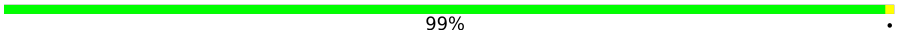
• Molecule 10: ATPase subunit 9, putative

Chain X1:



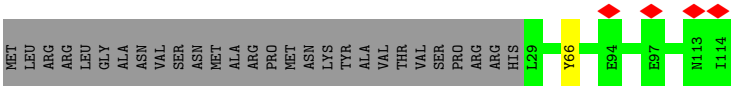
• Molecule 11: ATP synthase subunit a

Chain a:



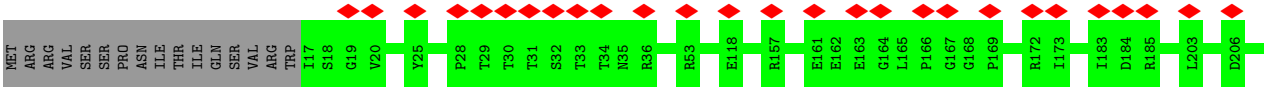
• Molecule 12: subunit-8

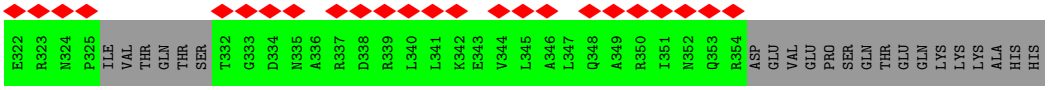
Chain c:



• Molecule 13: subunit-d

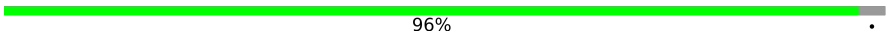
Chain d:





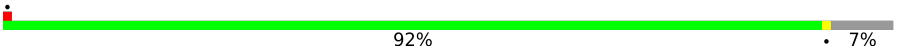
• Molecule 14: ATPTB1

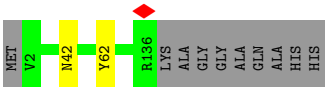
Chain e:



• Molecule 15: subunit-f

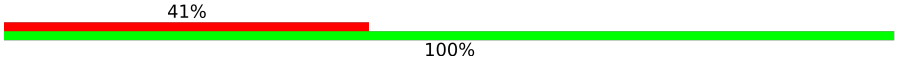
Chain f:

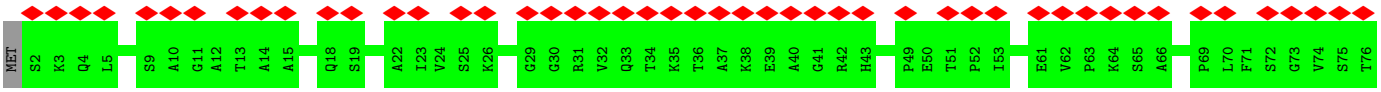


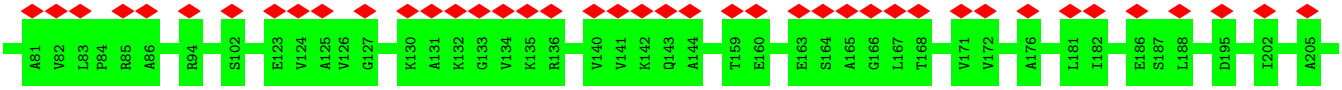


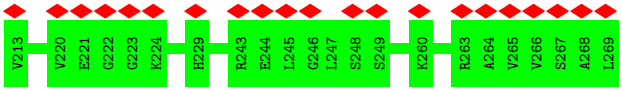
• Molecule 16: ATPTB3

Chain g:



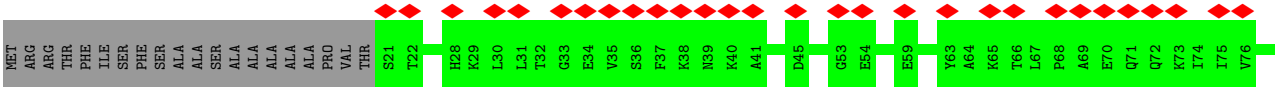


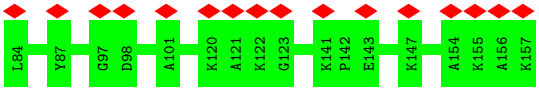




• Molecule 17: ATPTB4

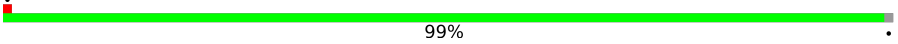
Chain h:





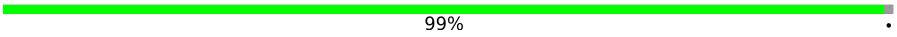
• Molecule 18: subunit-i/j

Chain i:



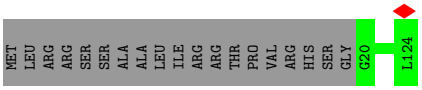
• Molecule 19: ATPTB6

Chain j:



• Molecule 20: subunit-k

Chain k:

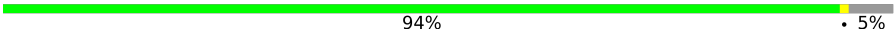


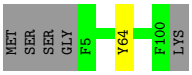
• Molecule 21: ATPTB11

Chain n:

• Molecule 22: ATPTB12

Chain o:



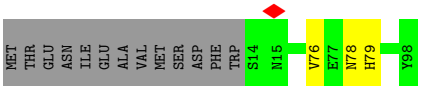


• Molecule 23: subunit-b

Chain p:

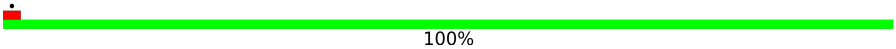
• Molecule 24: ATPEG3

Chain q:



• Molecule 25: ATPEG4

Chain r:




M1
HG2

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32482	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	0.120	Depositor
Minimum map value	-0.067	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	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

5.1 Standard geometry

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

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	A1	0.25	0/4159	0.46	0/5632
1	B1	0.24	0/4111	0.46	0/5566
1	C1	0.24	0/4113	0.47	0/5569
2	D1	0.24	0/3745	0.46	0/5077
2	E1	0.24	0/3738	0.46	0/5067
2	F1	0.24	0/3760	0.46	0/5098
3	G1	0.25	0/2427	0.49	0/3268
4	H1	0.25	0/1274	0.45	0/1728
5	I1	0.23	0/547	0.48	0/738
6	J1	0.24	0/1342	0.39	0/1810
6	K1	0.23	0/1342	0.39	0/1810
6	L1	0.24	0/1337	0.39	0/1803
7	L	0.25	0/547	0.43	0/735
7	l	0.24	0/547	0.43	0/735
8	M	0.26	0/1049	0.42	0/1423
8	m	0.26	0/1049	0.42	0/1423
9	M1	0.24	0/1916	0.40	0/2591
10	O1	0.25	0/574	0.41	0/777
10	P1	0.25	0/574	0.41	0/777
10	Q1	0.25	0/574	0.40	0/777
10	R1	0.25	0/574	0.41	0/777
10	S1	0.25	0/574	0.40	0/777
10	T1	0.25	0/574	0.41	0/777
10	U1	0.25	0/574	0.41	0/777
10	V1	0.25	0/574	0.38	0/777
10	W1	0.25	0/574	0.39	0/777
10	X1	0.25	0/574	0.41	0/777
11	a	0.37	0/2111	0.42	0/2861
12	c	0.35	0/772	0.45	0/1054
13	d	0.26	0/2786	0.51	0/3760
14	e	0.30	0/3305	0.46	0/4482
15	f	0.34	0/1183	0.50	0/1601

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	g	0.24	0/1953	0.44	0/2650
17	h	0.24	0/1088	0.39	0/1466
18	i	0.33	0/913	0.47	0/1240
19	j	0.28	0/1462	0.48	0/1973
20	k	0.29	0/904	0.49	0/1228
21	n	0.33	0/1166	0.45	0/1581
22	o	0.28	0/814	0.39	0/1100
23	p	0.30	0/707	0.45	0/957
24	q	0.31	0/799	0.50	0/1091
25	r	0.34	0/567	0.46	0/767
All	All	0.26	0/63273	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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	4084	4197	4196	23	0
1	B1	4038	4162	4160	28	0
1	C1	4039	4155	4154	22	0
2	D1	3689	3742	3741	24	0
2	E1	3682	3733	3733	27	0
2	F1	3703	3759	3758	28	0
3	G1	2387	2387	2387	39	0
4	H1	1251	1232	1231	14	0
5	I1	533	513	513	2	0
6	J1	1315	1276	1276	11	0
6	K1	1315	1276	1276	6	0
6	L1	1310	1271	1271	2	0
7	L	537	545	545	2	0
7	l	537	545	545	0	0
8	M	1027	1042	1042	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	m	1027	1042	1042	0	0
9	M1	1877	1873	1873	9	0
10	O1	565	600	599	10	0
10	P1	565	600	599	7	0
10	Q1	565	600	599	5	0
10	R1	565	600	599	2	0
10	S1	565	601	599	2	0
10	T1	565	601	599	5	0
10	U1	565	600	599	5	0
10	V1	565	600	599	0	0
10	W1	565	600	599	5	0
10	X1	565	600	599	8	0
11	a	2032	2044	2044	0	0
12	c	745	715	715	0	0
13	d	2737	2762	2763	0	0
14	e	3220	3050	3061	0	0
15	f	1145	1111	1111	0	0
16	g	1933	2020	2020	0	0
17	h	1070	1088	1088	0	0
18	i	883	857	857	0	0
19	j	1424	1411	1411	0	0
20	k	873	876	876	0	0
21	n	1128	1082	1082	0	0
22	o	789	767	767	0	0
23	p	684	651	651	0	0
24	q	766	720	720	0	0
25	r	542	498	498	0	0
26	A1	31	12	12	0	0
26	B1	31	12	12	0	0
26	C1	31	12	12	0	0
26	F1	31	12	12	1	0
27	A1	1	0	0	0	0
27	B1	1	0	0	0	0
27	C1	1	0	0	0	0
27	D1	1	0	0	0	0
27	F1	1	0	0	0	0
28	D1	27	12	12	0	0
29	H1	29	11	11	0	0
30	L	100	156	156	0	0
30	M	100	156	156	1	0
30	c	100	156	156	0	0
30	e	500	780	780	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	f	100	156	156	0	0
30	j	200	312	312	0	0
30	l	100	156	156	0	0
30	m	100	156	156	0	0
30	q	100	156	156	0	0
31	M	51	82	82	1	0
31	f	51	82	82	0	0
31	m	51	82	82	0	0
32	a	54	88	88	0	0
32	f	108	176	176	0	0
32	i	54	88	88	0	0
33	e	35	39	46	0	0
33	j	35	39	46	0	0
34	e	48	60	0	0	0
34	n	59	70	0	0	0
All	All	64103	65465	65342	252	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (252) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F1:184:GLY:O	2:F1:189:LYS:NZ	2.23	0.72
3:G1:76:ILE:O	3:G1:90:ILE:HD13	1.90	0.71
10:O1:44:ALA:HB3	10:X1:41:SER:O	1.92	0.70
1:B1:531:PHE:O	1:B1:532:THR:HG22	1.92	0.69
1:A1:75:ALA:HB3	1:A1:78:THR:HG21	1.74	0.68
1:C1:533:LEU:HD22	1:C1:542:LEU:HD22	1.75	0.67
3:G1:90:ILE:HD11	3:G1:162:ASN:OD1	1.95	0.66
3:G1:241:ARG:O	3:G1:245:VAL:HG23	1.97	0.65
10:R1:86:LEU:HD11	10:S1:84:PRO:HB3	1.80	0.64
1:A1:398:GLN:NE2	1:A1:463:ASN:OD1	2.32	0.63
10:U1:48:GLN:O	10:U1:51:HIS:ND1	2.29	0.62
2:D1:184:GLY:O	2:D1:189:LYS:NZ	2.31	0.62
2:E1:165:LYS:NZ	2:E1:486:VAL:O	2.27	0.62
4:H1:46:ASN:N	4:H1:46:ASN:OD1	2.30	0.62
9:M1:210:ASP:OD1	9:M1:210:ASP:N	2.30	0.61
10:O1:84:PRO:O	10:O1:87:THR:HG23	2.01	0.60
3:G1:198:ASN:O	4:H1:37:ASN:ND2	2.34	0.60
2:F1:486:VAL:HG21	2:F1:492:VAL:HG22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:66:GLN:HG3	7:L:68:VAL:HG23	1.83	0.60
9:M1:110:MET:CE	9:M1:122:VAL:HG21	2.31	0.60
3:G1:93:CYS:O	3:G1:97:VAL:HG23	2.03	0.59
2:F1:178:LYS:NZ	2:F1:322:ILE:O	2.27	0.59
3:G1:209:GLU:HB2	3:G1:213:LEU:HD22	1.84	0.59
8:M:103:PHE:CE2	8:M:107:LEU:HD11	2.39	0.58
6:K1:28:ASP:OD1	6:K1:32:TYR:N	2.37	0.57
2:E1:263:LEU:HD21	2:E1:321:ARG:HB2	1.86	0.57
1:A1:438:ALA:O	1:A1:441:SER:OG	2.17	0.57
2:E1:416:VAL:O	3:G1:34:ARG:NH1	2.37	0.57
2:E1:410:LEU:O	2:E1:414:ILE:HG23	2.05	0.56
7:L:10:LEU:HD13	8:M:83:ILE:HD11	1.87	0.56
2:E1:130:ASP:O	6:L1:32:TYR:OH	2.23	0.56
2:D1:347:ALA:HB3	2:D1:348:PRO:HD3	1.87	0.56
10:O1:111:LEU:HD11	10:P1:113:PHE:HE1	1.70	0.56
1:B1:107:LEU:HD12	1:B1:111:ILE:HG23	1.88	0.55
2:E1:416:VAL:HG13	3:G1:30:LEU:HD11	1.88	0.55
1:C1:515:LYS:O	6:K1:134:ARG:NH1	2.40	0.55
2:F1:118:LEU:HA	2:F1:242:VAL:HG22	1.89	0.55
6:K1:70:ILE:O	6:K1:74:ASN:ND2	2.40	0.54
1:A1:457:ARG:NH2	1:A1:488:VAL:O	2.40	0.54
1:B1:180:ASN:OD1	1:B1:181:TYR:N	2.40	0.54
3:G1:51:GLU:O	3:G1:55:SER:N	2.40	0.54
3:G1:255:LEU:O	3:G1:259:THR:HG23	2.08	0.54
1:C1:523:GLU:N	1:C1:523:GLU:OE1	2.37	0.54
3:G1:246:GLU:O	3:G1:250:THR:HG23	2.07	0.54
9:M1:110:MET:HE2	9:M1:122:VAL:HG21	1.89	0.54
2:E1:68:ARG:NH1	2:E1:92:THR:O	2.38	0.54
3:G1:186:ASP:OD2	3:G1:199:ARG:NH2	2.41	0.53
4:H1:39:ASP:OD1	4:H1:39:ASP:N	2.40	0.53
4:H1:132:THR:HG21	4:H1:137:LEU:HD21	1.90	0.53
1:B1:173:ILE:HG23	1:B1:174:VAL:HG13	1.90	0.53
1:B1:239:ILE:HG23	1:B1:267:THR:HG23	1.91	0.53
6:J1:117:GLU:O	6:J1:121:THR:HG23	2.07	0.53
10:O1:70:GLY:HA2	10:X1:72:ILE:HD11	1.91	0.53
1:C1:447:VAL:HG12	1:C1:449:THR:HG23	1.90	0.53
3:G1:188:ALA:HB1	10:Q1:85:ASN:HD21	1.74	0.53
2:D1:91:GLN:OE1	2:D1:91:GLN:N	2.42	0.53
1:C1:514:ASN:O	1:C1:518:TYR:OH	2.20	0.53
1:C1:59:ASP:OD1	2:F1:300:ARG:NH2	2.42	0.52
30:M:201:CDL:H261	31:M:202:PEE:H44	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K1:165:ALA:O	6:K1:169:GLY:N	2.42	0.52
1:B1:199:GLY:N	1:B1:357:SER:OG	2.43	0.52
10:O1:100:LEU:HD22	10:P1:98:PHE:CZ	2.44	0.52
1:B1:508:MET:O	6:J1:179:GLN:NE2	2.42	0.52
4:H1:54:LEU:HD21	4:H1:131:CYS:SG	2.50	0.52
1:B1:328:ARG:NH2	2:F1:345:ASP:OD1	2.43	0.52
9:M1:162:HIS:NE2	9:M1:168:LEU:O	2.39	0.52
2:E1:412:ASP:O	2:E1:416:VAL:HG23	2.09	0.52
1:B1:75:ALA:HB3	1:B1:78:THR:HG21	1.92	0.51
1:B1:141:ASN:OD1	1:B1:145:HIS:N	2.43	0.51
8:M:119:ARG:NH2	8:M:122:ILE:O	2.44	0.51
1:A1:292:GLU:O	1:A1:296:ASN:ND2	2.42	0.51
10:O1:110:MET:SD	10:O1:111:LEU:HD12	2.51	0.51
2:D1:270:ARG:NH1	2:D1:323:THR:O	2.44	0.51
2:F1:272:VAL:HG12	2:F1:272:VAL:O	2.11	0.51
1:C1:454:ARG:NH1	1:C1:481:LEU:O	2.44	0.50
2:E1:416:VAL:CG1	3:G1:30:LEU:HD11	2.41	0.50
3:G1:7:LEU:O	3:G1:7:LEU:HD12	2.11	0.50
1:A1:188:LYS:NZ	1:A1:461:LEU:O	2.33	0.50
2:F1:120:ARG:NE	2:F1:130:ASP:OD2	2.43	0.50
2:D1:414:ILE:HG13	2:D1:422:LEU:HD11	1.93	0.50
2:F1:178:LYS:HG2	2:F1:355:LEU:HD23	1.92	0.50
3:G1:213:LEU:C	3:G1:213:LEU:HD23	2.32	0.50
1:B1:301:CYS:SG	1:B1:302:LEU:N	2.85	0.50
4:H1:161:ALA:O	4:H1:165:VAL:HG23	2.12	0.50
2:D1:486:VAL:HG21	2:D1:492:VAL:HG22	1.94	0.49
2:F1:180:GLY:HA3	2:F1:355:LEU:HD13	1.94	0.49
1:B1:531:PHE:O	1:B1:532:THR:CG2	2.60	0.49
10:T1:45:ILE:HD12	10:U1:45:ILE:HG21	1.94	0.49
1:B1:203:LEU:HD13	1:B1:379:VAL:HG11	1.93	0.49
1:C1:317:GLN:NE2	2:F1:313:GLU:OE1	2.44	0.49
3:G1:47:LEU:HD11	3:G1:228:ASN:HB2	1.95	0.49
8:M:103:PHE:CZ	8:M:107:LEU:HD11	2.47	0.49
3:G1:7:LEU:HD12	3:G1:7:LEU:C	2.32	0.49
4:H1:171:VAL:O	4:H1:175:VAL:HG23	2.13	0.49
2:E1:301:ILE:HG23	3:G1:279:LEU:HD13	1.94	0.49
2:E1:303:ALA:N	2:E1:307:TYR:O	2.39	0.49
10:O1:84:PRO:HB3	10:X1:86:LEU:HD11	1.95	0.49
10:O1:111:LEU:HD11	10:P1:113:PHE:CE1	2.47	0.48
10:T1:43:VAL:O	10:U1:45:ILE:HA	2.13	0.48
2:D1:448:GLU:O	2:D1:452:GLY:N	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F1:91:GLN:OE1	2:F1:91:GLN:N	2.46	0.48
1:A1:212:LYS:HG2	1:A1:389:LEU:HD12	1.96	0.48
1:A1:514:ASN:O	1:A1:518:TYR:OH	2.21	0.48
2:F1:347:ALA:HB3	2:F1:348:PRO:CD	2.43	0.48
1:B1:110:ASN:O	1:B1:114:VAL:HG23	2.14	0.48
3:G1:81:GLY:O	3:G1:241:ARG:NH1	2.47	0.48
10:W1:45:ILE:O	10:X1:48:GLN:N	2.46	0.48
10:O1:45:ILE:HD12	10:P1:45:ILE:HG21	1.95	0.48
6:K1:79:CYS:O	6:K1:83:SER:OG	2.21	0.48
6:J1:181:GLY:O	6:J1:185:VAL:HG23	2.14	0.47
1:C1:203:LEU:HD13	1:C1:379:VAL:CG1	2.43	0.47
2:E1:81:ASP:OD1	2:E1:84:THR:N	2.44	0.47
2:E1:164:ILE:HD12	2:E1:167:ILE:HD12	1.95	0.47
2:F1:263:LEU:HD21	2:F1:321:ARG:HB2	1.96	0.47
4:H1:61:LEU:HD12	4:H1:61:LEU:H	1.80	0.47
1:C1:203:LEU:HD13	1:C1:379:VAL:HG11	1.96	0.47
1:A1:398:GLN:NE2	1:A1:459:VAL:O	2.47	0.47
1:C1:168:THR:OG1	1:C1:345:ARG:NH2	2.47	0.47
1:A1:166:VAL:HG12	1:A1:166:VAL:O	2.14	0.47
2:F1:41:ILE:HG23	2:F1:41:ILE:O	2.15	0.47
3:G1:134:SER:OG	5:I1:45:ARG:NH2	2.48	0.47
3:G1:237:GLU:OE2	3:G1:241:ARG:NH2	2.48	0.47
6:J1:165:ALA:O	6:J1:169:GLY:N	2.48	0.47
2:D1:174:CYS:HB3	2:D1:383:ILE:HG21	1.96	0.46
3:G1:29:THR:HG21	3:G1:241:ARG:HD2	1.97	0.46
10:S1:86:LEU:HD22	10:T1:84:PRO:HB3	1.97	0.46
2:E1:174:CYS:HB3	2:E1:383:ILE:HD13	1.98	0.46
9:M1:110:MET:HE1	9:M1:122:VAL:HG21	1.96	0.46
2:E1:182:PHE:CD1	2:E1:358:THR:HG23	2.51	0.46
2:F1:137:GLU:OE1	2:F1:137:GLU:N	2.42	0.46
4:H1:82:TYR:O	10:T1:83:GLN:NE2	2.49	0.46
1:C1:166:VAL:HG12	1:C1:166:VAL:O	2.16	0.46
8:M:88:TYR:O	8:M:91:GLN:NE2	2.49	0.46
2:F1:260:GLN:OE1	2:F1:260:GLN:N	2.49	0.46
1:B1:531:PHE:O	1:B1:532:THR:CB	2.64	0.46
1:C1:531:PHE:O	1:C1:532:THR:CB	2.63	0.46
1:B1:111:ILE:HD12	1:B1:276:PRO:HB3	1.98	0.45
8:M:46:HIS:O	8:M:50:GLY:N	2.50	0.45
10:W1:43:VAL:O	10:X1:45:ILE:HA	2.16	0.45
4:H1:119:ASN:OD1	4:H1:120:ASN:N	2.48	0.45
6:J1:107:MET:O	6:J1:112:ARG:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:225:ARG:NH2	1:C1:522:GLN:OE1	2.49	0.45
3:G1:194:ASP:OD1	3:G1:195:ASN:N	2.50	0.45
1:B1:109:ASP:OD1	1:B1:109:ASP:N	2.50	0.45
2:F1:116:GLU:OE1	2:F1:116:GLU:N	2.44	0.45
2:F1:347:ALA:HB3	2:F1:348:PRO:HD3	1.98	0.45
1:A1:524:LEU:HD23	1:A1:527:LEU:HD12	1.98	0.45
3:G1:202:PHE:CZ	3:G1:206:LEU:HD12	2.52	0.45
1:B1:323:ARG:HA	2:E1:301:ILE:HD12	1.98	0.45
2:F1:232:VAL:HG11	2:F1:241:CYS:SG	2.58	0.44
10:P1:62:LEU:HD11	10:P1:109:LEU:HD13	1.99	0.44
6:J1:73:TYR:OH	6:J1:111:ASN:OD1	2.35	0.44
1:A1:537:ILE:HD12	1:A1:537:ILE:N	2.32	0.44
3:G1:22:VAL:HG12	3:G1:249:LEU:HG	2.00	0.44
10:Q1:111:LEU:HD23	10:Q1:114:LEU:HD12	2.00	0.44
2:F1:150:LEU:HD23	2:F1:150:LEU:O	2.17	0.44
2:F1:243:LEU:HD22	2:F1:245:TYR:HE2	1.81	0.44
9:M1:118:LEU:O	9:M1:122:VAL:HG23	2.17	0.44
1:A1:399:ARG:NH2	2:D1:398:GLN:OE1	2.51	0.44
6:J1:124:MET:HB3	6:J1:154:LEU:HD23	2.00	0.44
1:B1:107:LEU:CD1	1:B1:111:ILE:HG23	2.48	0.44
2:F1:270:ARG:NH1	2:F1:323:THR:O	2.48	0.44
1:A1:285:TYR:OH	1:A1:338:LEU:HD12	2.18	0.44
2:D1:180:GLY:HA3	2:D1:355:LEU:HD13	2.00	0.44
4:H1:94:PRO:O	4:H1:95:SER:OG	2.30	0.44
10:W1:47:VAL:HG23	10:X1:47:VAL:CG1	2.48	0.44
1:B1:52:ILE:C	1:B1:52:ILE:HD12	2.39	0.43
1:C1:62:ILE:HD12	1:C1:62:ILE:C	2.38	0.43
2:D1:351:THR:O	2:D1:351:THR:HG22	2.18	0.43
2:D1:470:LEU:HD23	2:D1:470:LEU:O	2.18	0.43
2:F1:166:VAL:HG12	2:F1:440:LEU:HD22	2.00	0.43
10:X1:70:GLY:O	10:X1:74:GLY:N	2.45	0.43
2:D1:75:GLU:OE2	2:D1:144:HIS:NE2	2.44	0.43
3:G1:47:LEU:HD11	3:G1:228:ASN:CB	2.48	0.43
3:G1:213:LEU:HD23	3:G1:214:ILE:N	2.33	0.43
1:A1:65:LEU:HD22	1:A1:120:VAL:HG21	2.01	0.43
1:B1:532:THR:HG23	1:B1:534:ASN:H	1.83	0.43
2:E1:172:PRO:O	2:E1:383:ILE:HD11	2.19	0.43
2:E1:305:VAL:HG12	2:E1:305:VAL:O	2.17	0.43
2:E1:360:VAL:HG21	2:E1:378:GLU:HG3	2.00	0.43
1:A1:131:VAL:HG11	1:A1:293:TYR:HB2	1.99	0.43
1:C1:411:VAL:HG11	1:C1:415:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E1:410:LEU:HD13	2:E1:430:VAL:HG23	2.00	0.43
10:P1:86:LEU:HD11	10:Q1:84:PRO:HB3	2.01	0.43
10:W1:84:PRO:O	10:W1:87:THR:HG23	2.18	0.43
1:A1:495:PHE:CE2	1:A1:499:LEU:HD11	2.52	0.43
1:A1:61:THR:HG22	1:A1:111:ILE:CD1	2.49	0.43
1:C1:537:ILE:N	1:C1:537:ILE:HD12	2.34	0.43
1:B1:295:MET:HB2	1:B1:358:VAL:HG23	2.00	0.43
1:B1:454:ARG:NH1	1:B1:481:LEU:O	2.52	0.43
2:E1:170:ILE:HG22	2:E1:170:ILE:O	2.19	0.43
2:D1:263:LEU:HD21	2:D1:321:ARG:HB2	2.01	0.43
6:J1:132:GLN:OE1	6:J1:135:LEU:HD12	2.19	0.43
2:E1:273:GLU:OE1	2:E1:275:GLN:NE2	2.52	0.42
1:B1:523:GLU:CB	6:J1:135:LEU:HD11	2.50	0.42
2:D1:130:ASP:O	6:K1:32:TYR:OH	2.28	0.42
2:D1:392:ASP:O	2:D1:396:VAL:HG23	2.19	0.42
3:G1:52:LEU:HD11	4:H1:35:VAL:HB	2.01	0.42
9:M1:66:ILE:HD12	9:M1:66:ILE:N	2.33	0.42
10:T1:45:ILE:HD12	10:U1:45:ILE:CG2	2.48	0.42
1:C1:135:VAL:HG12	1:C1:135:VAL:O	2.20	0.42
2:D1:288:THR:HG23	2:D1:311:LEU:HD13	2.00	0.42
2:F1:189:LYS:N	26:F1:601:ATP:O1B	2.49	0.42
3:G1:95:ASP:O	3:G1:98:VAL:HG23	2.20	0.42
10:W1:47:VAL:HG23	10:X1:47:VAL:HG13	2.02	0.42
1:B1:56:HIS:HB2	1:B1:66:ILE:HG23	2.02	0.42
2:E1:39:GLN:NE2	2:E1:46:ASP:OD2	2.49	0.42
3:G1:293:VAL:HG11	9:M1:109:TRP:CZ2	2.55	0.42
10:U1:47:VAL:HB	10:U1:50:LEU:HG	2.02	0.42
1:C1:80:ILE:HD12	1:C1:80:ILE:C	2.40	0.42
2:D1:282:ASP:HA	2:D1:283:ASN:HA	1.81	0.42
2:E1:432:ARG:NH1	2:E1:471:LEU:O	2.53	0.42
2:F1:446:VAL:HG12	2:F1:446:VAL:O	2.20	0.42
3:G1:52:LEU:O	3:G1:199:ARG:HD2	2.20	0.42
1:B1:80:ILE:HD12	1:B1:80:ILE:C	2.40	0.42
3:G1:8:TYR:CZ	3:G1:262:LEU:HD13	2.55	0.42
9:M1:90:VAL:CG2	9:M1:108:VAL:HG22	2.50	0.42
10:Q1:65:VAL:HG13	10:Q1:101:THR:HG22	2.02	0.42
6:J1:36:THR:HG22	6:J1:36:THR:O	2.20	0.42
3:G1:58:GLN:HE21	3:G1:58:GLN:HA	1.85	0.42
5:I1:70:ILE:N	5:I1:70:ILE:HD12	2.34	0.42
1:A1:203:LEU:HD13	1:A1:379:VAL:CG1	2.50	0.41
2:E1:282:ASP:HA	2:E1:283:ASN:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G1:22:VAL:HG13	3:G1:245:VAL:HG13	2.01	0.41
4:H1:97:LEU:HD23	4:H1:98:THR:N	2.36	0.41
1:A1:508:MET:O	6:L1:179:GLN:NE2	2.53	0.41
1:C1:52:ILE:HD12	1:C1:53:GLY:N	2.35	0.41
2:D1:170:ILE:HD12	2:D1:170:ILE:N	2.35	0.41
1:A1:511:THR:O	1:A1:511:THR:HG22	2.20	0.41
6:J1:86:LYS:HD2	6:J1:91:VAL:HG21	2.03	0.41
3:G1:12:LEU:O	3:G1:12:LEU:HD12	2.21	0.41
3:G1:30:LEU:HD12	3:G1:30:LEU:O	2.21	0.41
1:A1:135:VAL:O	1:A1:135:VAL:HG12	2.21	0.41
2:F1:110:SER:O	2:F1:140:ARG:NH1	2.54	0.41
1:A1:61:THR:HG21	2:D1:313:GLU:OE2	2.20	0.41
2:D1:263:LEU:HD13	2:D1:322:ILE:HG12	2.01	0.41
2:D1:305:VAL:HG12	2:D1:305:VAL:O	2.20	0.41
3:G1:95:ASP:HA	3:G1:98:VAL:HG23	2.03	0.41
10:R1:96:LEU:HD23	10:R1:96:LEU:O	2.20	0.41
1:B1:471:MET:N	1:B1:525:ASN:OD1	2.54	0.41
2:E1:347:ALA:HB3	2:E1:348:PRO:CD	2.51	0.41
10:O1:72:ILE:HD11	10:P1:70:GLY:HA2	2.02	0.41
1:B1:226:ILE:O	1:B1:230:ILE:HG12	2.21	0.40
1:C1:301:CYS:SG	1:C1:302:LEU:N	2.94	0.40
1:C1:531:PHE:O	1:C1:532:THR:HB	2.22	0.40
2:D1:343:ILE:HD11	2:D1:352:PHE:CZ	2.56	0.40
2:F1:62:VAL:HG21	2:F1:72:LEU:HD23	2.03	0.40
2:E1:91:GLN:N	2:E1:91:GLN:OE1	2.54	0.40
10:Q1:55:THR:HG23	10:Q1:112:ALA:HB1	2.03	0.40
2:D1:263:LEU:HD21	2:D1:321:ARG:CB	2.52	0.40
3:G1:58:GLN:HE21	3:G1:58:GLN:CA	2.34	0.40
4:H1:85:HIS:HB3	4:H1:118:ILE:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	526/584 (90%)	521 (99%)	5 (1%)	0	100	100
1	B1	517/584 (88%)	508 (98%)	8 (2%)	1 (0%)	47	78
1	C1	517/584 (88%)	512 (99%)	5 (1%)	0	100	100
2	D1	485/519 (93%)	478 (99%)	6 (1%)	1 (0%)	47	78
2	E1	484/519 (93%)	476 (98%)	8 (2%)	0	100	100
2	F1	487/519 (94%)	479 (98%)	8 (2%)	0	100	100
3	G1	298/305 (98%)	288 (97%)	10 (3%)	0	100	100
4	H1	159/182 (87%)	155 (98%)	4 (2%)	0	100	100
5	I1	63/75 (84%)	63 (100%)	0	0	100	100
6	J1	164/188 (87%)	163 (99%)	1 (1%)	0	100	100
6	K1	164/188 (87%)	160 (98%)	4 (2%)	0	100	100
6	L1	163/188 (87%)	161 (99%)	2 (1%)	0	100	100
7	L	63/92 (68%)	63 (100%)	0	0	100	100
7	l	63/92 (68%)	63 (100%)	0	0	100	100
8	M	127/144 (88%)	127 (100%)	0	0	100	100
8	m	127/144 (88%)	127 (100%)	0	0	100	100
9	M1	230/255 (90%)	225 (98%)	5 (2%)	0	100	100
10	O1	76/118 (64%)	75 (99%)	1 (1%)	0	100	100
10	P1	76/118 (64%)	76 (100%)	0	0	100	100
10	Q1	76/118 (64%)	76 (100%)	0	0	100	100
10	R1	76/118 (64%)	76 (100%)	0	0	100	100
10	S1	76/118 (64%)	76 (100%)	0	0	100	100
10	T1	76/118 (64%)	76 (100%)	0	0	100	100
10	U1	76/118 (64%)	75 (99%)	1 (1%)	0	100	100
10	V1	76/118 (64%)	76 (100%)	0	0	100	100
10	W1	76/118 (64%)	76 (100%)	0	0	100	100
10	X1	76/118 (64%)	76 (100%)	0	0	100	100
11	a	229/231 (99%)	224 (98%)	5 (2%)	0	100	100
12	c	84/114 (74%)	82 (98%)	2 (2%)	0	100	100
13	d	328/370 (89%)	319 (97%)	9 (3%)	0	100	100
14	e	381/396 (96%)	376 (99%)	5 (1%)	0	100	100
15	f	133/145 (92%)	129 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	g	266/269 (99%)	264 (99%)	2 (1%)	0	100	100
17	h	135/157 (86%)	134 (99%)	1 (1%)	0	100	100
18	i	101/104 (97%)	100 (99%)	1 (1%)	0	100	100
19	j	166/169 (98%)	162 (98%)	4 (2%)	0	100	100
20	k	103/124 (83%)	101 (98%)	2 (2%)	0	100	100
21	n	137/156 (88%)	129 (94%)	8 (6%)	0	100	100
22	o	94/101 (93%)	94 (100%)	0	0	100	100
23	p	78/105 (74%)	76 (97%)	2 (3%)	0	100	100
24	q	83/98 (85%)	81 (98%)	2 (2%)	0	100	100
25	r	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
All	All	7775/8943 (87%)	7657 (98%)	116 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B1	532	THR
2	D1	305	VAL

