Full wwPDB EM Validation Report ⓘ

Mar 31, 2022 – 07:46 pm BST

PDB ID	:	7PSA
EMDB ID	:	EMD-13611
Title	:	The acetogenin-bound complex I of Mus musculus resolved to 3.4 angstroms
Authors	:	Grba, D.; Hirst, J.
Deposited on	:	2021-09-22
Resolution	:	3.40 Å(reported)
Based on initial model	:	6ZR2

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

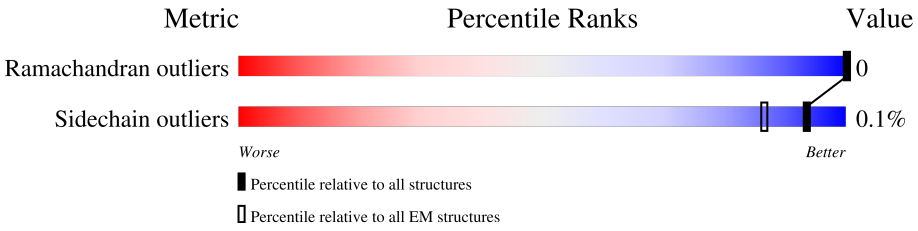
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 3.40 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	115	57% 100%
2	B	224	13% 69% 30%
3	C	263	18% 79% 21%
4	D	463	22% 92% 7%
5	E	248	40% 85% 15%
6	F	464	38% 92% 8%
7	G	727	37% 94% 5%
8	H	318	43% 100%
9	I	212	12% 84% 16%