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	A1	439/479 (92%)	437 (100%)	2 (0%)	88	94
1	B1	435/479 (91%)	434 (100%)	1 (0%)	93	97
1	C1	434/479 (91%)	432 (100%)	2 (0%)	88	94
2	D1	398/420 (95%)	397 (100%)	1 (0%)	92	96
2	E1	397/420 (94%)	396 (100%)	1 (0%)	92	96
2	F1	400/420 (95%)	399 (100%)	1 (0%)	92	96
3	G1	253/257 (98%)	239 (94%)	14 (6%)	21	53
4	H1	137/156 (88%)	134 (98%)	3 (2%)	52	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	I1	58/67 (87%)	58 (100%)	0	100	100
6	J1	145/162 (90%)	145 (100%)	0	100	100
6	K1	145/162 (90%)	145 (100%)	0	100	100
6	L1	145/162 (90%)	144 (99%)	1 (1%)	84	91
7	L	55/75 (73%)	55 (100%)	0	100	100
7	l	55/75 (73%)	55 (100%)	0	100	100
8	M	111/124 (90%)	111 (100%)	0	100	100
8	m	111/124 (90%)	111 (100%)	0	100	100
9	M1	200/215 (93%)	198 (99%)	2 (1%)	76	86
10	O1	56/89 (63%)	56 (100%)	0	100	100
10	P1	56/89 (63%)	55 (98%)	1 (2%)	59	77
10	Q1	56/89 (63%)	55 (98%)	1 (2%)	59	77
10	R1	56/89 (63%)	55 (98%)	1 (2%)	59	77
10	S1	56/89 (63%)	55 (98%)	1 (2%)	59	77
10	T1	56/89 (63%)	55 (98%)	1 (2%)	59	77
10	U1	56/89 (63%)	55 (98%)	1 (2%)	59	77
10	V1	56/89 (63%)	56 (100%)	0	100	100
10	W1	56/89 (63%)	56 (100%)	0	100	100
10	X1	56/89 (63%)	55 (98%)	1 (2%)	59	77
11	a	225/225 (100%)	223 (99%)	2 (1%)	78	88
12	c	80/104 (77%)	79 (99%)	1 (1%)	69	83
13	d	297/334 (89%)	297 (100%)	0	100	100
14	e	334/341 (98%)	333 (100%)	1 (0%)	92	96
15	f	119/124 (96%)	117 (98%)	2 (2%)	60	79
16	g	205/206 (100%)	205 (100%)	0	100	100
17	h	110/123 (89%)	110 (100%)	0	100	100
18	i	95/96 (99%)	95 (100%)	0	100	100
19	j	149/150 (99%)	149 (100%)	0	100	100
20	k	91/107 (85%)	91 (100%)	0	100	100
21	n	123/137 (90%)	123 (100%)	0	100	100
22	o	82/86 (95%)	81 (99%)	1 (1%)	71	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	p	75/94 (80%)	75 (100%)	0	100 100
24	q	80/92 (87%)	77 (96%)	3 (4%)	33 61
25	r	56/56 (100%)	56 (100%)	0	100 100
All	All	6599/7441 (89%)	6554 (99%)	45 (1%)	84 91

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	181	TYR
1	A1	281	TYR
1	B1	181	TYR
1	C1	181	TYR
1	C1	511	THR
2	D1	171	LEU
2	E1	171	LEU
2	F1	171	LEU
3	G1	6	ARG
3	G1	7	LEU
3	G1	9	LYS
3	G1	12	LEU
3	G1	18	PHE
3	G1	23	LYS
3	G1	30	LEU
3	G1	58	GLN
3	G1	83	CYS
3	G1	171	ARG
3	G1	182	LYS
3	G1	206	LEU
3	G1	262	LEU
3	G1	296	ASN
4	H1	39	ASP
4	H1	46	ASN
4	H1	87	TYR
6	L1	167	THR
9	M1	87	THR
9	M1	210	ASP
10	P1	98	PHE
10	Q1	104	ILE
10	R1	87	THR
10	S1	82	ARG
10	T1	106	LEU

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Mol	Chain	Res	Type
10	U1	83	GLN
10	X1	107	PHE
11	a	144	PHE
11	a	169	PHE
12	c	66	TYR
14	e	268	TYR
15	f	42	ASN
15	f	62	TYR
22	o	64	TYR
24	q	76	VAL
24	q	78	ASN
24	q	79	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	339	HIS
1	A1	398	GLN
1	B1	56	HIS
1	B1	296	ASN
2	E1	275	GLN
2	E1	456	HIS
2	F1	354	HIS
3	G1	58	GLN
3	G1	212	GLN
4	H1	44	HIS
6	J1	93	ASN
6	K1	82	GLN
6	L1	140	GLN
10	P1	83	GLN
10	Q1	85	ASN
10	S1	85	ASN
10	T1	51	HIS
10	T1	83	GLN
10	V1	75	ASN
12	c	113	ASN
14	e	69	ASN
24	q	72	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
14	AME	e	1	14	9,10,11	0.25	0	9,11,13	0.47	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
14	AME	e	1	14	-	3/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	e	1	AME	N-CA-CB-CG
14	e	1	AME	C-CA-N-CT1
14	e	1	AME	CB-CA-N-CT1

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	$\#\|Z\| > 2$
30	CDL	f	201	-	99,99,99	0.29	0	105,111,111	0.27	0
30	CDL	m	201	-	99,99,99	0.30	0	105,111,111	0.25	0
34	Q7G	e	407	-	54,54,90	0.13	0	82,84,138	0.31	0
34	Q7G	n	201	-	66,66,90	0.13	0	100,102,138	0.29	0
26	ATP	C1	601	27	26,33,33	0.62	0	31,52,52	0.61	1 (3%)
28	ADP	D1	601	27	24,29,29	0.70	0	29,45,45	0.78	1 (3%)
33	LMT	e	406	-	36,36,36	0.10	0	47,47,47	0.15	0
30	CDL	e	403	-	99,99,99	0.29	0	105,111,111	0.27	0
30	CDL	e	404	-	99,99,99	0.29	0	105,111,111	0.26	0
30	CDL	e	401	-	99,99,99	0.29	0	105,111,111	0.26	0
32	PC1	a	301	-	53,53,53	0.29	0	59,61,61	0.27	0
31	PEE	M	202	-	50,50,50	0.74	2 (4%)	53,55,55	0.48	0
26	ATP	F1	601	27	26,33,33	0.62	0	31,52,52	0.60	1 (3%)
30	CDL	q	101	-	99,99,99	0.29	0	105,111,111	0.29	0
30	CDL	j	202	-	99,99,99	0.29	0	105,111,111	0.26	0
30	CDL	M	201	-	99,99,99	0.29	0	105,111,111	0.32	1 (0%)
26	ATP	B1	601	27	26,33,33	0.61	0	31,52,52	0.60	1 (3%)
32	PC1	f	204	-	53,53,53	0.27	0	59,61,61	0.27	0
26	ATP	A1	601	27	26,33,33	0.62	0	31,52,52	0.61	1 (3%)
30	CDL	L	101	-	99,99,99	0.30	0	105,111,111	0.26	0
33	LMT	j	203	-	36,36,36	0.12	0	47,47,47	0.18	0
30	CDL	j	201	-	99,99,99	0.29	0	105,111,111	0.26	0
30	CDL	l	101	-	99,99,99	0.29	0	105,111,111	0.26	0
32	PC1	i	201	-	53,53,53	0.29	0	59,61,61	0.27	0
32	PC1	f	203	-	53,53,53	0.28	0	59,61,61	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	PEE	m	202	-	50,50,50	0.75	2 (4%)	53,55,55	0.48	0
31	PEE	f	202	-	50,50,50	0.76	2 (4%)	53,55,55	0.48	0
30	CDL	e	402	-	99,99,99	0.29	0	105,111,111	0.27	0
29	UTP	H1	201	-	22,30,30	1.02	1 (4%)	27,47,47	0.97	1 (3%)
30	CDL	c	201	-	99,99,99	0.29	0	105,111,111	0.27	0
30	CDL	e	405	-	99,99,99	0.30	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
30	CDL	f	201	-	-	21/110/110/110	-
30	CDL	m	201	-	-	29/110/110/110	-
34	Q7G	e	407	-	1/1/19/34	5/15/123/200	0/7/7/10
34	Q7G	n	201	-	2/2/24/34	6/20/148/200	0/8/8/10
26	ATP	C1	601	27	-	5/18/38/38	0/3/3/3
28	ADP	D1	601	27	-	1/12/32/32	0/3/3/3
33	LMT	e	406	-	-	1/21/61/61	0/2/2/2
30	CDL	e	403	-	-	27/110/110/110	-
30	CDL	e	404	-	-	21/110/110/110	-
30	CDL	e	401	-	-	22/110/110/110	-
32	PC1	a	301	-	-	12/57/57/57	-
31	PEE	M	202	-	-	26/54/54/54	-
26	ATP	F1	601	27	-	4/18/38/38	0/3/3/3
30	CDL	q	101	-	-	28/110/110/110	-
30	CDL	j	202	-	-	27/110/110/110	-
30	CDL	M	201	-	-	28/110/110/110	-
26	ATP	B1	601	27	-	8/18/38/38	0/3/3/3
32	PC1	f	204	-	-	5/57/57/57	-
26	ATP	A1	601	27	-	4/18/38/38	0/3/3/3
30	CDL	L	101	-	-	17/110/110/110	-
33	LMT	j	203	-	-	5/21/61/61	0/2/2/2
30	CDL	j	201	-	-	23/110/110/110	-
30	CDL	l	101	-	-	18/110/110/110	-
32	PC1	i	201	-	-	8/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PC1	f	203	-	-	7/57/57/57	-
31	PEE	m	202	-	-	23/54/54/54	-
31	PEE	f	202	-	-	19/54/54/54	-
30	CDL	e	402	-	-	24/110/110/110	-
29	UTP	H1	201	-	-	3/20/38/38	0/2/2/2
30	CDL	c	201	-	-	23/110/110/110	-
30	CDL	e	405	-	-	28/110/110/110	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	f	202	PEE	C39-C38	3.57	1.52	1.31
31	f	202	PEE	C18-C19	3.56	1.52	1.31
31	m	202	PEE	C18-C19	3.55	1.52	1.31
31	M	202	PEE	C18-C19	3.52	1.52	1.31
31	m	202	PEE	C39-C38	3.50	1.52	1.31
31	M	202	PEE	C39-C38	3.45	1.51	1.31
29	H1	201	UTP	C4-N3	3.09	1.38	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	H1	201	UTP	C5-C4-N3	-3.85	114.83	123.31
26	A1	601	ATP	C5-C6-N6	2.32	123.88	120.35
26	B1	601	ATP	C5-C6-N6	2.32	123.87	120.35
28	D1	601	ADP	C5-C6-N6	2.32	123.87	120.35
26	F1	601	ATP	C5-C6-N6	2.30	123.84	120.35
26	C1	601	ATP	C5-C6-N6	2.29	123.83	120.35
30	M	201	CDL	C27-C26-C25	2.10	129.38	113.42

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
34	e	407	Q7G	C1B
34	n	201	Q7G	C1B
34	n	201	Q7G	C1C

All (478) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A1	601	ATP	PB-O3B-PG-O2G
26	A1	601	ATP	C5'-O5'-PA-O1A
26	B1	601	ATP	PB-O3B-PG-O2G
26	C1	601	ATP	PB-O3B-PG-O2G
26	F1	601	ATP	PB-O3B-PG-O2G
29	H1	201	UTP	C5'-O5'-PA-O3A
30	L	101	CDL	CA2-OA2-PA1-OA4
30	M	201	CDL	CA2-C1-CB2-OB2
30	M	201	CDL	CA3-OA5-PA1-OA3
30	M	201	CDL	OA6-CA4-CA6-OA8
30	M	201	CDL	CB2-OB2-PB2-OB4
30	M	201	CDL	C51-CB5-OB6-CB4
30	c	201	CDL	CB2-OB2-PB2-OB3
30	c	201	CDL	CB3-OB5-PB2-OB4
30	e	401	CDL	CB2-OB2-PB2-OB3
30	e	401	CDL	CB2-OB2-PB2-OB4
30	e	401	CDL	CB3-OB5-PB2-OB3
30	e	402	CDL	CA3-OA5-PA1-OA2
30	e	402	CDL	CA3-OA5-PA1-OA3
30	e	402	CDL	CA3-OA5-PA1-OA4
30	e	403	CDL	CB2-OB2-PB2-OB3
30	e	404	CDL	O1-C1-CA2-OA2
30	e	404	CDL	CA3-OA5-PA1-OA4
30	e	404	CDL	CB3-OB5-PB2-OB3
30	e	404	CDL	CB3-OB5-PB2-OB4
30	e	405	CDL	CA3-OA5-PA1-OA3
30	e	405	CDL	CA3-OA5-PA1-OA4
30	f	201	CDL	CA2-OA2-PA1-OA4
30	j	201	CDL	CA2-OA2-PA1-OA3
30	j	201	CDL	CA3-OA5-PA1-OA2
30	j	201	CDL	CA3-OA5-PA1-OA3
30	j	201	CDL	CA3-OA5-PA1-OA4
30	j	202	CDL	CB3-OB5-PB2-OB4
30	l	101	CDL	CA2-OA2-PA1-OA4
30	m	201	CDL	CA2-C1-CB2-OB2
30	m	201	CDL	CA3-OA5-PA1-OA3
30	m	201	CDL	OA6-CA4-CA6-OA8
30	m	201	CDL	CB2-OB2-PB2-OB4
30	m	201	CDL	C51-CB5-OB6-CB4
30	q	101	CDL	CA2-C1-CB2-OB2
30	q	101	CDL	OA5-CA3-CA4-OA6
30	q	101	CDL	CB2-OB2-PB2-OB3
30	q	101	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
30	q	101	CDL	CB3-OB5-PB2-OB3
31	M	202	PEE	C1-O3P-P-O2P
31	M	202	PEE	O4P-C4-C5-N
31	f	202	PEE	O4P-C4-C5-N
31	m	202	PEE	C1-O3P-P-O2P
31	m	202	PEE	O4P-C4-C5-N
32	a	301	PC1	C11-O13-P-O14
32	a	301	PC1	C1-O11-P-O12
32	a	301	PC1	C1-O11-P-O14
32	f	203	PC1	C11-O13-P-O12
32	f	203	PC1	C1-O11-P-O14
32	f	204	PC1	O13-C11-C12-N
32	i	201	PC1	C11-O13-P-O12
32	i	201	PC1	C11-O13-P-O14
32	i	201	PC1	C11-O13-P-O11
32	i	201	PC1	O13-C11-C12-N
33	e	406	LMT	C2-C1-O1'-C1'
33	j	203	LMT	C2'-C1'-O1'-C1
33	j	203	LMT	O5'-C1'-O1'-C1
33	j	203	LMT	C2-C1-O1'-C1'
34	e	407	Q7G	C2B-C1B-O1B-C24
34	e	407	Q7G	O5B-C1B-O1B-C24
34	e	407	Q7G	CG1-C22-C23-C48
34	n	201	Q7G	C2B-C1B-O1B-C24
30	M	201	CDL	OB7-CB5-OB6-CB4
30	m	201	CDL	OB7-CB5-OB6-CB4
30	q	101	CDL	OA7-CA5-OA6-CA4
30	M	201	CDL	O1-C1-CB2-OB2
30	m	201	CDL	O1-C1-CB2-OB2
30	q	101	CDL	O1-C1-CB2-OB2
30	e	403	CDL	C11-CA5-OA6-CA4
30	q	101	CDL	C11-CA5-OA6-CA4
30	e	404	CDL	CB2-C1-CA2-OA2
30	e	404	CDL	CA2-C1-CB2-OB2
30	e	403	CDL	OA7-CA5-OA6-CA4
30	e	402	CDL	C31-CA7-OA8-CA6
31	M	202	PEE	C31-C30-O3-C3
31	m	202	PEE	C31-C30-O3-C3
30	e	405	CDL	OB5-CB3-CB4-OB6
30	e	403	CDL	O1-C1-CA2-OA2
30	e	404	CDL	O1-C1-CB2-OB2
30	e	402	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
30	e	405	CDL	CA7-C31-C32-C33
30	m	201	CDL	CA5-C11-C12-C13
31	m	202	PEE	O5-C30-O3-C3
30	M	201	CDL	CA5-C11-C12-C13
34	n	201	Q7G	O5B-C1B-O1B-C24
31	M	202	PEE	O5-C30-O3-C3
30	e	403	CDL	C51-CB5-OB6-CB4
30	e	401	CDL	C77-C78-C79-C80
30	L	101	CDL	CA2-OA2-PA1-OA5
30	L	101	CDL	CA3-OA5-PA1-OA2
30	M	201	CDL	CA3-OA5-PA1-OA2
30	M	201	CDL	CB2-OB2-PB2-OB5
30	c	201	CDL	CB3-OB5-PB2-OB2
30	e	401	CDL	CB2-OB2-PB2-OB5
30	e	404	CDL	CA3-OA5-PA1-OA2
30	e	404	CDL	CB3-OB5-PB2-OB2
30	e	405	CDL	CA3-OA5-PA1-OA2
30	e	405	CDL	CB3-OB5-PB2-OB2
30	f	201	CDL	CA2-OA2-PA1-OA5
30	f	201	CDL	CB3-OB5-PB2-OB2
30	j	202	CDL	CB3-OB5-PB2-OB2
30	l	101	CDL	CA2-OA2-PA1-OA5
30	l	101	CDL	CA3-OA5-PA1-OA2
30	m	201	CDL	CA3-OA5-PA1-OA2
30	m	201	CDL	CB2-OB2-PB2-OB5
30	q	101	CDL	CB2-OB2-PB2-OB5
31	M	202	PEE	C1-O3P-P-O4P
31	f	202	PEE	C4-O4P-P-O3P
31	m	202	PEE	C1-O3P-P-O4P
31	m	202	PEE	C4-O4P-P-O3P
32	a	301	PC1	C11-O13-P-O11
32	a	301	PC1	C1-O11-P-O13
32	f	203	PC1	C11-O13-P-O11
32	f	204	PC1	C11-O13-P-O11
30	e	403	CDL	OB7-CB5-OB6-CB4
30	e	405	CDL	C11-CA5-OA6-CA4
30	j	202	CDL	C11-CA5-OA6-CA4
30	e	405	CDL	OA7-CA5-OA6-CA4
30	j	202	CDL	OA7-CA5-OA6-CA4
30	e	403	CDL	C71-C72-C73-C74
30	j	201	CDL	CA4-CA3-OA5-PA1
30	j	201	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
30	j	202	CDL	C74-C75-C76-C77
30	e	405	CDL	C57-C58-C59-C60
30	j	201	CDL	OB5-CB3-CB4-CB6
30	j	202	CDL	C78-C79-C80-C81
34	e	407	Q7G	CG1-C22-C23-C24
30	c	201	CDL	C55-C56-C57-C58
30	e	403	CDL	C14-C15-C16-C17
30	L	101	CDL	C31-CA7-OA8-CA6
30	l	101	CDL	C31-CA7-OA8-CA6
30	e	402	CDL	C11-CA5-OA6-CA4
30	l	101	CDL	C11-CA5-OA6-CA4
31	f	202	PEE	C11-C10-O2-C2
30	m	201	CDL	C12-C13-C14-C15
30	j	201	CDL	CA7-C31-C32-C33
30	c	201	CDL	C34-C35-C36-C37
30	M	201	CDL	C12-C13-C14-C15
30	j	201	CDL	C81-C82-C83-C84
30	M	201	CDL	C73-C74-C75-C76
31	f	202	PEE	C42-C43-C44-C45
30	j	202	CDL	C15-C16-C17-C18
30	e	404	CDL	C17-C18-C19-C20
30	L	101	CDL	C11-CA5-OA6-CA4
30	e	404	CDL	C11-CA5-OA6-CA4
30	f	201	CDL	C11-CA5-OA6-CA4
30	j	202	CDL	C51-CB5-OB6-CB4
30	e	404	CDL	OA5-CA3-CA4-OA6
30	j	202	CDL	OB7-CB5-OB6-CB4
30	l	101	CDL	OA7-CA5-OA6-CA4
30	m	201	CDL	C73-C74-C75-C76
33	j	203	LMT	O5B-C5B-C6B-O6B
31	M	202	PEE	C22-C23-C24-C25
34	n	201	Q7G	O5C-C5C-C6C-O6C
31	M	202	PEE	C17-C18-C19-C20
31	m	202	PEE	C17-C18-C19-C20
30	e	402	CDL	C78-C79-C80-C81
30	L	101	CDL	OA7-CA5-OA6-CA4
30	e	402	CDL	OA7-CA5-OA6-CA4
31	M	202	PEE	C4-O4P-P-O3P
32	f	203	PC1	C1-O11-P-O13
30	L	101	CDL	OA9-CA7-OA8-CA6
30	l	101	CDL	OA9-CA7-OA8-CA6
30	q	101	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
30	e	403	CDL	C78-C79-C80-C81
31	M	202	PEE	C31-C32-C33-C34
30	c	201	CDL	C51-C52-C53-C54
30	q	101	CDL	CB7-C71-C72-C73
30	e	402	CDL	C81-C82-C83-C84
30	e	404	CDL	OA7-CA5-OA6-CA4
30	e	401	CDL	C18-C19-C20-C21
30	e	401	CDL	C56-C57-C58-C59
30	m	201	CDL	C78-C79-C80-C81
30	e	403	CDL	C17-C18-C19-C20
30	e	403	CDL	CB3-CB4-CB6-OB8
30	f	201	CDL	C77-C78-C79-C80
30	j	201	CDL	C62-C63-C64-C65
30	m	201	CDL	CA3-CA4-CA6-OA8
31	m	202	PEE	C1-C2-C3-O3
30	l	101	CDL	C14-C15-C16-C17
30	e	402	CDL	C11-C12-C13-C14
31	m	202	PEE	C22-C23-C24-C25
30	M	201	CDL	C78-C79-C80-C81
30	e	402	CDL	CA6-CA4-OA6-CA5
30	q	101	CDL	CB3-CB4-OB6-CB5
30	c	201	CDL	CA4-CA3-OA5-PA1
30	m	201	CDL	OA5-CA3-CA4-OA6
30	L	101	CDL	C14-C15-C16-C17
30	q	101	CDL	CA5-C11-C12-C13
30	e	403	CDL	OB6-CB4-CB6-OB8
30	f	201	CDL	OB6-CB4-CB6-OB8
32	f	203	PC1	O21-C2-C3-O31
31	f	202	PEE	O4-C10-O2-C2
30	j	201	CDL	C34-C35-C36-C37
30	j	202	CDL	C79-C80-C81-C82
26	F1	601	ATP	PG-O3B-PB-O1B
32	f	204	PC1	C37-C38-C39-C3A
30	f	201	CDL	OA7-CA5-OA6-CA4
30	c	201	CDL	CA4-CA6-OA8-CA7
30	M	201	CDL	OA5-CA3-CA4-CA6
30	e	405	CDL	OB5-CB3-CB4-CB6
30	m	201	CDL	OA5-CA3-CA4-CA6
30	j	202	CDL	C76-C77-C78-C79
30	q	101	CDL	C77-C78-C79-C80
31	m	202	PEE	C31-C32-C33-C34
30	e	405	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
31	M	202	PEE	C2-C1-O3P-P
31	m	202	PEE	C2-C1-O3P-P
30	e	402	CDL	C75-C76-C77-C78
30	M	201	CDL	CA3-CA4-CA6-OA8
30	e	404	CDL	CB3-CB4-CB6-OB8
30	e	405	CDL	CB3-CB4-CB6-OB8
30	j	202	CDL	CB3-CB4-CB6-OB8
31	M	202	PEE	C1-C2-C3-O3
32	f	203	PC1	C1-C2-C3-O31
30	M	201	CDL	C21-C22-C23-C24
30	c	201	CDL	C39-C40-C41-C42
30	c	201	CDL	CB2-OB2-PB2-OB5
30	e	401	CDL	CB3-OB5-PB2-OB2
30	q	101	CDL	CA2-OA2-PA1-OA5
30	M	201	CDL	OA5-CA3-CA4-OA6
30	c	201	CDL	OA5-CA3-CA4-OA6
30	f	201	CDL	OA5-CA3-CA4-OA6
30	j	201	CDL	OB5-CB3-CB4-OB6
30	j	202	CDL	OA5-CA3-CA4-OA6
30	m	201	CDL	C21-C22-C23-C24
30	L	101	CDL	OA6-CA4-CA6-OA8
30	l	101	CDL	OA6-CA4-CA6-OA8
30	q	101	CDL	CB2-C1-CA2-OA2
34	n	201	Q7G	C24-C23-C48-O1C
32	i	201	PC1	C2C-C2D-C2E-C2F
30	e	405	CDL	CA4-CA3-OA5-PA1
30	f	201	CDL	CB4-CB3-OB5-PB2
30	j	201	CDL	C1-CB2-OB2-PB2
32	a	301	PC1	C2-C1-O11-P
30	e	403	CDL	C62-C63-C64-C65
30	e	405	CDL	C76-C77-C78-C79
30	c	201	CDL	OA5-CA3-CA4-CA6
30	j	202	CDL	OA5-CA3-CA4-CA6
30	M	201	CDL	C42-C43-C44-C45
30	c	201	CDL	CA3-CA4-CA6-OA8
30	e	402	CDL	C1-CB2-OB2-PB2
30	l	101	CDL	CA4-CA3-OA5-PA1
31	f	202	PEE	C1-C2-C3-O3
30	j	202	CDL	O1-C1-CB2-OB2
26	B1	601	ATP	PB-O3B-PG-O3G
30	l	101	CDL	C31-C32-C33-C34
30	e	404	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
30	e	405	CDL	OB6-CB4-CB6-OB8
31	m	202	PEE	O2-C2-C3-O3
30	e	403	CDL	C12-C13-C14-C15
30	c	201	CDL	C38-C39-C40-C41
26	B1	601	ATP	PA-O3A-PB-O2B
30	c	201	CDL	C40-C41-C42-C43
34	n	201	Q7G	C16-C17-O20-CG1
30	e	401	CDL	C81-C82-C83-C84
30	c	201	CDL	C83-C84-C85-C86
30	e	403	CDL	CB2-OB2-PB2-OB5
30	l	101	CDL	CB2-OB2-PB2-OB5
30	L	101	CDL	CA4-CA3-OA5-PA1
30	e	402	CDL	CA4-CA3-OA5-PA1
29	H1	201	UTP	C5'-O5'-PA-O2A
30	L	101	CDL	CA2-OA2-PA1-OA3
30	L	101	CDL	CA3-OA5-PA1-OA3
30	M	201	CDL	CA3-OA5-PA1-OA4
30	e	401	CDL	CB3-OB5-PB2-OB4
30	e	405	CDL	CB3-OB5-PB2-OB3
30	f	201	CDL	CB3-OB5-PB2-OB3
30	l	101	CDL	CA2-OA2-PA1-OA3
30	l	101	CDL	CA3-OA5-PA1-OA3
30	m	201	CDL	CA3-OA5-PA1-OA4
31	M	202	PEE	C4-O4P-P-O2P
31	f	202	PEE	C4-O4P-P-O2P
31	f	202	PEE	C4-O4P-P-O1P
31	m	202	PEE	C4-O4P-P-O2P
31	m	202	PEE	C4-O4P-P-O1P
32	f	204	PC1	C11-O13-P-O12
30	L	101	CDL	C31-C32-C33-C34
30	e	405	CDL	OA5-CA3-CA4-OA6
34	e	407	Q7G	C23-C24-O1B-C1B
30	f	201	CDL	C13-C14-C15-C16
30	c	201	CDL	O1-C1-CA2-OA2
30	j	201	CDL	O1-C1-CA2-OA2
30	j	202	CDL	CA3-CA4-CA6-OA8
32	a	301	PC1	O13-C11-C12-N
32	f	203	PC1	O13-C11-C12-N
31	M	202	PEE	O2-C2-C3-O3
31	f	202	PEE	O2-C2-C3-O3
30	j	201	CDL	C72-C73-C74-C75
30	j	202	CDL	CB4-CB3-OB5-PB2