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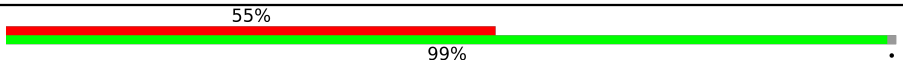
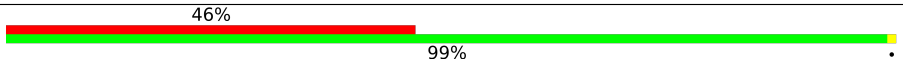
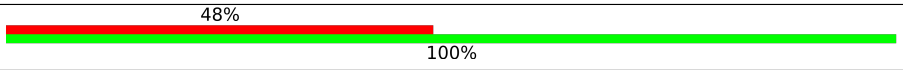
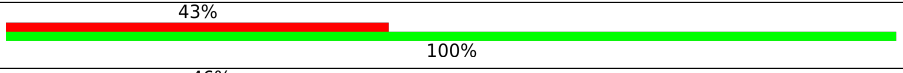
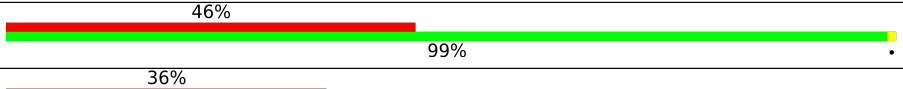
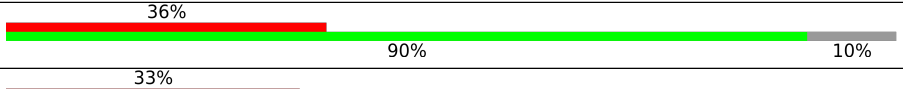
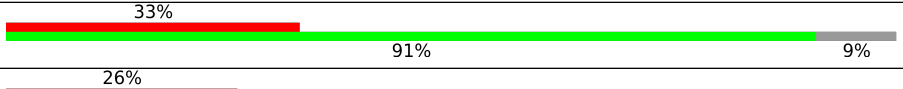
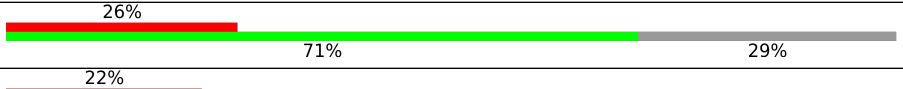
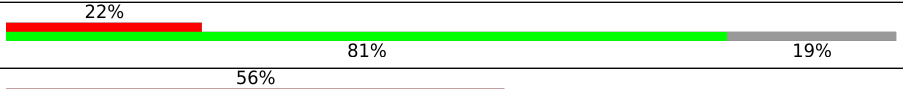
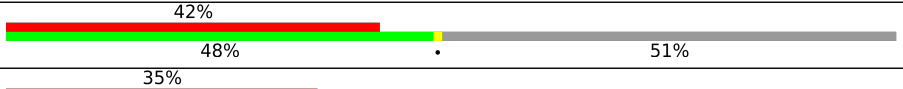
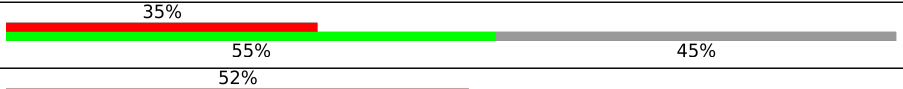
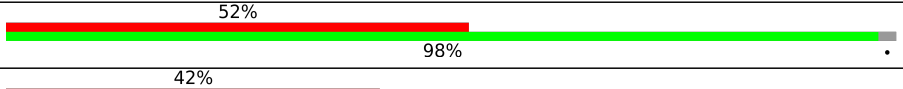
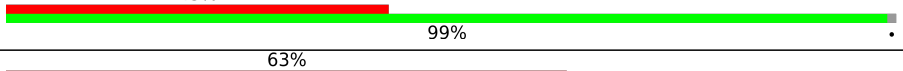
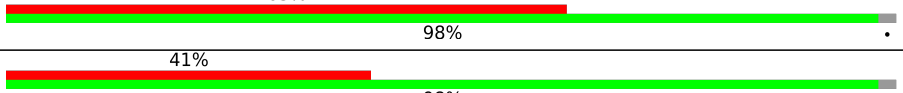
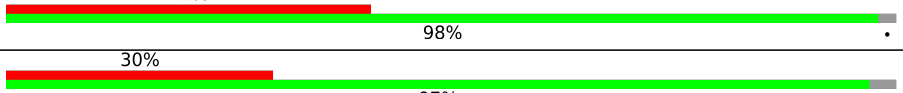
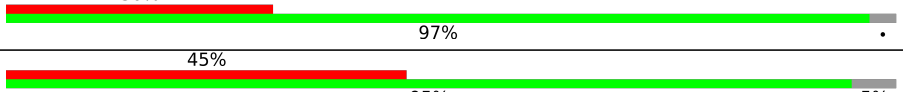
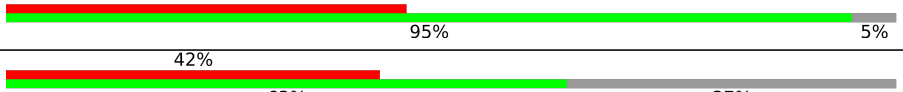
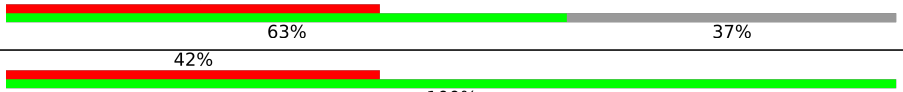
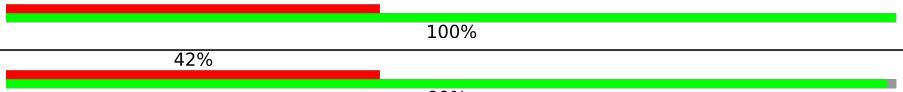
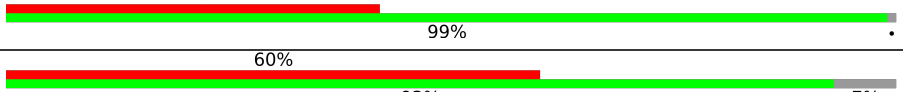
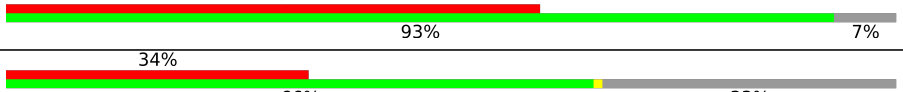
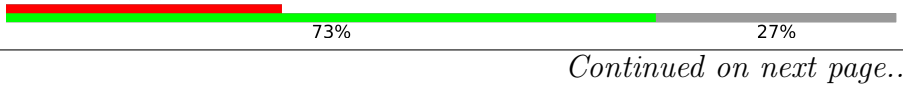
Mol	Chain	Length	Quality of chain
10	J	172	
11	K	98	
12	L	607	
13	M	459	
14	N	345	
15	O	355	
16	P	377	
17	Q	175	
18	R	116	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	131	
23	X	172	
24	Y	143	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	
29	d	120	
30	e	106	
31	f	57	
32	g	151	
33	h	189	