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Mol	Chain	Res	Type	Atoms
30	f	201	CDL	C12-C13-C14-C15
31	m	202	PEE	C41-C42-C43-C44
30	j	202	CDL	CB3-CB4-OB6-CB5
30	e	404	CDL	OA5-CA3-CA4-CA6
30	e	403	CDL	CB2-C1-CA2-OA2
32	i	201	PC1	C2A-C2B-C2C-C2D
31	m	202	PEE	C36-C37-C38-C39
30	e	401	CDL	CB4-CB3-OB5-PB2
30	e	405	CDL	C40-C41-C42-C43
30	j	202	CDL	C61-C62-C63-C64
30	L	101	CDL	CB2-OB2-PB2-OB5
30	c	201	CDL	CA3-OA5-PA1-OA2
30	q	101	CDL	CA3-OA5-PA1-OA2
30	q	101	CDL	CB3-OB5-PB2-OB2
31	f	202	PEE	C1-O3P-P-O4P
30	f	201	CDL	CB3-CB4-CB6-OB8
30	j	201	CDL	C55-C56-C57-C58
31	f	202	PEE	C19-C20-C21-C22
26	A1	601	ATP	PG-O3B-PB-O2B
26	C1	601	ATP	PG-O3B-PB-O2B
26	F1	601	ATP	PG-O3B-PB-O2B
34	n	201	Q7G	C18-C17-O20-CG1
33	j	203	LMT	C2-C3-C4-C5
30	m	201	CDL	C71-CB7-OB8-CB6
30	q	101	CDL	C1-CB2-OB2-PB2
30	c	201	CDL	CB2-C1-CA2-OA2
30	j	201	CDL	CB2-C1-CA2-OA2
30	M	201	CDL	C71-CB7-OB8-CB6
30	e	401	CDL	C13-C14-C15-C16
31	M	202	PEE	C39-C40-C41-C42
31	f	202	PEE	C18-C19-C20-C21
30	L	101	CDL	O1-C1-CA2-OA2
30	l	101	CDL	O1-C1-CA2-OA2
30	m	201	CDL	C42-C43-C44-C45
30	e	402	CDL	C74-C75-C76-C77
31	M	202	PEE	C36-C37-C38-C39
31	m	202	PEE	C23-C24-C25-C26
30	j	201	CDL	C77-C78-C79-C80
30	j	202	CDL	CA2-C1-CB2-OB2
31	f	202	PEE	O5-C30-O3-C3
26	F1	601	ATP	PB-O3B-PG-O1G
30	l	101	CDL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
30	M	201	CDL	C33-C34-C35-C36
30	L	101	CDL	C39-C40-C41-C42
30	e	404	CDL	CA6-CA4-OA6-CA5
30	j	201	CDL	CA3-CA4-OA6-CA5
30	e	401	CDL	OB7-CB5-OB6-CB4
30	e	405	CDL	C79-C80-C81-C82
31	f	202	PEE	C31-C30-O3-C3
30	m	201	CDL	OB9-CB7-OB8-CB6
30	e	402	CDL	C52-C51-CB5-OB6
32	f	204	PC1	O31-C31-C32-C33
30	e	402	CDL	C53-C54-C55-C56
30	e	403	CDL	C71-CB7-OB8-CB6
30	M	201	CDL	OB9-CB7-OB8-CB6
30	e	403	CDL	OA6-CA4-CA6-OA8
30	j	202	CDL	OA6-CA4-CA6-OA8
30	j	202	CDL	OB6-CB4-CB6-OB8
31	f	202	PEE	C16-C17-C18-C19
30	e	405	CDL	C53-C54-C55-C56
31	M	202	PEE	C23-C24-C25-C26
26	C1	601	ATP	PA-O3A-PB-O2B
30	m	201	CDL	C33-C34-C35-C36
30	e	403	CDL	OB9-CB7-OB8-CB6
30	M	201	CDL	CB3-CB4-CB6-OB8
30	e	403	CDL	CA3-CA4-CA6-OA8
30	e	404	CDL	C78-C79-C80-C81
30	f	201	CDL	C78-C79-C80-C81
31	M	202	PEE	C11-C10-O2-C2
30	e	404	CDL	C18-C19-C20-C21
30	c	201	CDL	C56-C57-C58-C59
31	f	202	PEE	C36-C37-C38-C39
31	m	202	PEE	C16-C17-C18-C19
30	e	401	CDL	OB5-CB3-CB4-OB6
30	e	402	CDL	OB5-CB3-CB4-OB6
30	c	201	CDL	CA5-C11-C12-C13
30	e	402	CDL	OB5-CB3-CB4-CB6
30	f	201	CDL	OA5-CA3-CA4-CA6
32	a	301	PC1	O11-C1-C2-C3
30	e	401	CDL	C51-CB5-OB6-CB4
31	m	202	PEE	C34-C35-C36-C37
30	e	403	CDL	C11-C12-C13-C14
30	c	201	CDL	OA6-CA4-CA6-OA8
30	m	201	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
30	e	405	CDL	C32-C31-CA7-OA8
32	i	201	PC1	O21-C21-C22-C23
30	e	403	CDL	C32-C31-CA7-OA8
31	f	202	PEE	O2-C10-C11-C12
26	A1	601	ATP	PB-O3B-PG-O1G
26	C1	601	ATP	PB-O3B-PG-O1G
28	D1	601	ADP	PA-O3A-PB-O1B
30	e	405	CDL	C56-C57-C58-C59
30	M	201	CDL	C12-C11-CA5-OA6
30	j	202	CDL	C12-C11-CA5-OA6
31	M	202	PEE	C16-C17-C18-C19
31	M	202	PEE	C38-C39-C40-C41
31	m	202	PEE	C38-C39-C40-C41
30	M	201	CDL	C19-C20-C21-C22
30	M	201	CDL	OA7-CA5-OA6-CA4
31	M	202	PEE	O4-C10-O2-C2
30	e	401	CDL	C16-C17-C18-C19
31	m	202	PEE	O2-C10-C11-C12
31	m	202	PEE	C18-C19-C20-C21
30	L	101	CDL	CA3-CA4-CA6-OA8
30	q	101	CDL	OB5-CB3-CB4-OB6
32	a	301	PC1	O11-C1-C2-O21
30	e	402	CDL	C72-C71-CB7-OB8
30	f	201	CDL	C72-C71-CB7-OB8
30	e	405	CDL	C81-C82-C83-C84
30	m	201	CDL	C12-C11-CA5-OA6
30	e	403	CDL	C52-C51-CB5-OB6
31	M	202	PEE	O2-C10-C11-C12
30	e	405	CDL	OA5-CA3-CA4-CA6
30	q	101	CDL	OB5-CB3-CB4-CB6
30	e	405	CDL	C74-C75-C76-C77
30	e	404	CDL	C32-C31-CA7-OA8
30	j	201	CDL	C52-C51-CB5-OB6
30	M	201	CDL	C12-C11-CA5-OA7
30	e	403	CDL	CB5-C51-C52-C53
31	M	202	PEE	C41-C42-C43-C44
30	e	401	CDL	C32-C31-CA7-OA8
30	e	405	CDL	C12-C11-CA5-OA6
26	B1	601	ATP	PG-O3B-PB-O1B
26	B1	601	ATP	PG-O3B-PB-O2B
26	B1	601	ATP	PA-O3A-PB-O1B
30	j	202	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
30	f	201	CDL	C12-C11-CA5-OA6
31	M	202	PEE	C18-C19-C20-C21
30	e	405	CDL	C32-C31-CA7-OA9
30	j	202	CDL	C59-C60-C61-C62
30	e	403	CDL	C32-C31-CA7-OA9
31	f	202	PEE	O4-C10-C11-C12
30	f	201	CDL	C72-C71-CB7-OB9
30	m	201	CDL	C12-C11-CA5-OA7
30	f	201	CDL	C37-C38-C39-C40
30	e	405	CDL	C12-C11-CA5-OA7
32	i	201	PC1	O22-C21-C22-C23
30	l	101	CDL	CA3-CA4-CA6-OA8
30	q	101	CDL	C72-C71-CB7-OB8
30	c	201	CDL	C62-C63-C64-C65
30	e	401	CDL	C63-C64-C65-C66
30	e	402	CDL	C72-C71-CB7-OB9
30	j	202	CDL	C12-C11-CA5-OA7
26	B1	601	ATP	C5'-O5'-PA-O1A
26	C1	601	ATP	C5'-O5'-PA-O1A
30	e	403	CDL	CB3-OB5-PB2-OB3
30	j	201	CDL	CA2-OA2-PA1-OA4
30	m	201	CDL	CB3-OB5-PB2-OB3
30	q	101	CDL	CA2-OA2-PA1-OA3
30	q	101	CDL	CA3-OA5-PA1-OA3
31	M	202	PEE	C4-O4P-P-O1P
31	f	202	PEE	C1-O3P-P-O1P
32	a	301	PC1	C11-O13-P-O12
30	m	201	CDL	C11-CA5-OA6-CA4
29	H1	201	UTP	O4'-C4'-C5'-O5'
30	e	403	CDL	C52-C51-CB5-OB7
30	f	201	CDL	C12-C11-CA5-OA7
31	m	202	PEE	O4-C10-C11-C12
30	j	202	CDL	C71-C72-C73-C74
31	M	202	PEE	C34-C35-C36-C37
31	M	202	PEE	O4-C10-C11-C12
26	B1	601	ATP	PB-O3B-PG-O1G
30	f	201	CDL	CA5-C11-C12-C13
30	e	401	CDL	C32-C31-CA7-OA9
30	e	401	CDL	C80-C81-C82-C83
30	j	201	CDL	CA6-CA4-OA6-CA5
32	a	301	PC1	C12-C11-O13-P
30	e	404	CDL	C32-C31-CA7-OA9

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Mol	Chain	Res	Type	Atoms
30	j	201	CDL	C52-C51-CB5-OB7
30	q	101	CDL	C71-C72-C73-C74
32	a	301	PC1	O31-C31-C32-C33
30	e	402	CDL	C19-C20-C21-C22
30	q	101	CDL	C73-C74-C75-C76
30	M	201	CDL	C72-C71-CB7-OB8
30	q	101	CDL	C72-C71-CB7-OB9
30	e	401	CDL	C52-C51-CB5-OB6
30	e	402	CDL	C32-C31-CA7-OA8
30	l	101	CDL	C60-C61-C62-C63
30	m	201	CDL	C14-C15-C16-C17
30	q	101	CDL	O1-C1-CA2-OA2
30	e	402	CDL	C32-C31-CA7-OA9
30	e	401	CDL	C43-C44-C45-C46
30	m	201	CDL	C72-C71-CB7-OB8

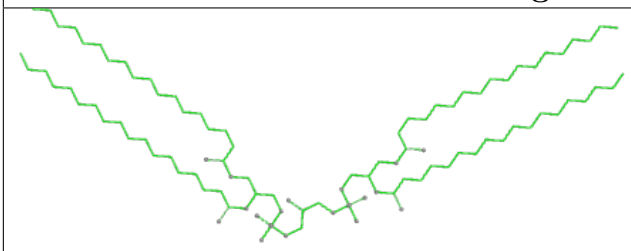
There are no ring outliers.

3 monomers are involved in 2 short contacts:

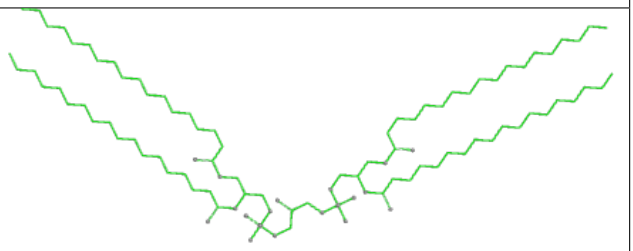
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	M	202	PEE	1	0
26	F1	601	ATP	1	0
30	M	201	CDL	1	0

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

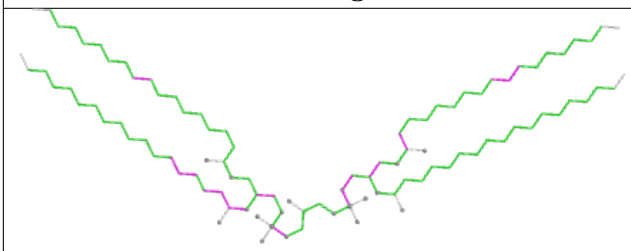
Ligand CDL f 201



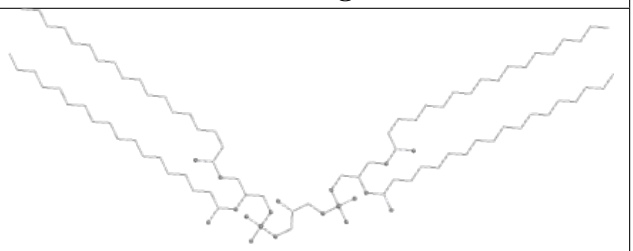
Bond lengths



Bond angles

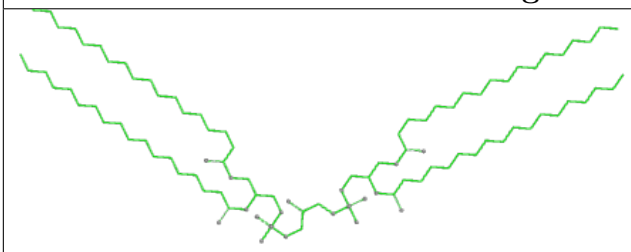


Torsions



Rings

Ligand CDL m 201



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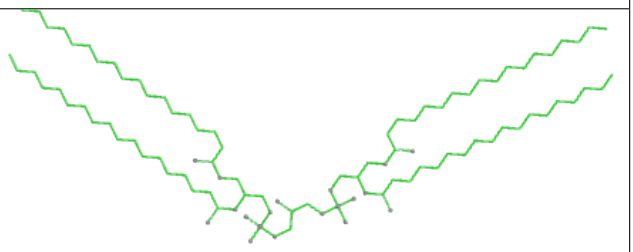
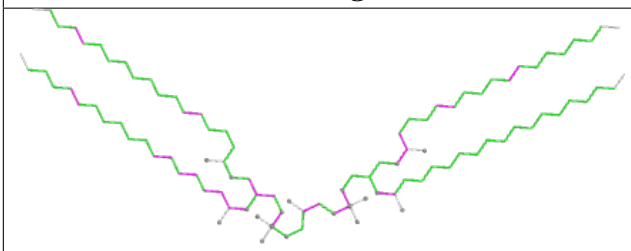
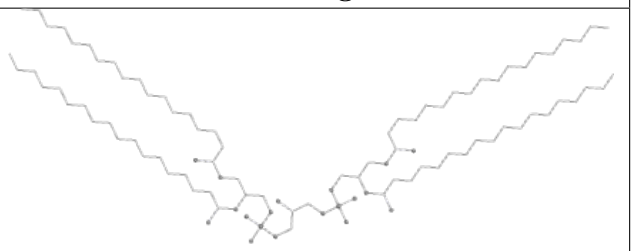


Bond angles

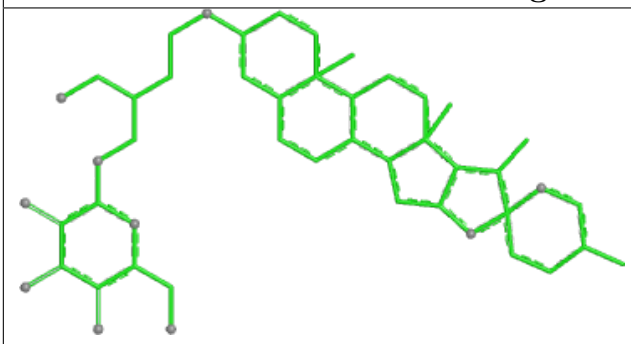


Torsions

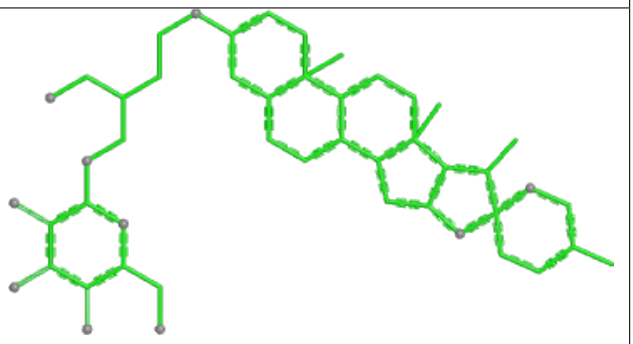


Rings

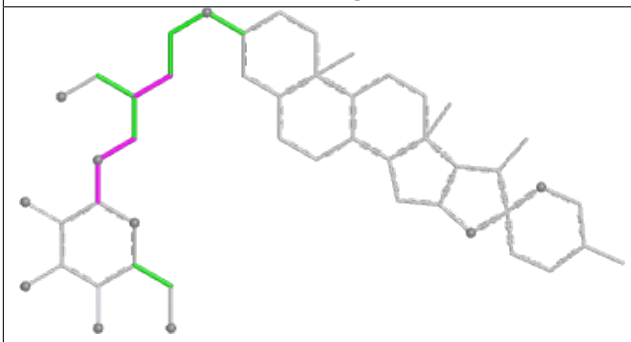
Ligand Q7G e 407



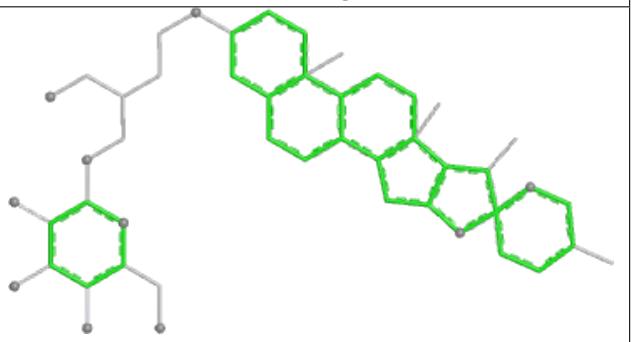
Bond lengths



Bond angles

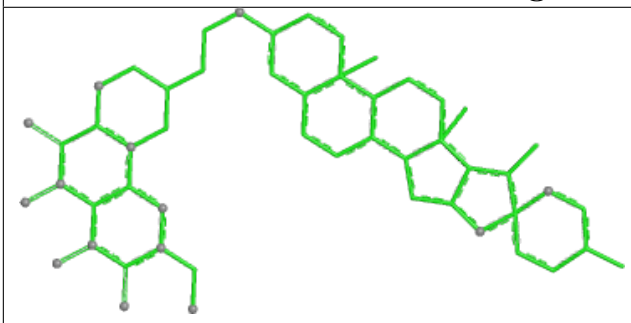


Torsions

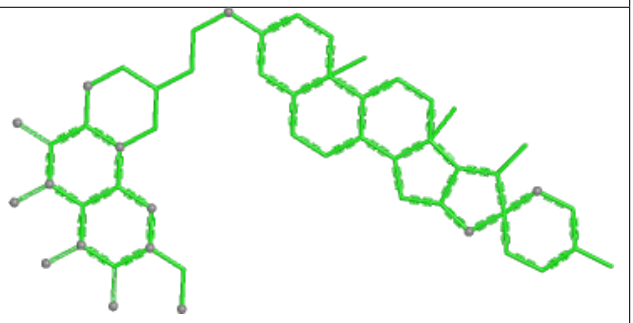


Rings

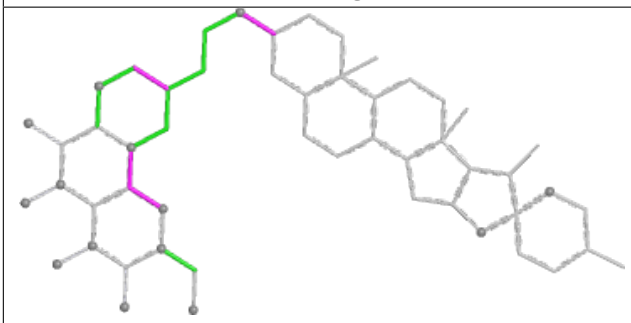
Ligand Q7G n 201



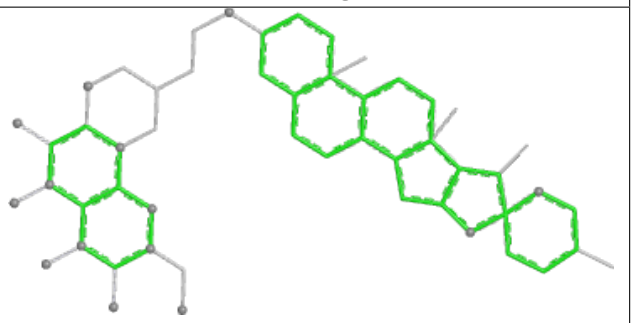
Bond lengths



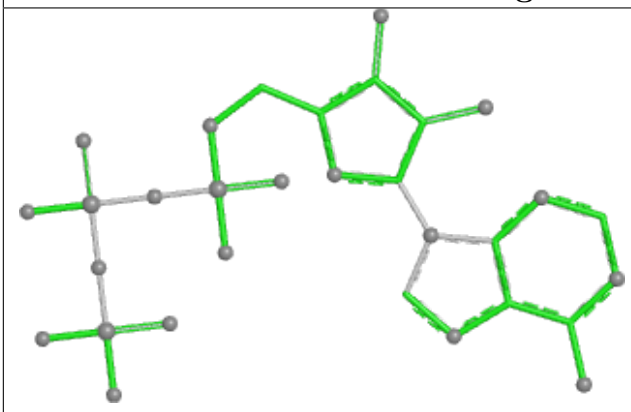
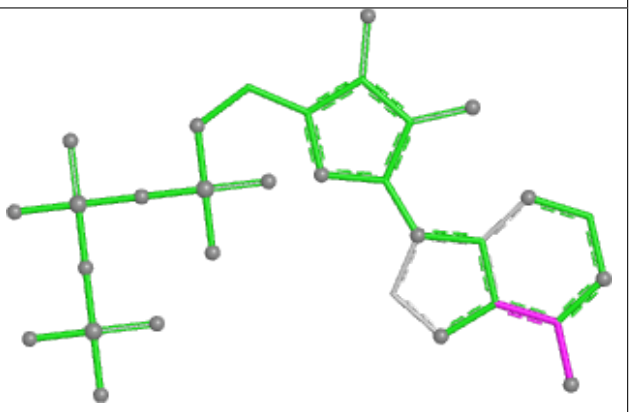
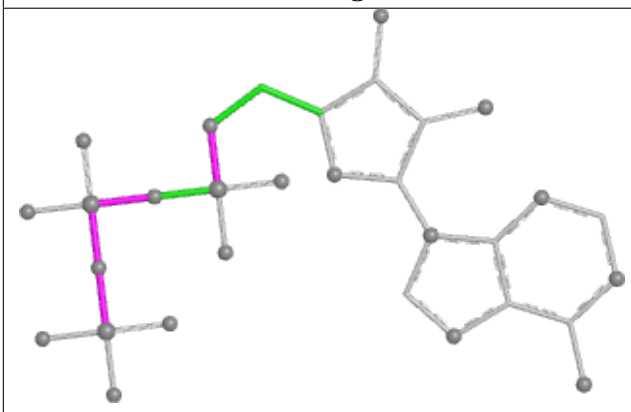
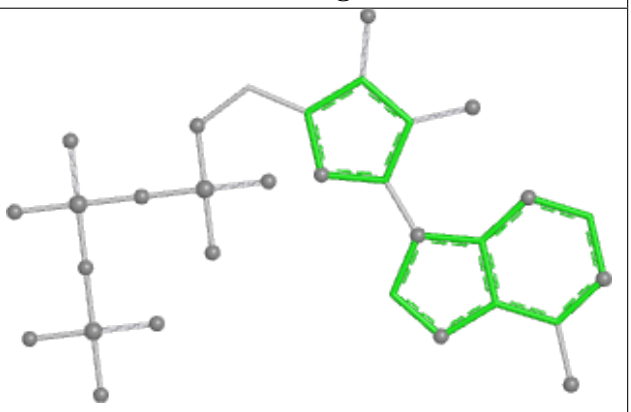
Bond angles

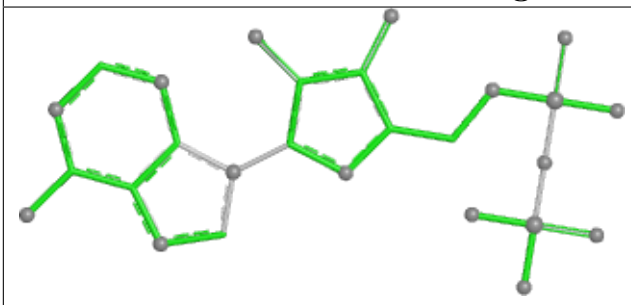
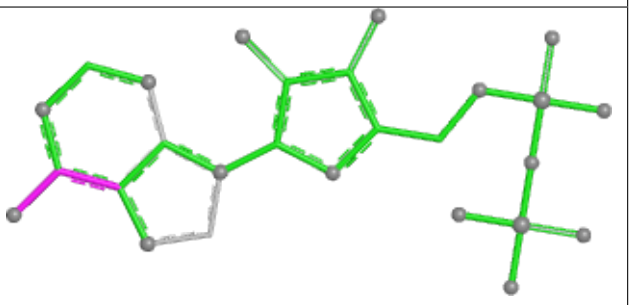
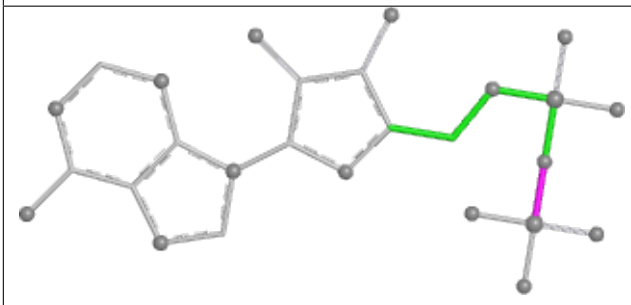
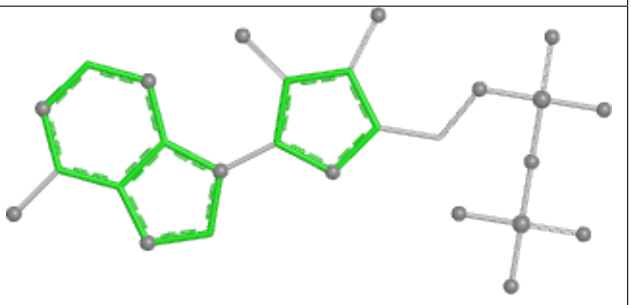


Torsions

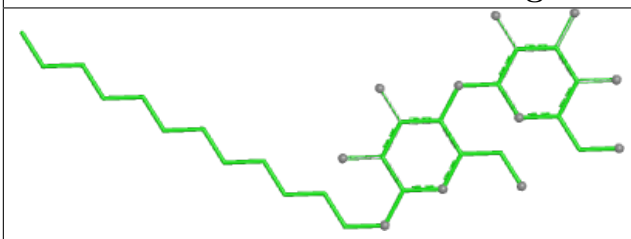


Rings

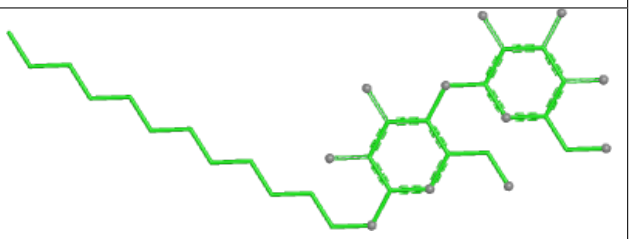
Ligand ATP C1 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP D1 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

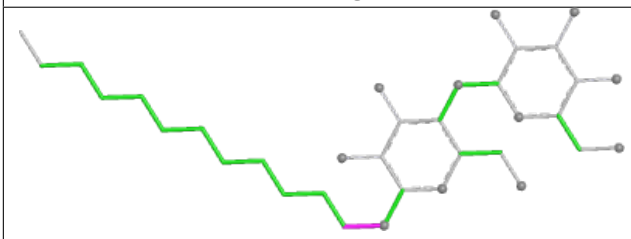
Ligand LMT e 406



Bond lengths



Bond angles



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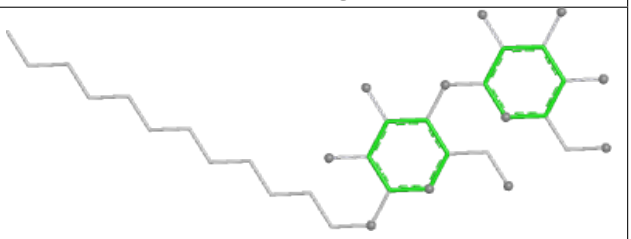
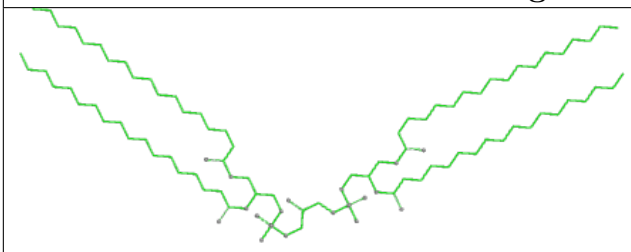


Rings

Ligand CDL e 403



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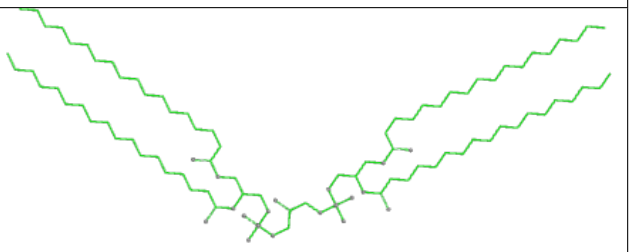

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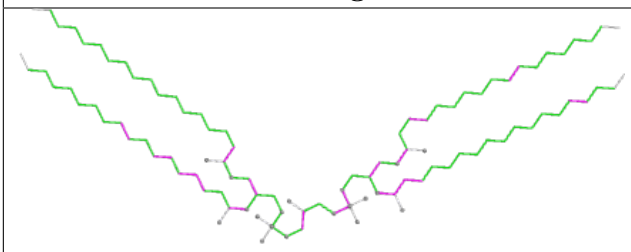

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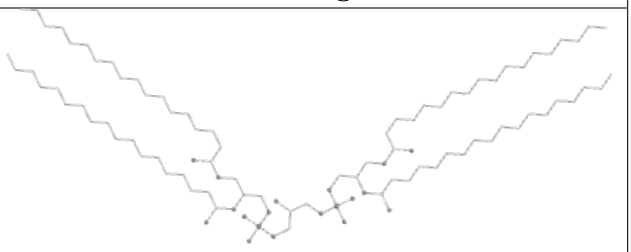
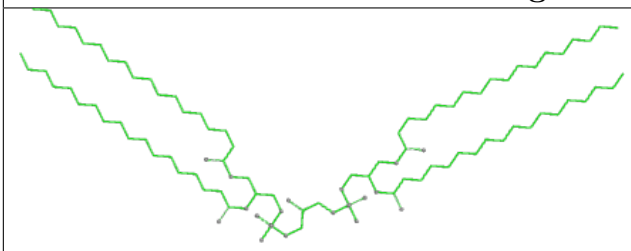


Rings

Ligand CDL e 404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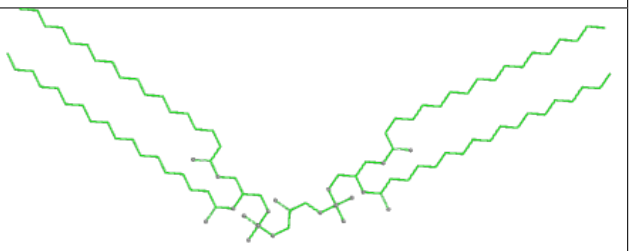
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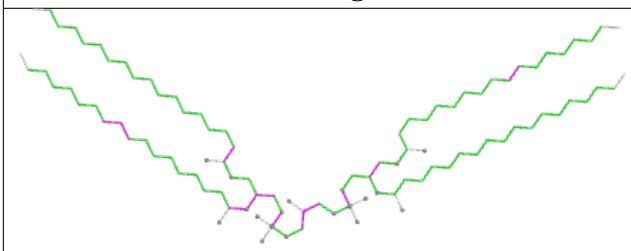
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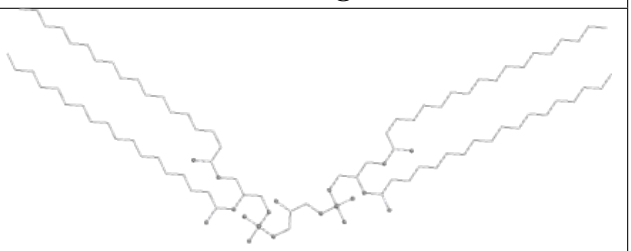
Rings

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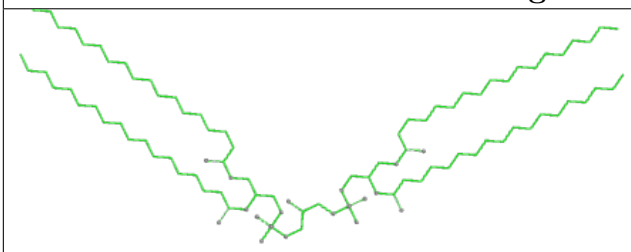
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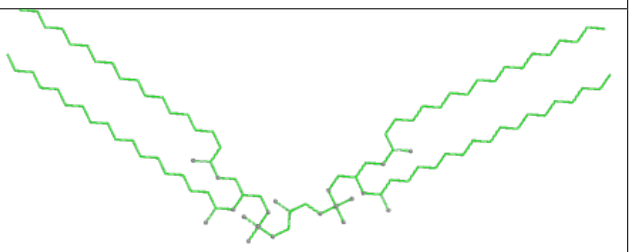
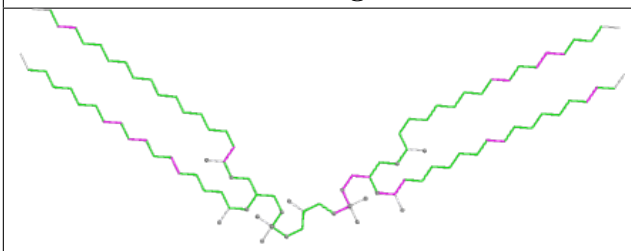
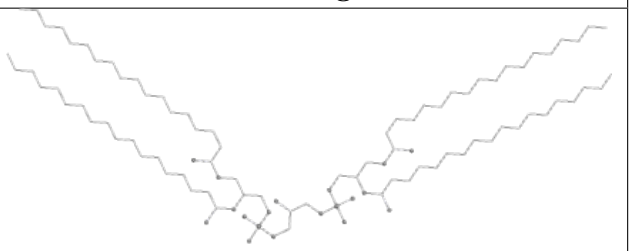
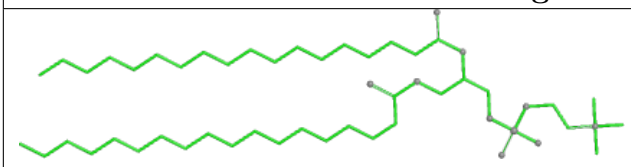

Bond angles


Torsions


Rings

Ligand PC1 a 301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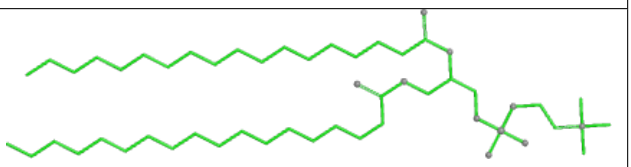
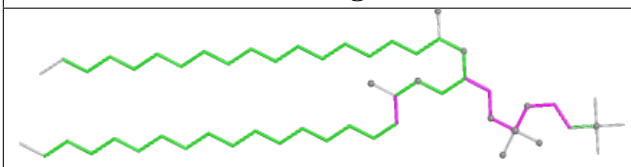

Bond angles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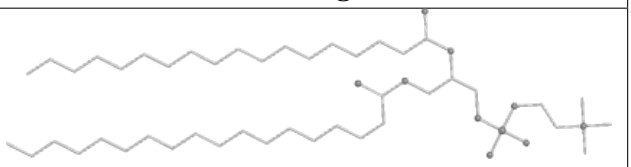
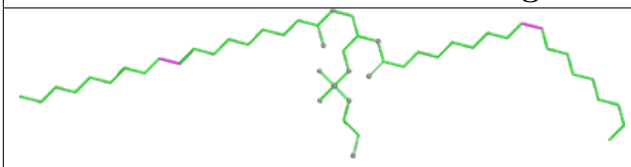
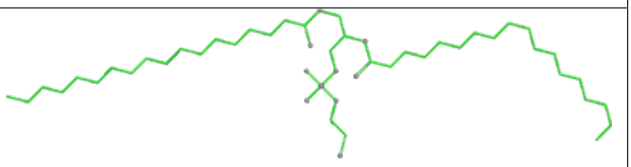
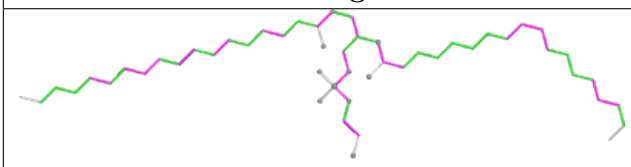
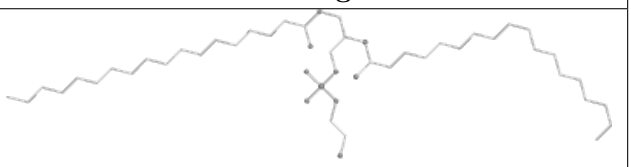
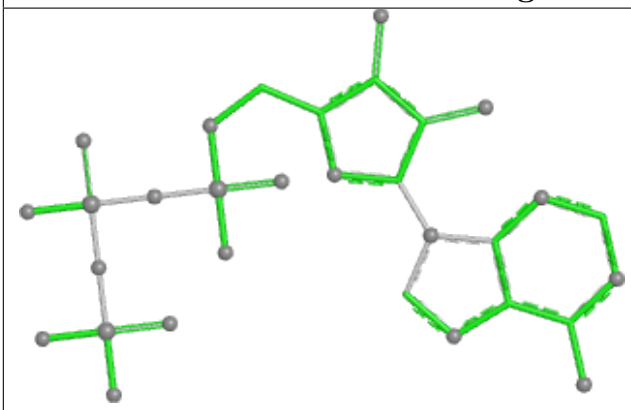
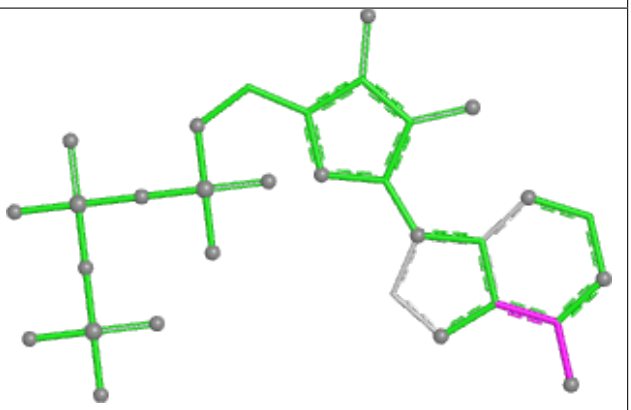
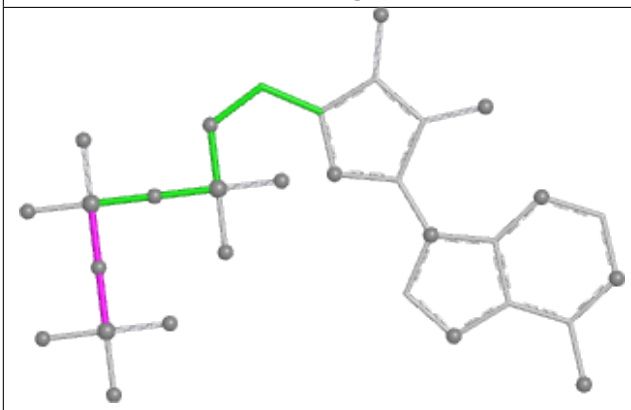
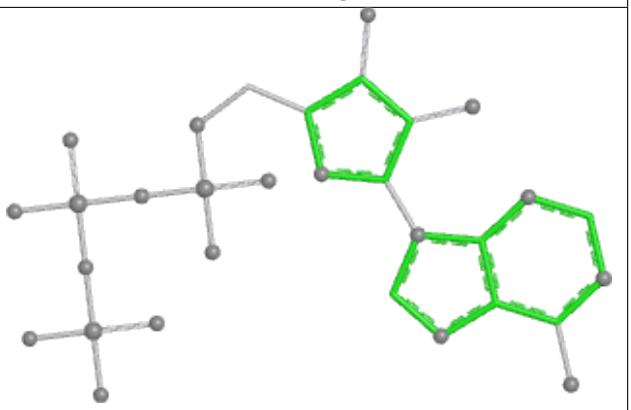
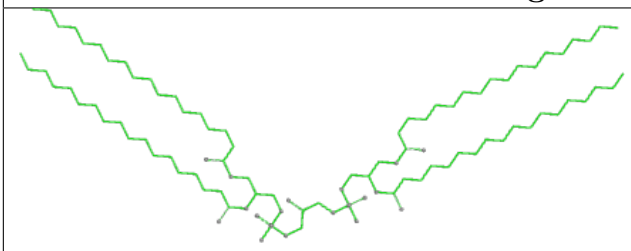

Rings

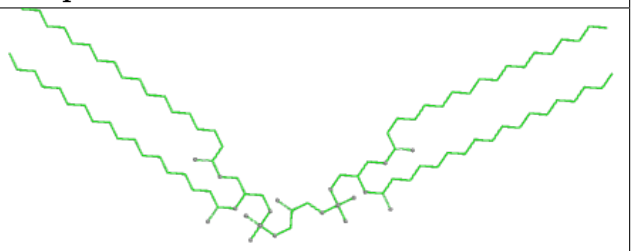
Ligand PEE M 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP F1 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

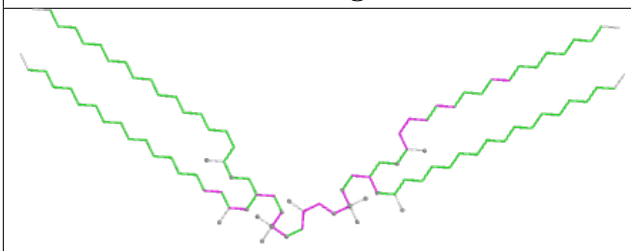
Ligand CDL q 101



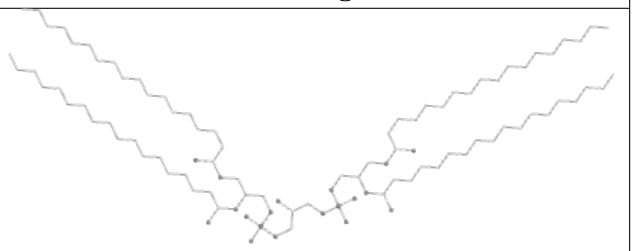
Bond lengths



Bond angles

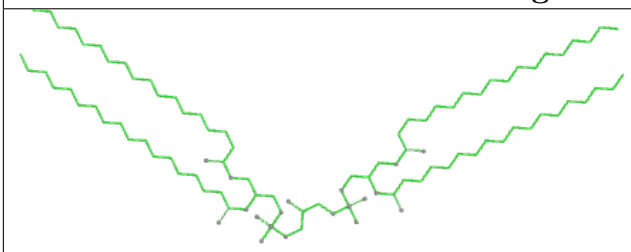


Torsions

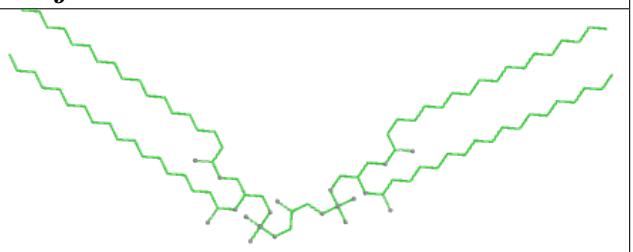


Rings

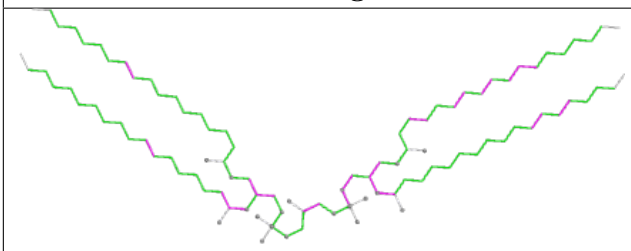
Ligand CDL j 202



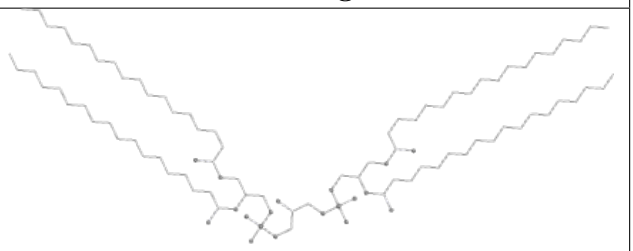
Bond lengths



Bond angles

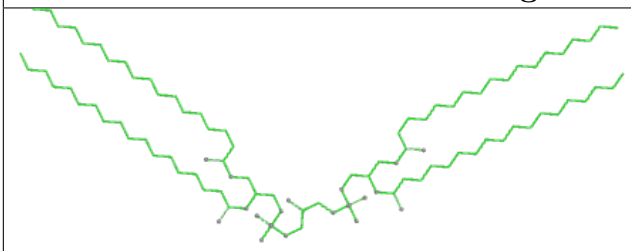


Torsions



Rings

Ligand CDL M 201



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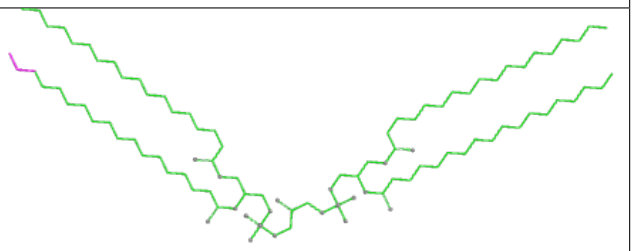