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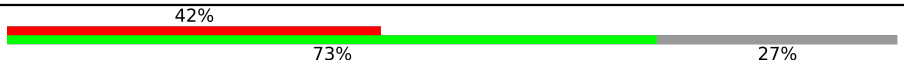
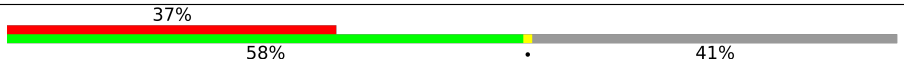
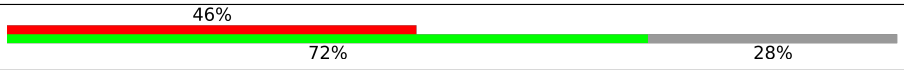
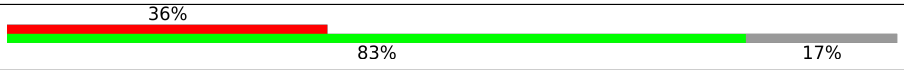
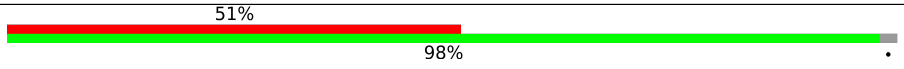
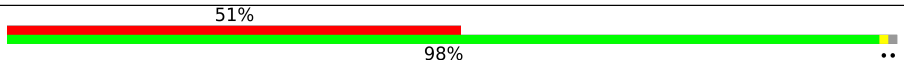
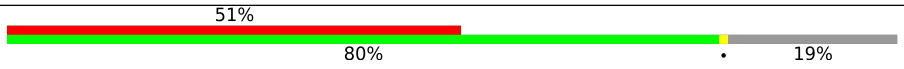
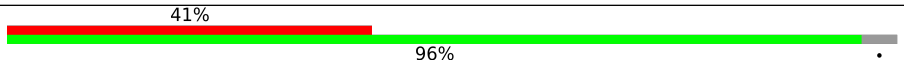
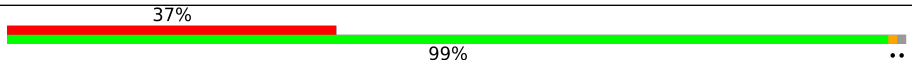
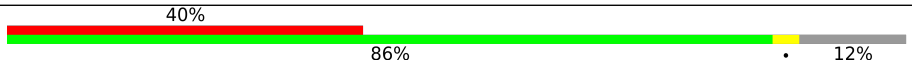
Mol	Chain	Length	Quality of chain
34	i	128	
35	j	105	
36	k	104	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	104	

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
55	EHZ	T	201	X	-	-	-
55	EHZ	U	201	X	-	-	-

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 134755 atoms, of which 67673 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 NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	115	1902	633	969	133	160	7	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	156	2502	796	1255	223	214	14	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	207	3402	1111	1681	296	311	3	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	430	6878	2215	3414	595	630	24	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	212	3287	1048	1639	277	312	11	0	0

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	428	Total	C	H	N	O	S	0	0
			6559	2080	3259	589	609	22		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	688	Total	C	H	N	O	S	0	0
			10618	3321	5322	919	1015	41		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	318	Total	C	H	N	O	S	0	0
			5166	1706	2626	384	428	22		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	178	Total	C	H	N	O	S	0	0
			2812	898	1381	245	276	12		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	171	Total	C	H	N	O	S	0	0
			2615	874	1315	185	226	15		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	98	Total	C	H	N	O	S	0	0
			1505	477	768	112	137	11		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	606	Total	C	H	N	O	S	0	0
			9785	3182	4985	746	827	45		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	459	Total	C	H	N	O	S	0	0
			7485	2408	3853	567	617	40		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	344	Total	C	H	N	O	S	0	0
			5591	1791	2895	416	452	37		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	320	Total	C	H	N	O	S	0	0
			5171	1674	2564	431	492	10		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	342	Total	C	H	N	O	S	0	0
			5514	1777	2766	483	481	7		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	125	Total	C	H	N	O	S	0	0
			2031	642	1016	179	190	4		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	94	Total	C	H	N	O	S	0	0
			1453	458	715	135	142	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	83	Total	C	H	N	O	S	0	0
			1353	419	686	126	119	3		