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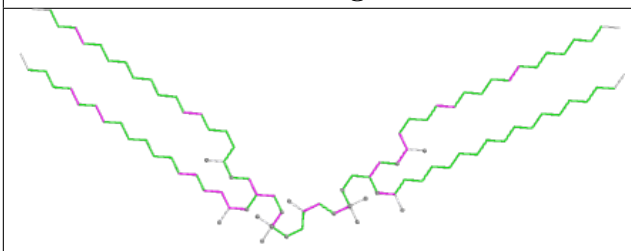

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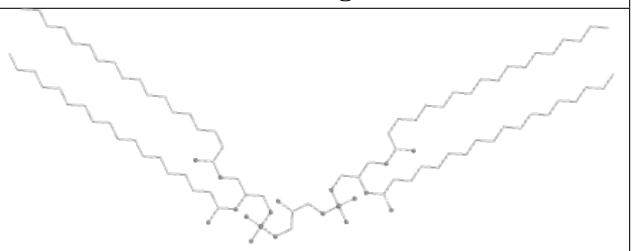
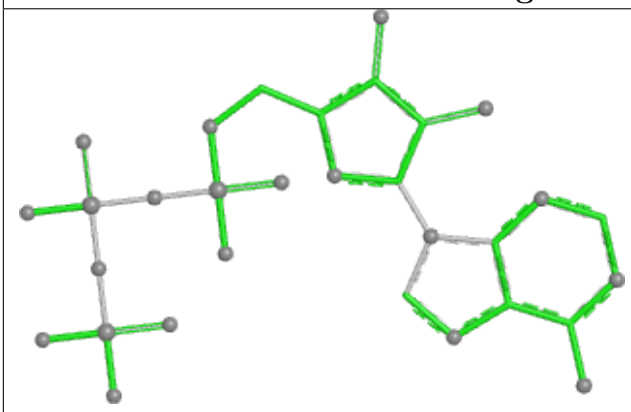


Rings

Ligand ATP B1 601



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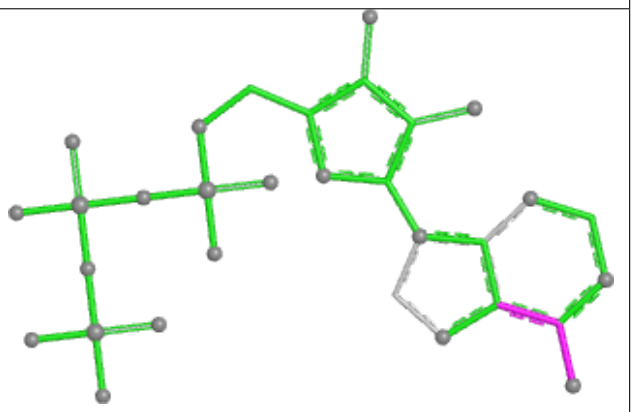

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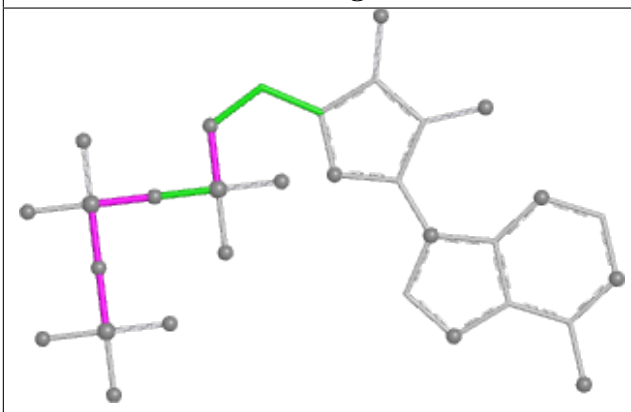

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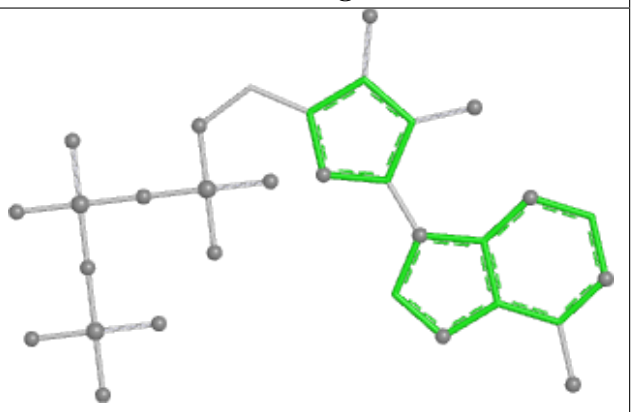
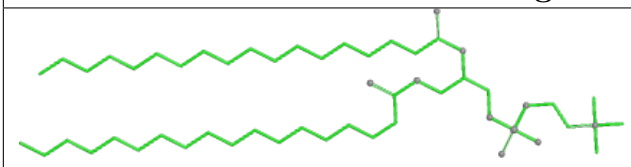
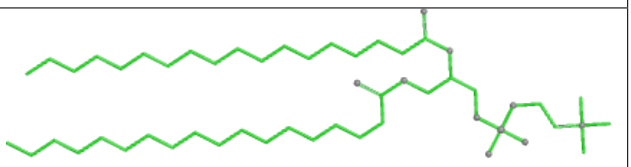
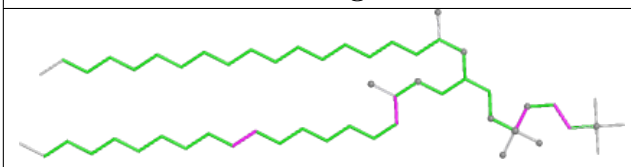
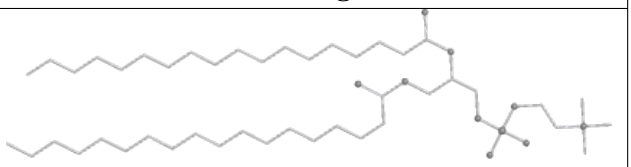
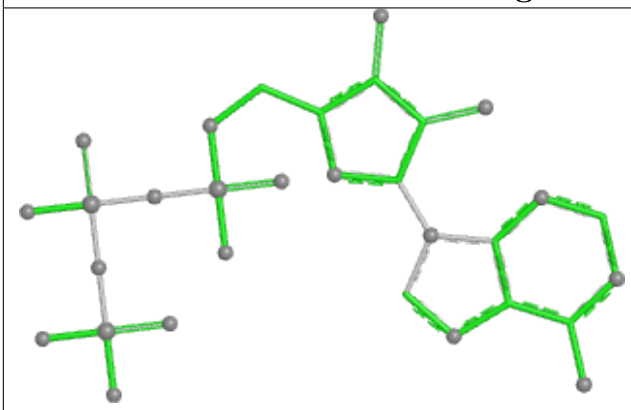
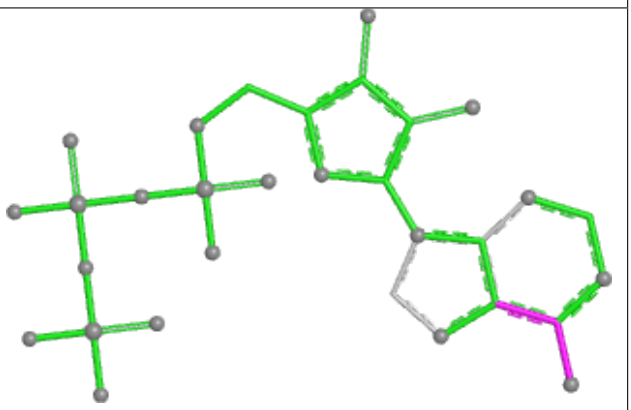
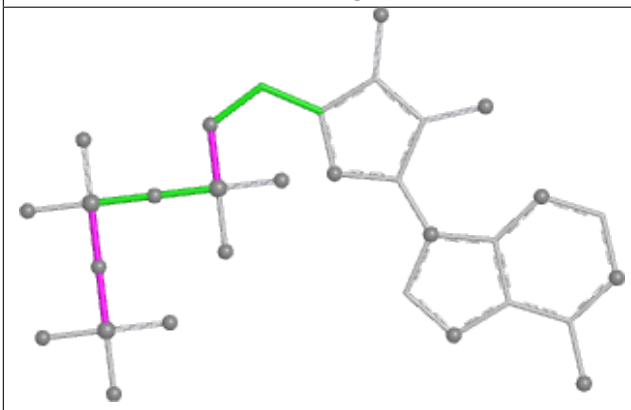
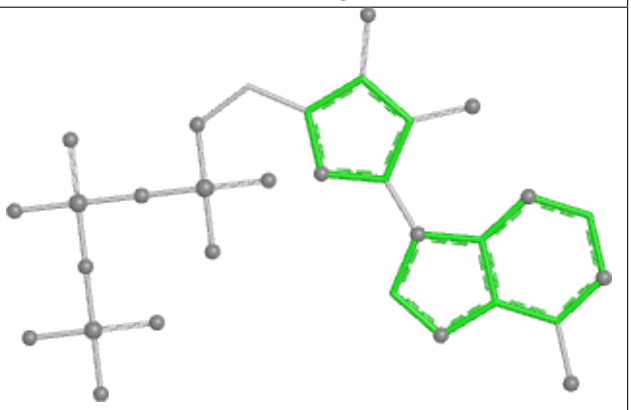
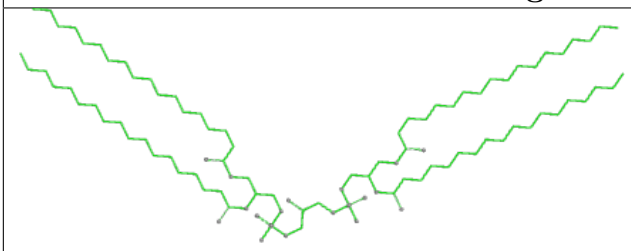


Rings

Ligand PC1 f 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP A1 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL L 101



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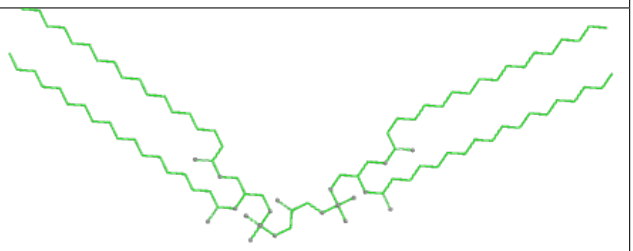

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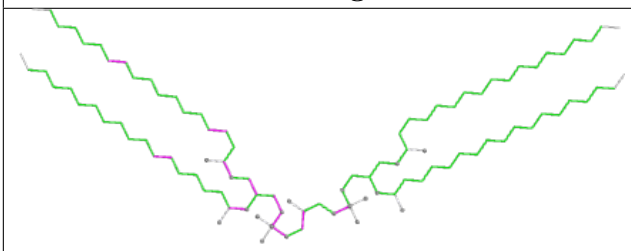

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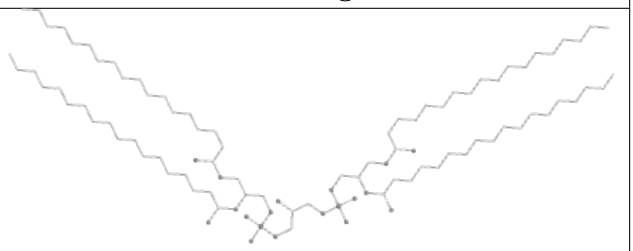
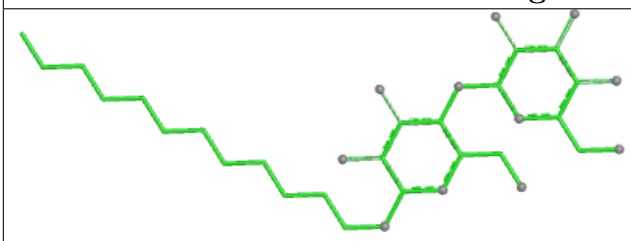


Rings

Ligand LMT j 203



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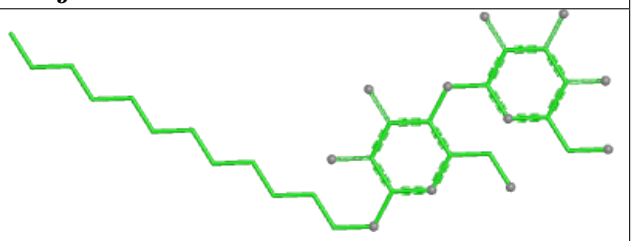

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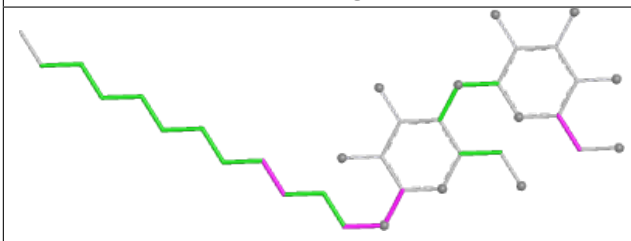

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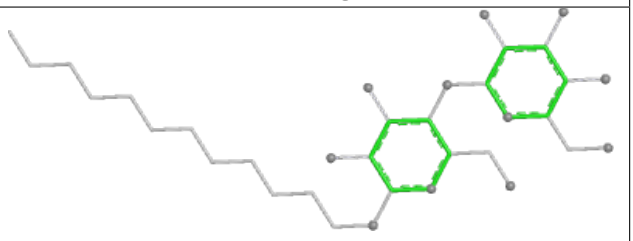
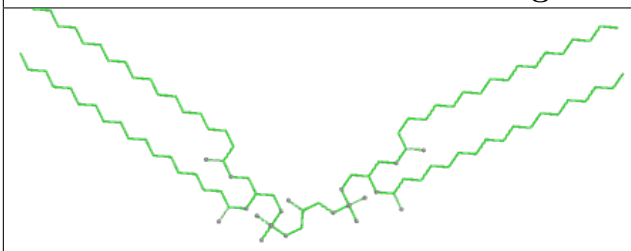


Rings

Ligand CDL j 201



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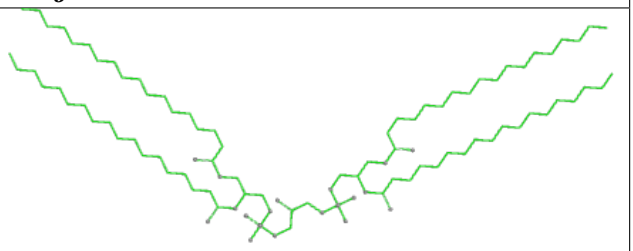

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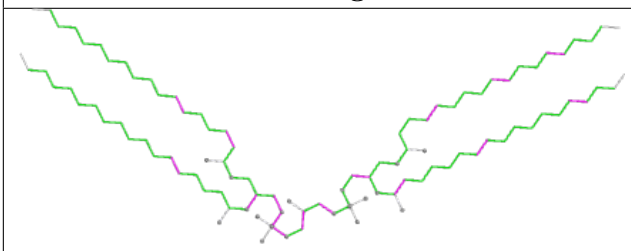

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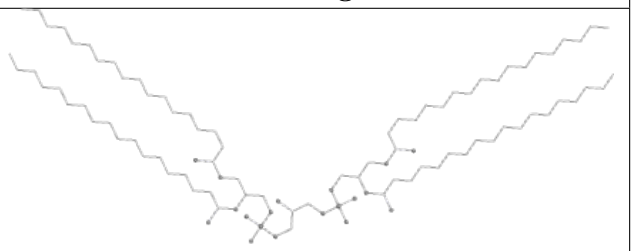
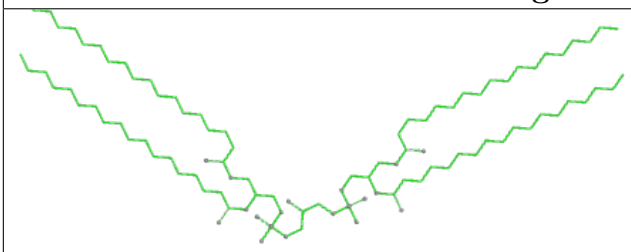


Rings

Ligand CDL l 101



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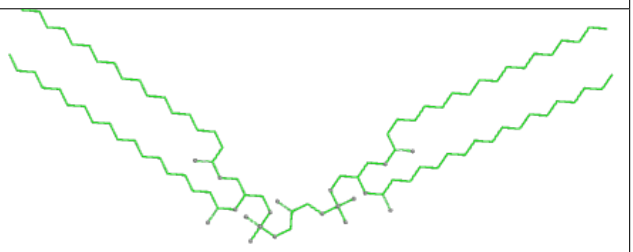

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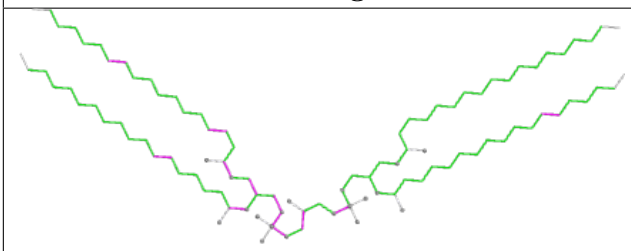

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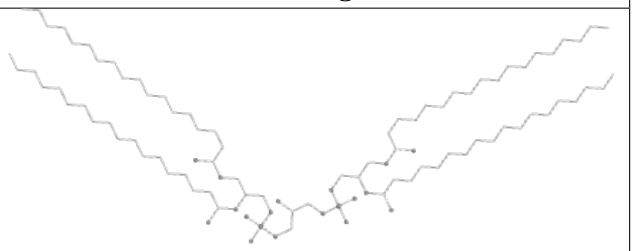
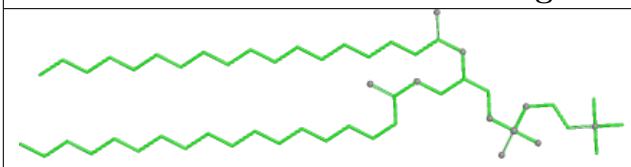


Rings

Ligand PC1 i 201



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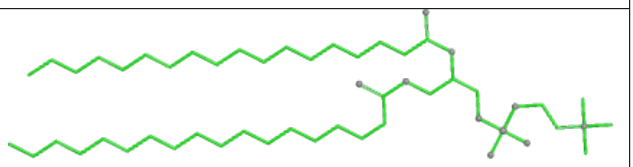

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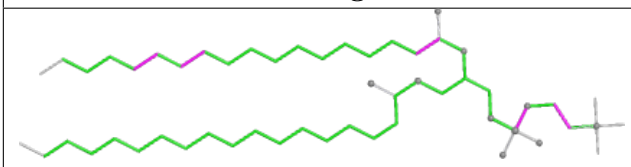

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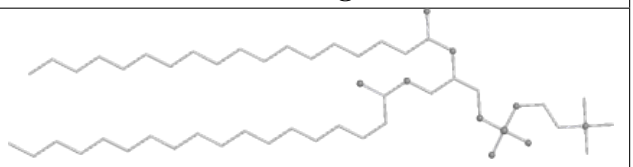
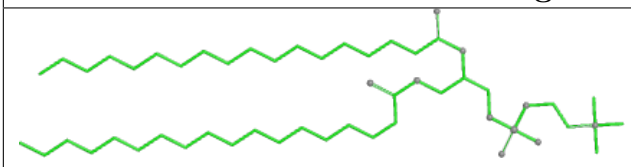
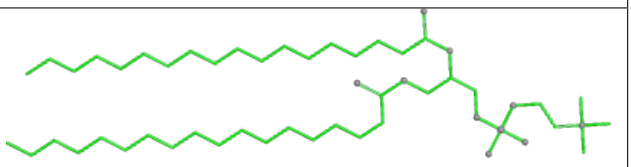
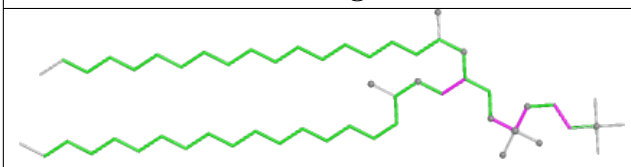
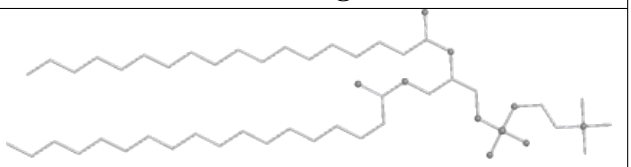
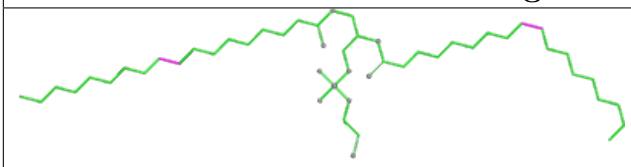
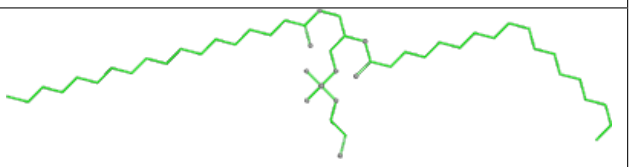
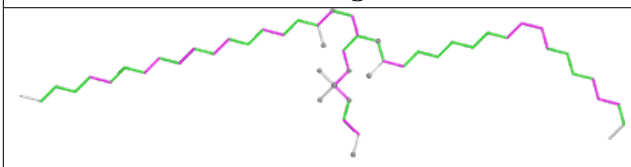
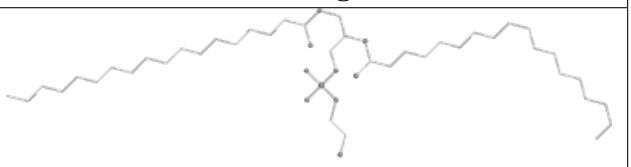
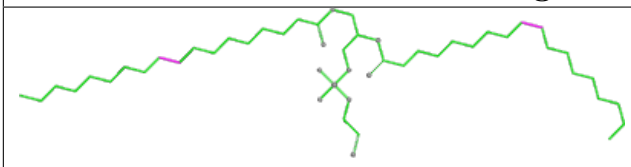
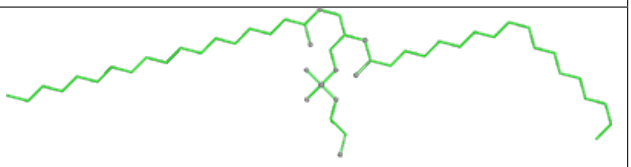
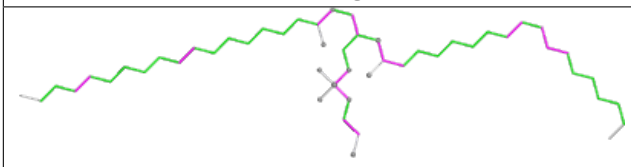
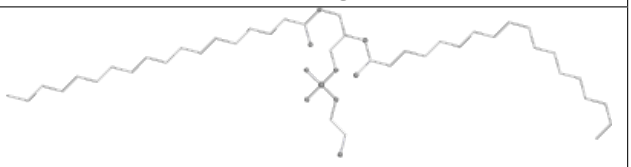