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	76	Total	C	H	N	O	S	0	0
			1213	392	602	90	124	5		
20	U	86	Total	C	H	N	O	S	0	0
			1378	446	686	102	139	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	V	114	Total	C	H	N	O	S	0	0
			1895	604	968	154	166	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	W	114	Total	C	H	N	O	S	0	0
			1961	619	991	180	165	6		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	X	171	Total	C	H	N	O	S	0	0
			2773	889	1377	250	247	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Y	140	Total	C	H	N	O	S	0	0
			2062	662	1025	175	192	8		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-2	MET	-	variant	UNP Q9D8B4
Y	-1	ALA	-	variant	UNP Q9D8B4
Y	39	SER	ARG	conflict	UNP Q9D8B4

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Z	141	Total	C	H	N	O	S	0	0
			2333	750	1166	207	202	8		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	a	68	Total	C	H	N	O	S	0	0
			1124	360	568	99	93	4		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	b	80	Total	C	H	N	O	S	0	0
			1256	414	628	99	111	4		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	c	48	Total	C	H	N	O	S	0	0
			797	261	399	69	67	1		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	d	120	Total	C	H	N	O	S	0	0
			1997	651	1001	171	165	9		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	e	105	Total	C	H	N	O	S	0	0
			1746	555	869	162	152	8		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	f	53	Total	C	H	N	O	S	0	0
			908	295	452	82	77	2		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	g	101	Total	C	H	N	O	S	0	0
			1633	549	783	136	161	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	h	138	Total	C	H	N	O	S	0	0
			2325	762	1163	194	203	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	i	94	Total	C	H	N	O	S	0	0
			1578	513	794	134	134	3		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	j	62	Total	C	H	N	O	S	0	0
			1033	355	496	88	93	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	k	75	Total	C	H	N	O	S	0	0
			1213	404	604	103	100	2		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	l	154	Total	C	H	N	O	S	0	0
			2481	834	1187	215	234	11		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	126	Total	C	H	N	O	0	0
			2111	676	1061	189	185		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	n	177	Total	C	H	N	O	S	0	0
			2998	981	1464	275	267	11		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	o	111	Total	C	H	N	O	S	0	0
			1894	605	937	176	168	8		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	p	169	Total	C	H	N	O	S	0	0
			2832	901	1399	257	267	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	q	144	Total	C	H	N	O	S	0	0
			2361	773	1158	213	212	5		

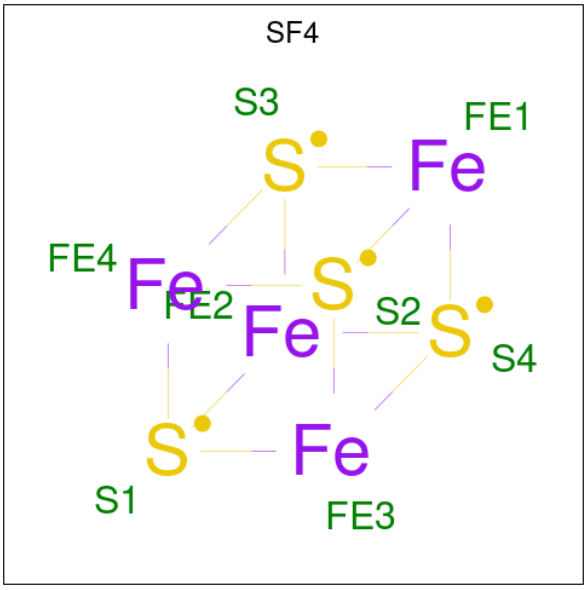
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	r	100	Total	C	H	N	O	S	0	0
			1638	507	836	149	143	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

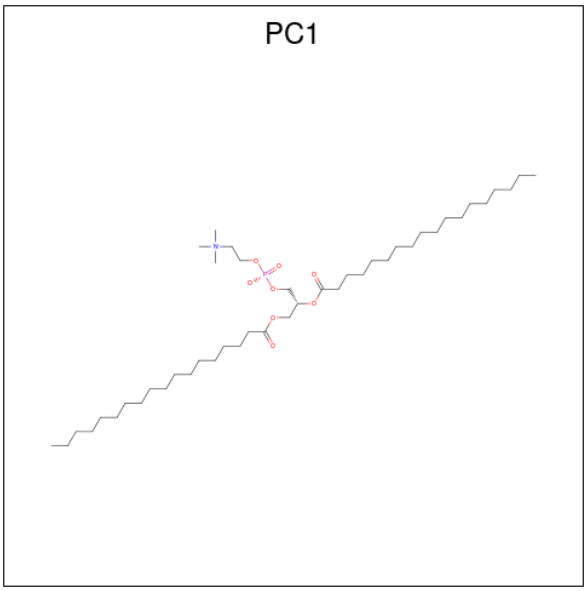
Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	41	Total	C	H	N	O	0	0
			668	215	324	61	68		

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



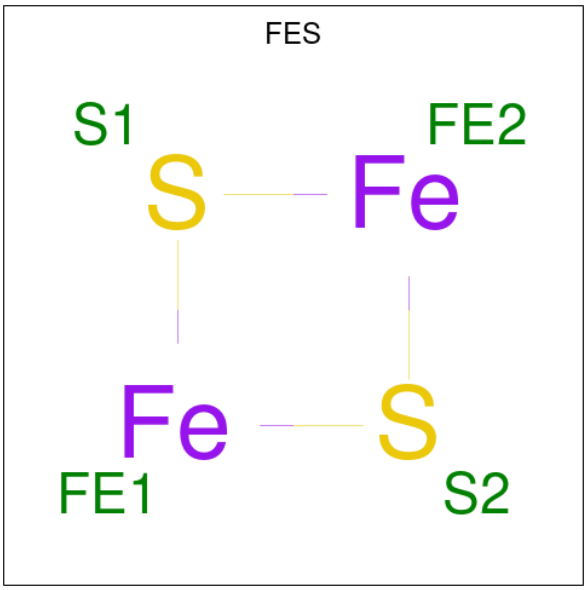
Mol	Chain	Residues	Atoms				AltConf
45	B	1	Total	Fe	S		0
			8	4	4		
45	F	1	Total	Fe	S		0
			8	4	4		
45	G	1	Total	Fe	S		0
			16	8	8		
45	G	1	Total	Fe	S		0
			16	8	8		
45	I	1	Total	Fe	S		0
			16	8	8		
45	I	1	Total	Fe	S		0
			16	8	8		

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



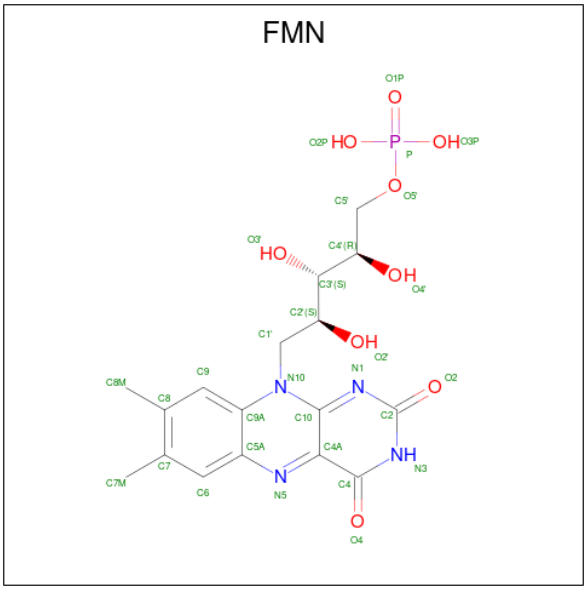
Mol	Chain	Residues	Atoms						AltConf
46	B	1	Total	C	H	N	O	P	0
			191	58	113	2	16	2	
46	B	1	Total	C	H	N	O	P	0
			191	58	113	2	16	2	
46	J	1	Total	C	H	N	O	P	0
			104	32	62	1	8	1	
46	Z	1	Total	C	H	N	O	P	0
			113	35	68	1	8	1	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



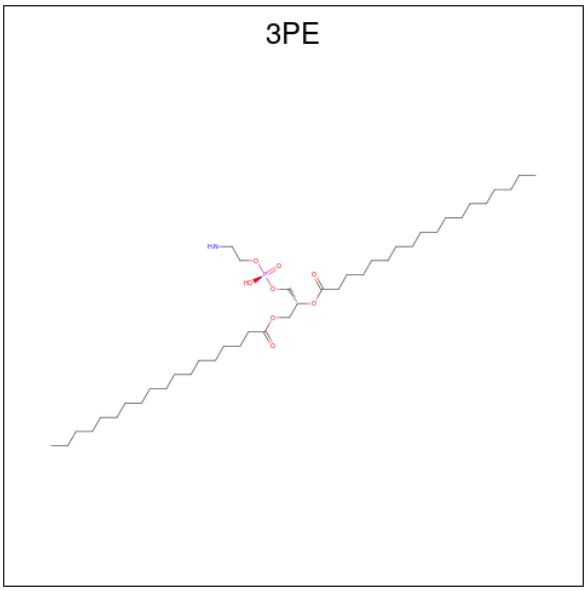
Mol	Chain	Residues	Atoms	AltConf
47	E	1	Total Fe S 4 2 2	0
47	G	1	Total Fe S 4 2 2	0