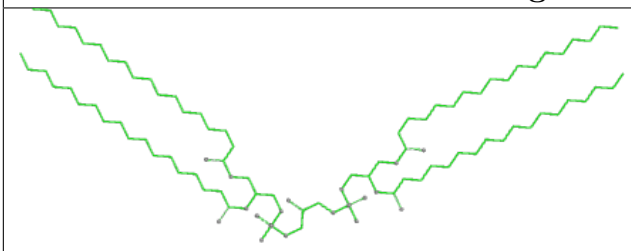
Rings

Ligand PC1 f 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

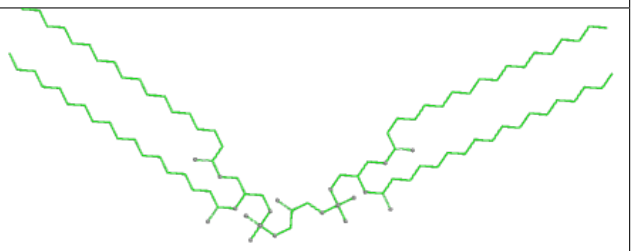
Ligand PEE m 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEE f 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

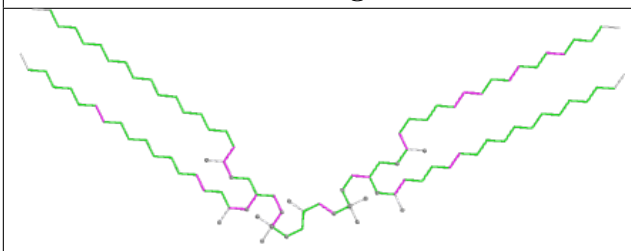
Ligand CDL e 402



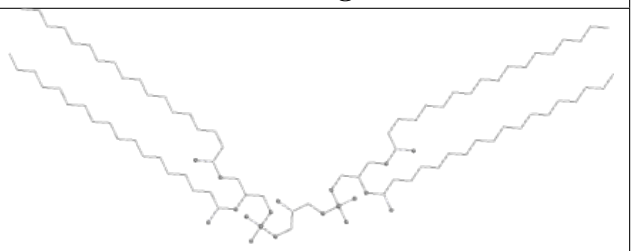
Bond lengths



Bond angles

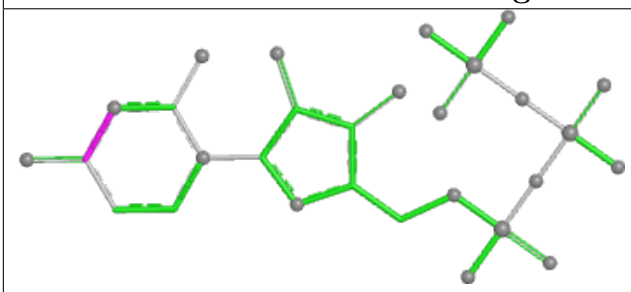


Torsions

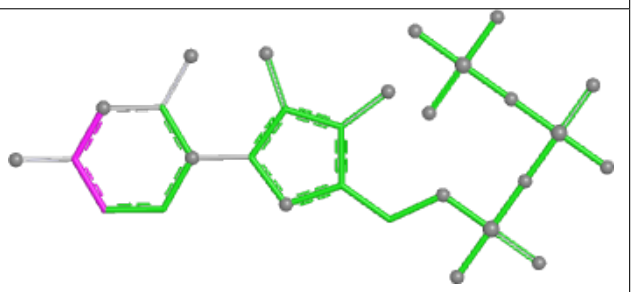


Rings

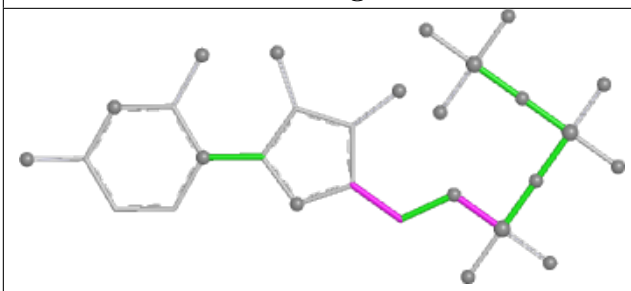
Ligand UTP H1 201



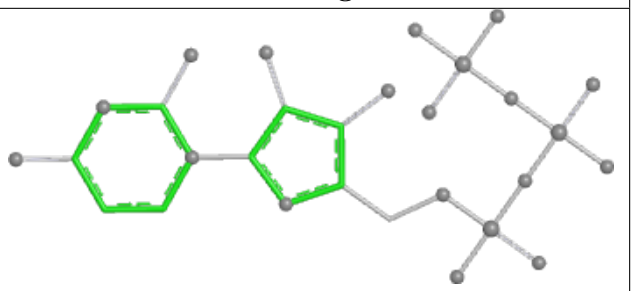
Bond lengths



Bond angles

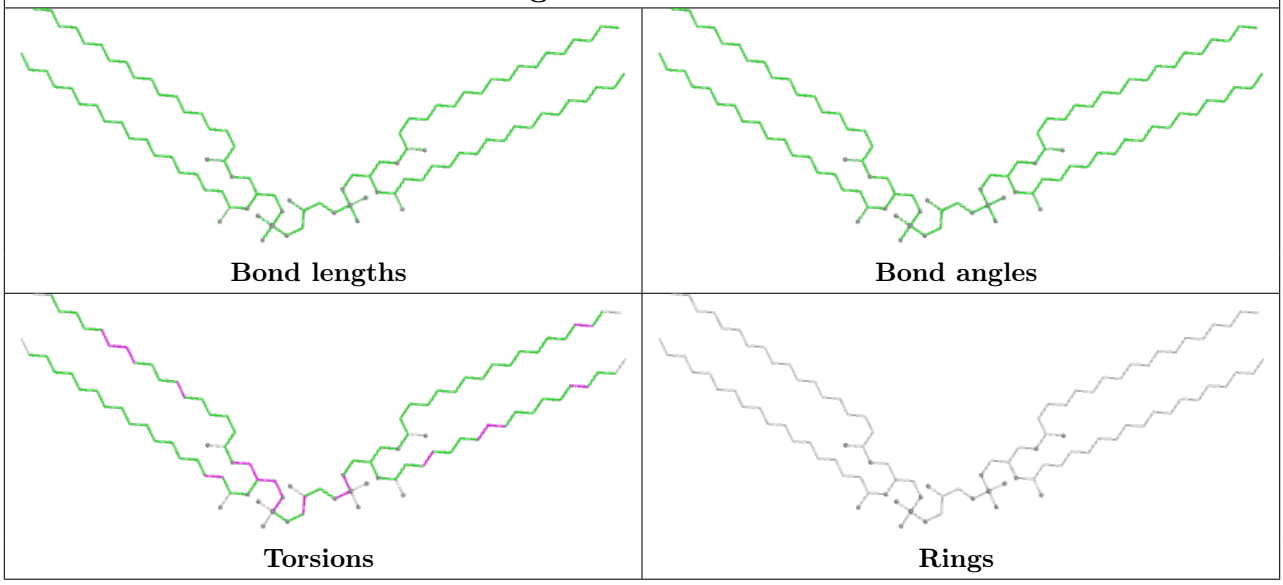


Torsions

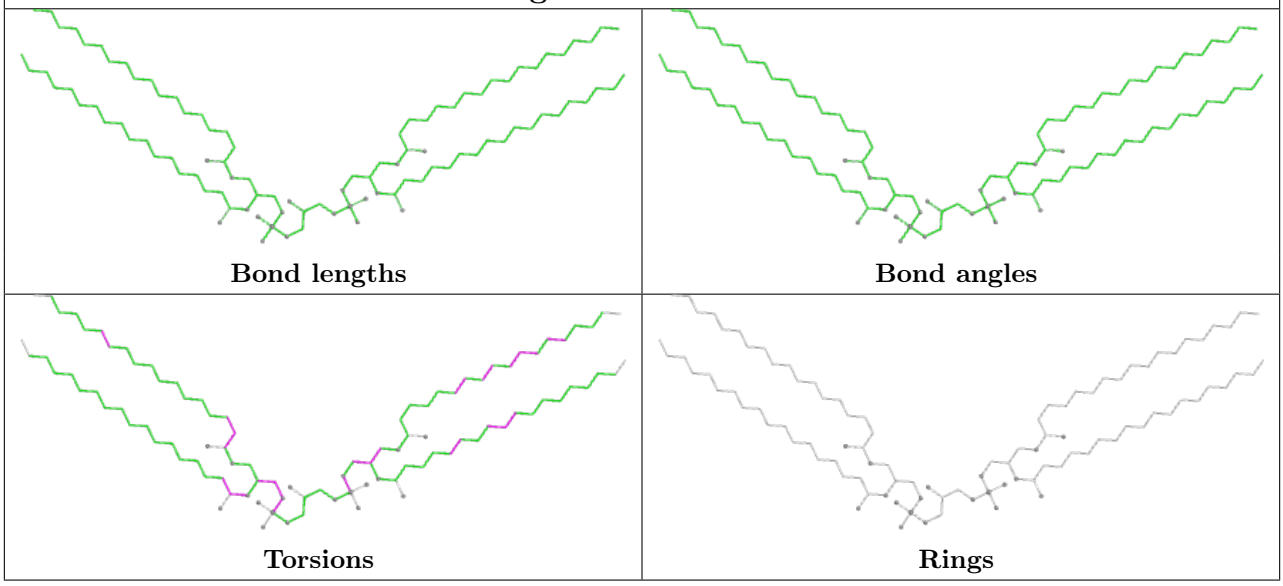


Rings

Ligand CDL c 201



Ligand CDL e 405



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.

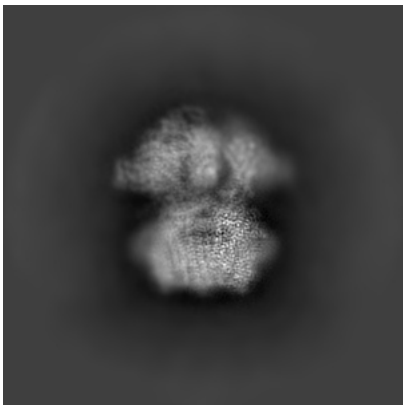
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15567. 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.

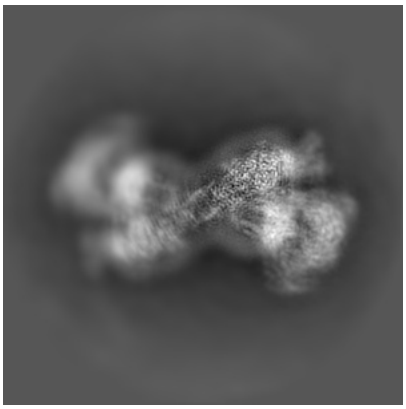
6.1 Orthogonal projections

6.1.1 Primary map



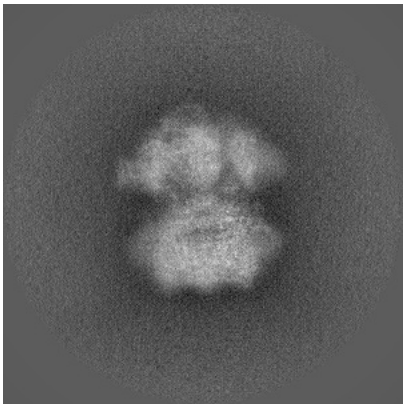
X

Y

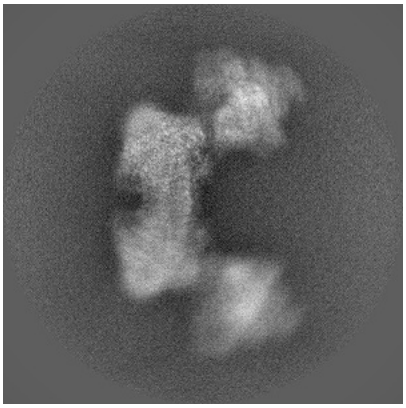


Z

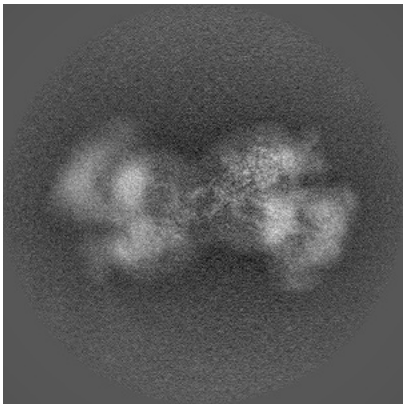
6.1.2 Raw map



X



Y

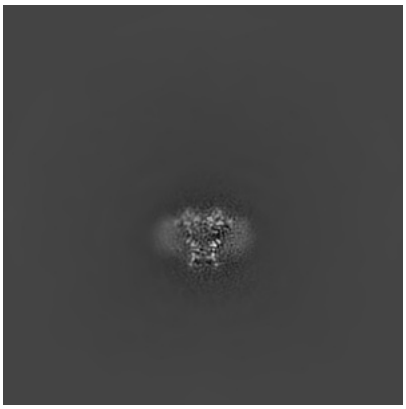


Z

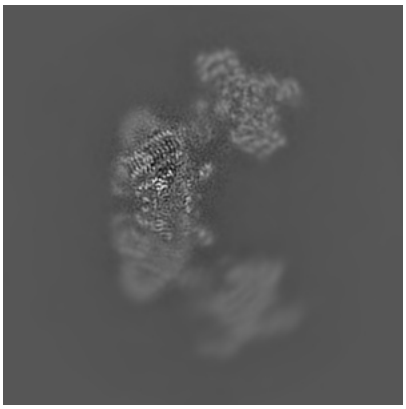
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

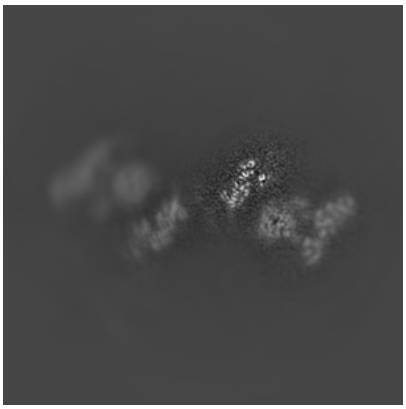
6.2.1 Primary map



X Index: 280

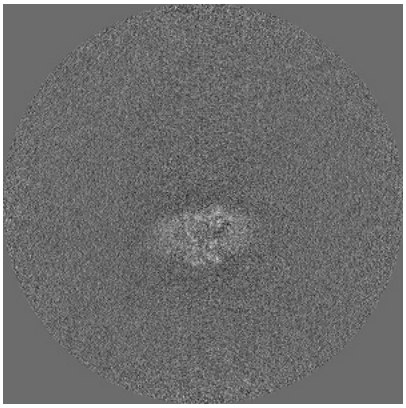


Y Index: 280

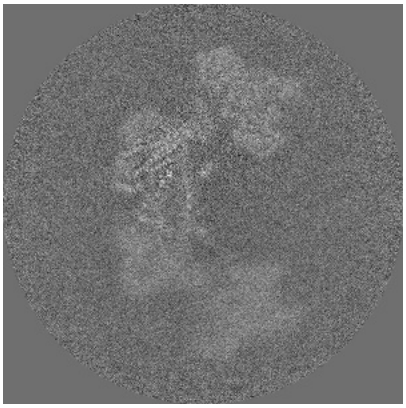


Z Index: 280

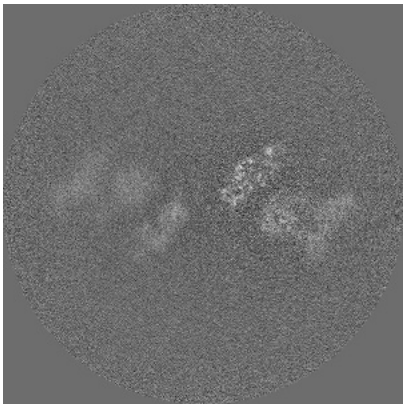
6.2.2 Raw map



X Index: 280



Y Index: 280

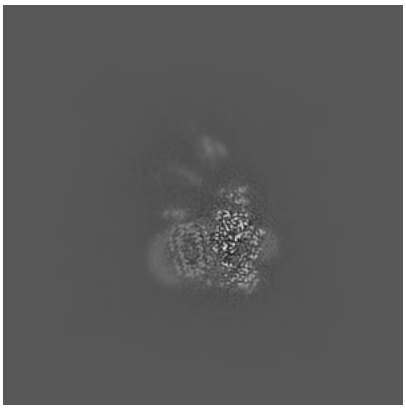


Z Index: 280

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

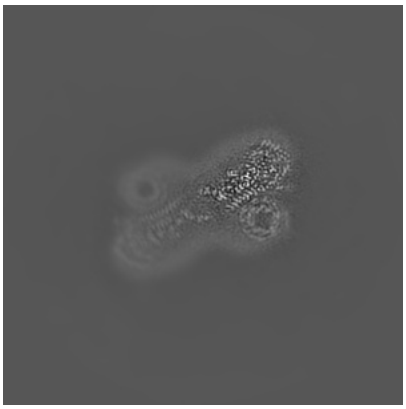
6.3 Largest variance slices (i)

6.3.1 Primary map



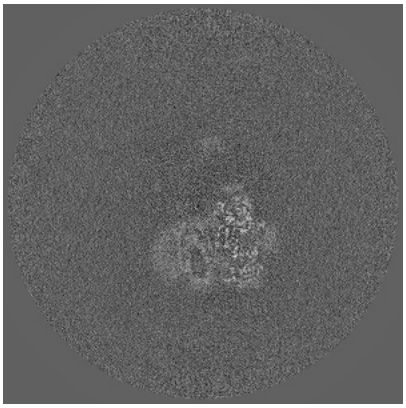
X Index: 352

Y Index: 319

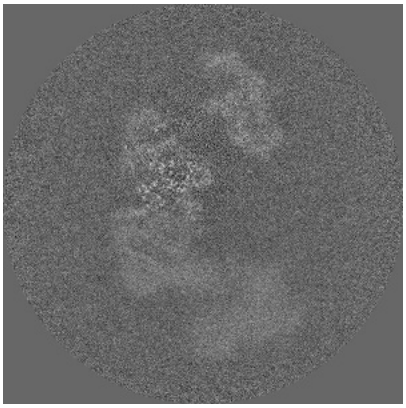


Z Index: 234

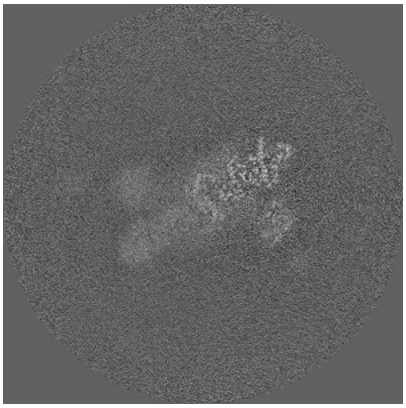
6.3.2 Raw map



X Index: 346



Y Index: 293



Z Index: 258

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

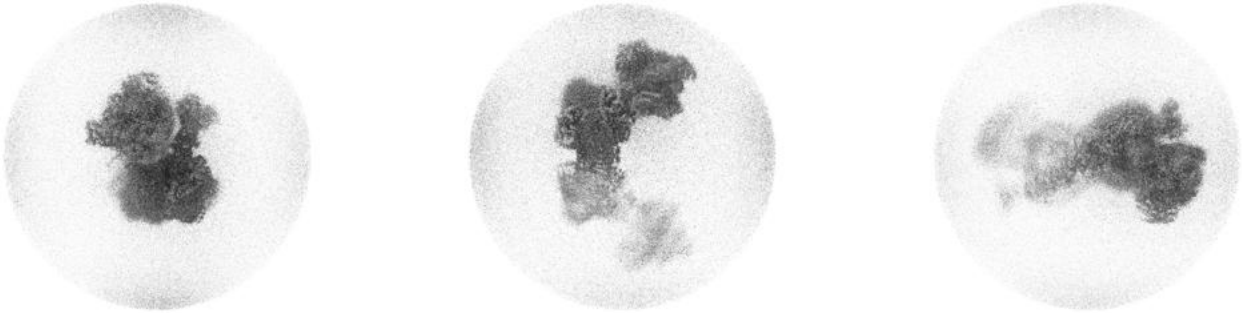
6.4 Orthogonal surface views (i)

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.

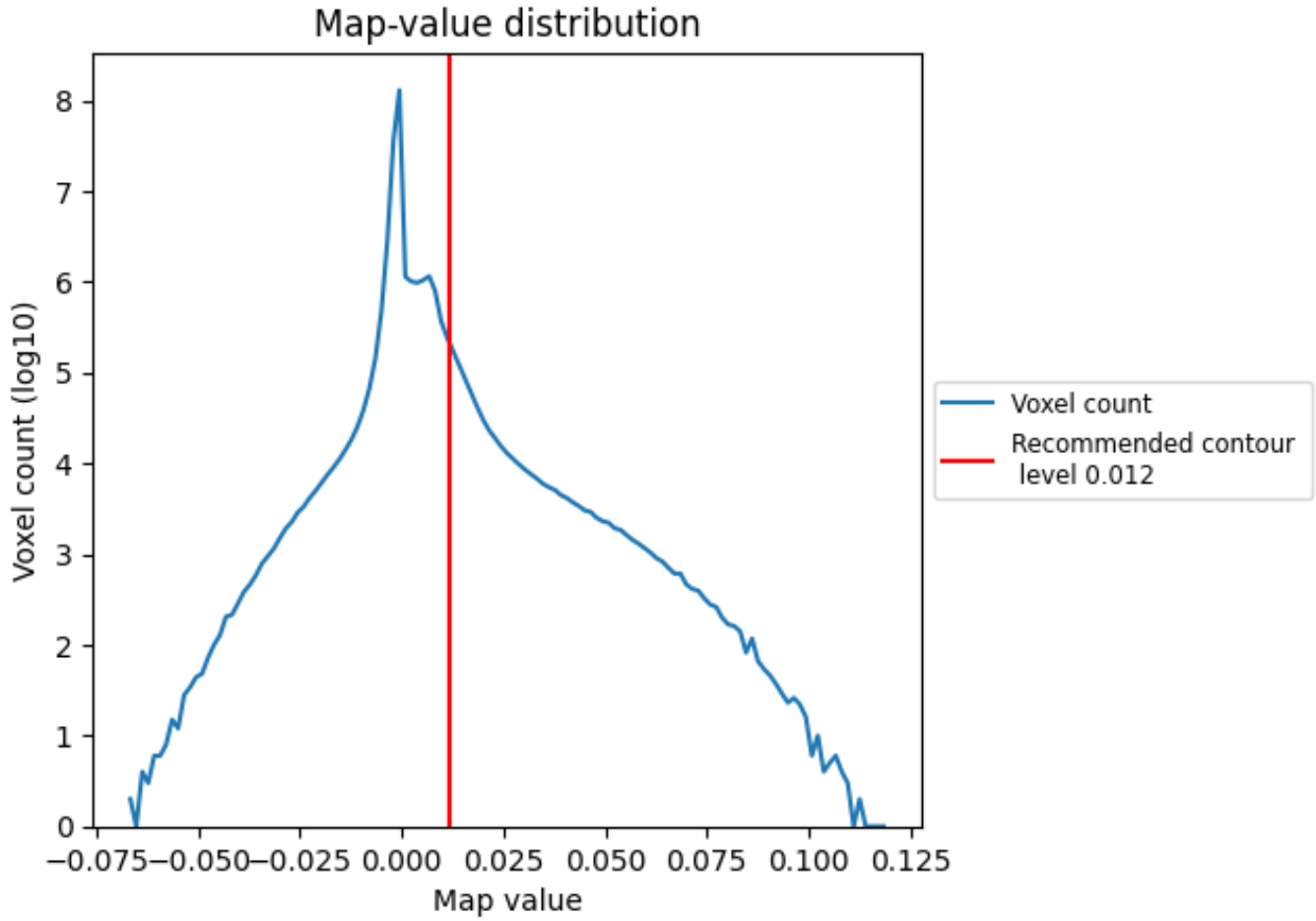
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

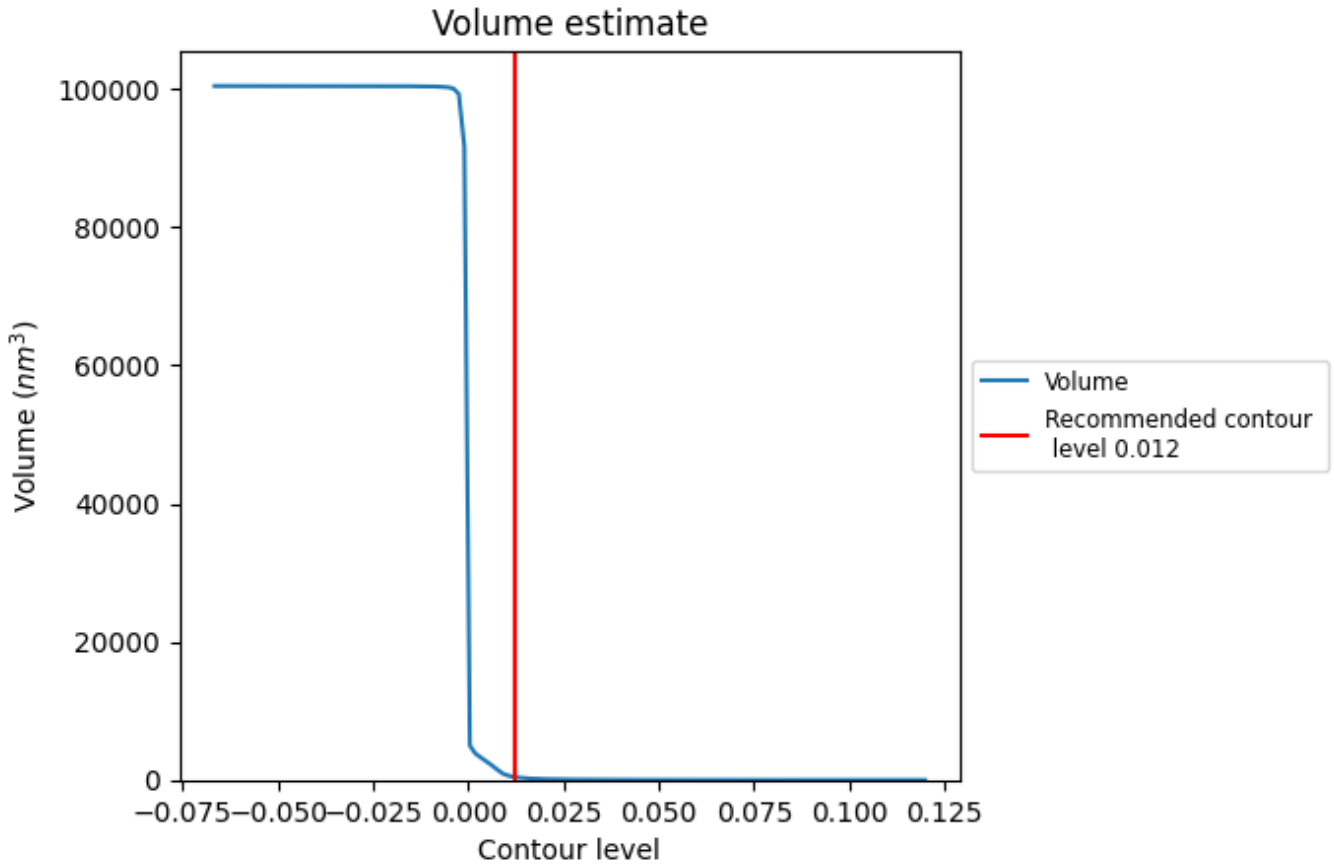
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

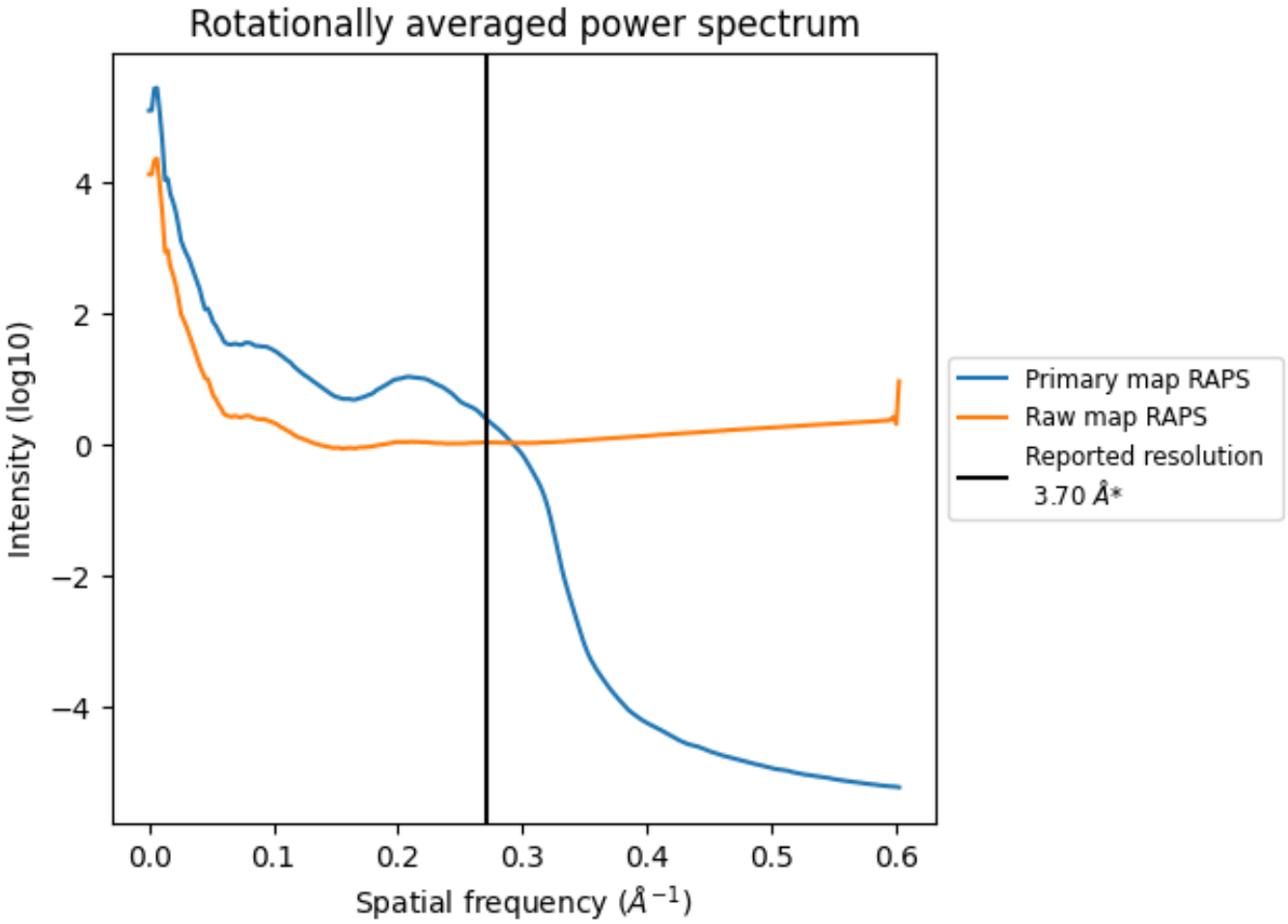
7.2 Volume estimate



The volume at the recommended contour level is 451 nm^3; this corresponds to an approximate mass of 407 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)

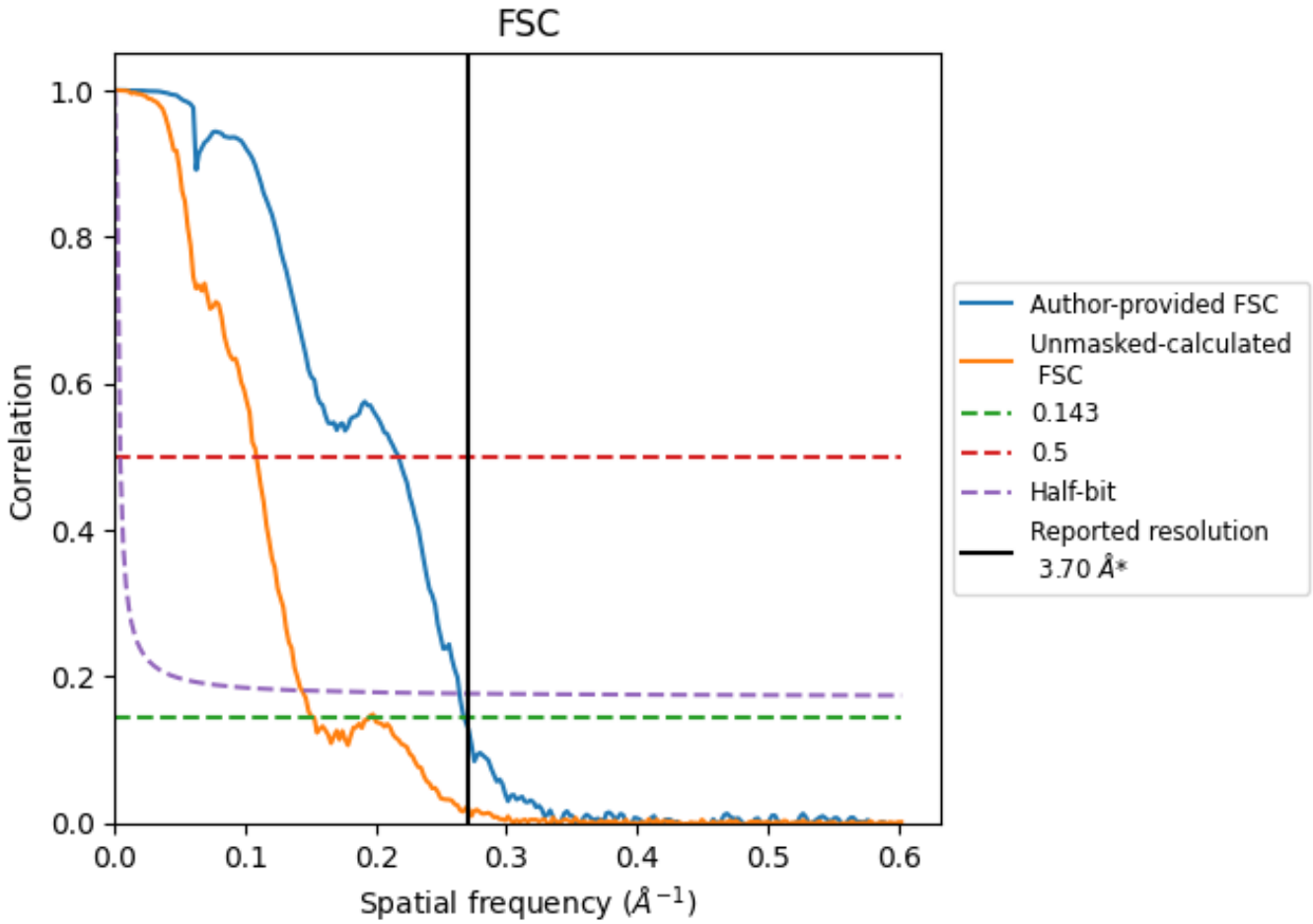


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

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)

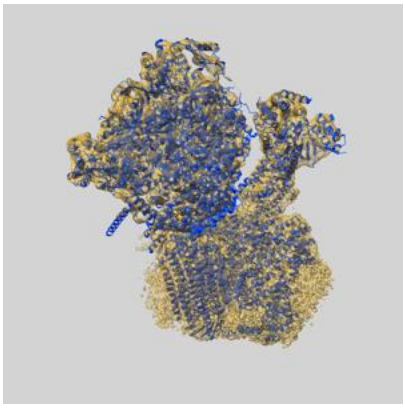
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.74	4.60	3.79
Unmasked-calculated*	6.54	9.22	6.97

*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 6.54 differs from the reported value 3.7 by more than 10 %

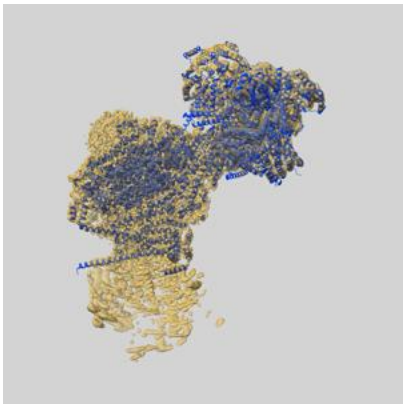
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15567 and PDB model 8APE. Per-residue inclusion information can be found in section 3 on page 16.

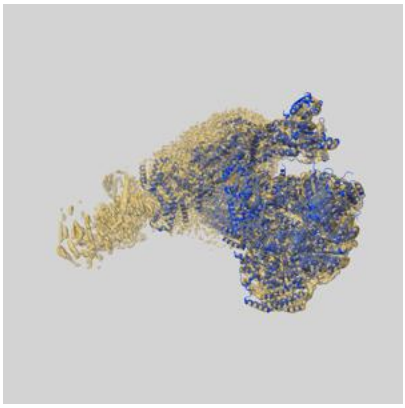
9.1 Map-model overlay



X



Y



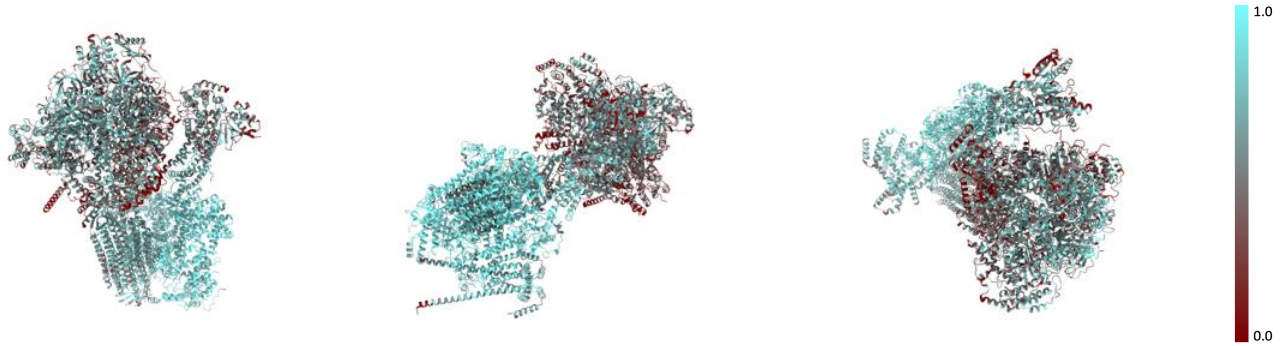
Z

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.

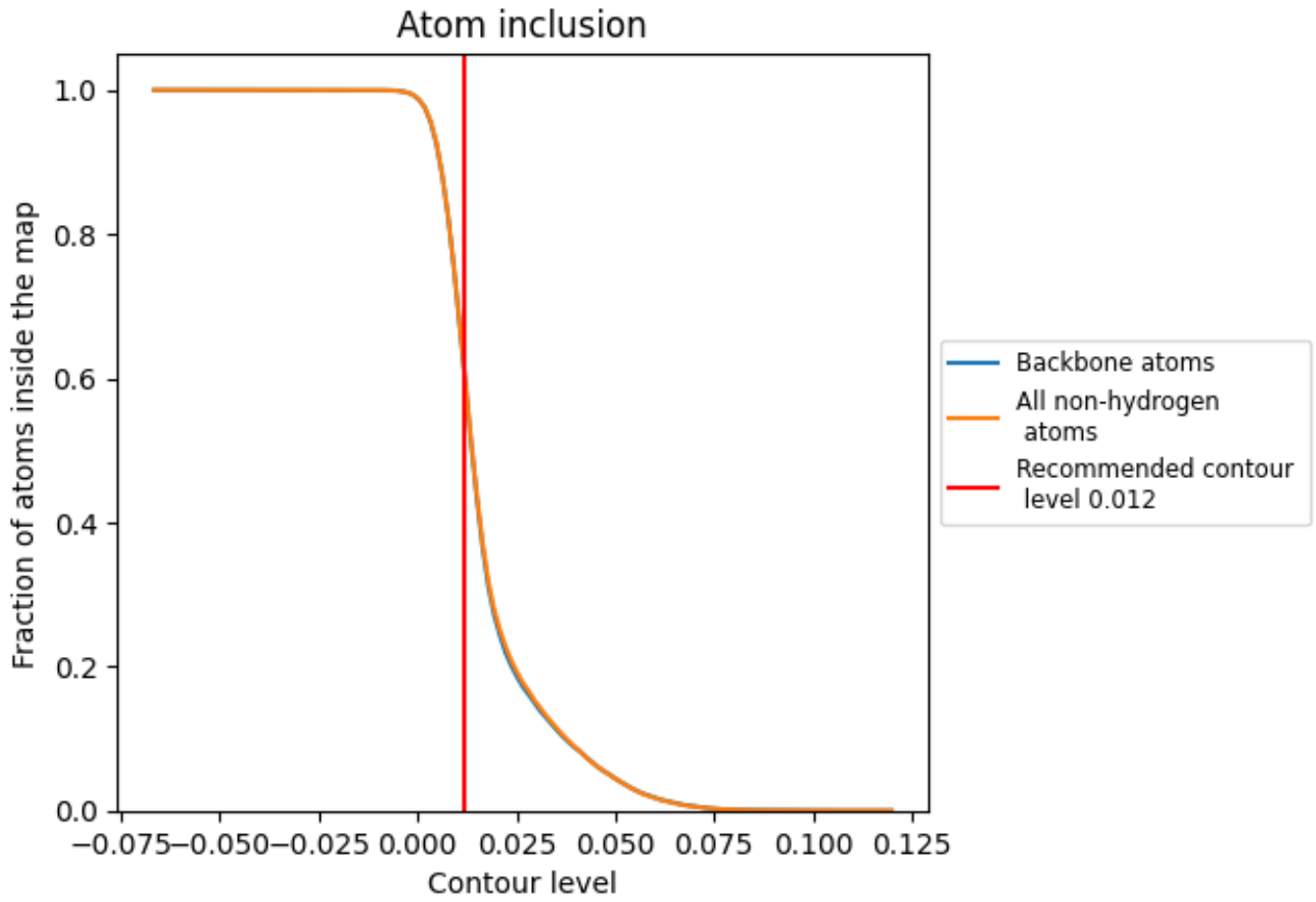
9.3 Atom inclusion mapped to coordinate model (i)



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, 60% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion
All	0.6018
A1	0.5458
B1	0.5218
C1	0.4460
D1	0.4630
E1	0.5268
F1	0.5037
G1	0.5696
H1	0.5406
I1	0.4186
J1	0.3387
K1	0.2579
L	0.6100
L1	0.4737
M	0.6543
M1	0.4841
O1	0.7148
P1	0.7576
Q1	0.7166
R1	0.6702
S1	0.6934
T1	0.6399
U1	0.6488
V1	0.6150
W1	0.6221
X1	0.6649
a	0.8647
c	0.7893
d	0.6641
e	0.8664
f	0.8344
g	0.4443
h	0.5066
i	0.8911
j	0.8430

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Chain	Atom inclusion
k	0.8452
l	0.6067
m	0.6742
n	0.8953
o	0.8579
p	0.8445
q	0.8655
r	0.8857