- Molecule 48 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



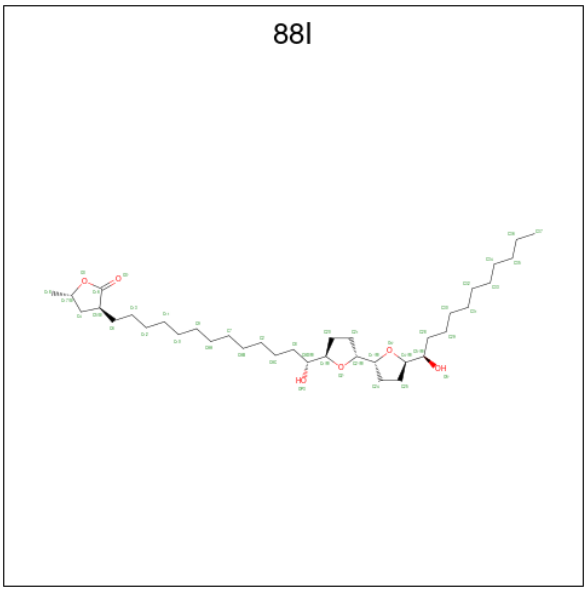
Mol	Chain	Residues	Atoms	AltConf
48	F	1	Total C H N O P 50 17 19 4 9 1	0

- Molecule 49 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



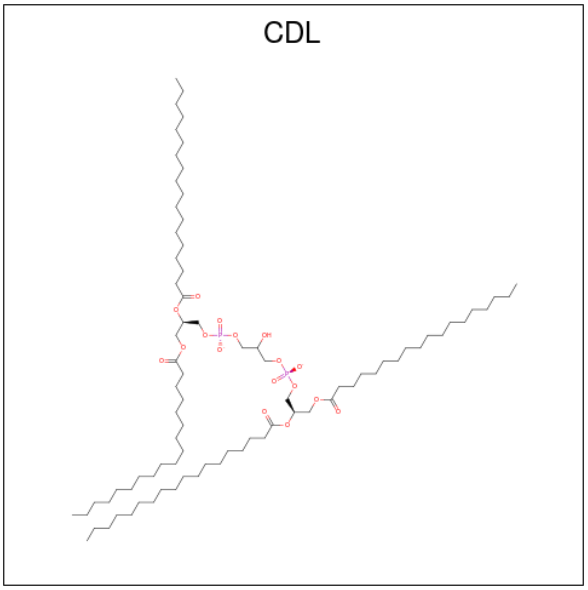
Mol	Chain	Residues	Atoms						AltConf
49	H	1	Total	C	H	N	O	P	0
			244	75	149	2	16	2	
49	H	1	Total	C	H	N	O	P	0
			244	75	149	2	16	2	
49	K	1	Total	C	H	N	O	P	0
			77	23	44	1	8	1	
49	L	1	Total	C	H	N	O	P	0
			357	110	217	3	24	3	
49	L	1	Total	C	H	N	O	P	0
			357	110	217	3	24	3	
49	L	1	Total	C	H	N	O	P	0
			357	110	217	3	24	3	
49	M	1	Total	C	H	N	O	P	0
			194	59	115	2	16	2	
49	M	1	Total	C	H	N	O	P	0
			194	59	115	2	16	2	
49	Y	1	Total	C	H	N	O	P	0
			101	31	60	1	8	1	

- Molecule 50 is (3 {S},5 {S})-5-methyl-3-[(13 {R})-13-oxidanyl-13-[(2 {R},5 {R})-5-[(2 {R},5 {R})-5-[(1 {R})-1-oxidanylundecyl]oxolan-2-yl]oxolan-2-yl]tridecyl]oxolan-2-one (three-letter code: 88I) (formula: $C_{37}H_{68}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
50	H	1	Total	C	H	O	0
			109	37	66	6	

- Molecule 51 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms					AltConf
51	L	1	Total	C	H	O	P	0
			174	55	100	17	2	
51	N	1	Total	C	H	O	P	0
			148	46	83	17	2	
51	X	1	Total	C	H	O	P	0
			154	48	87	17	2	

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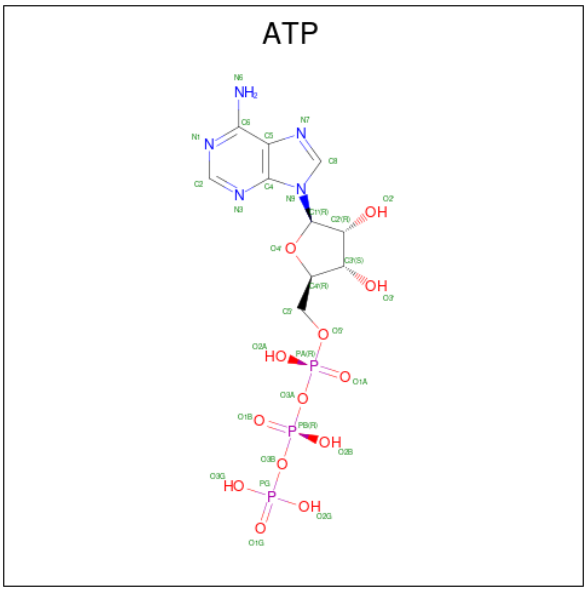
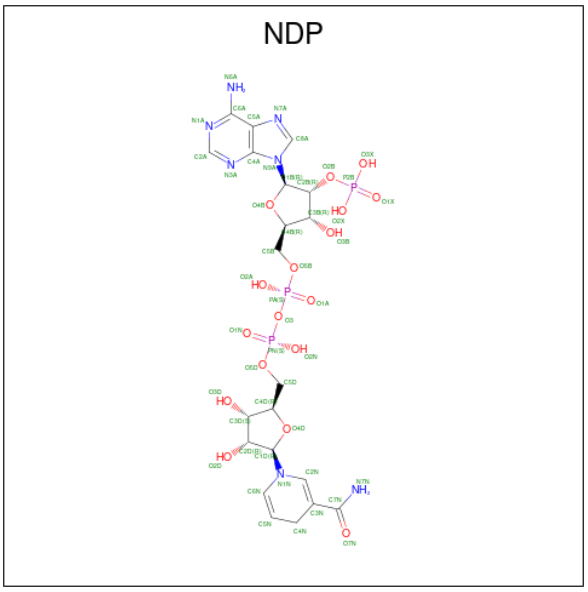
Mol	Chain	Residues	Atoms					AltConf
51	d	1	Total	C	H	O	P	0
			274	85	152	33	4	
51	d	1	Total	C	H	O	P	0
			274	85	152	33	4	
51	i	1	Total	C	H	O	P	0
			163	51	93	17	2	
51	r	1	Total	C	H	O	P	0
			123	38	66	17	2	

- Molecule 52 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
52	O	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 53 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

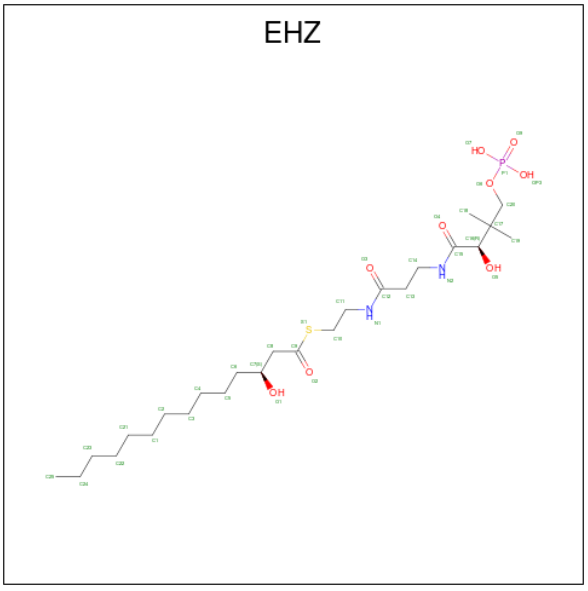


Mol	Chain	Residues	Atoms						AltConf
53	P	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	R	1	Total	Zn	0
			1	1	

- Molecule 55 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).

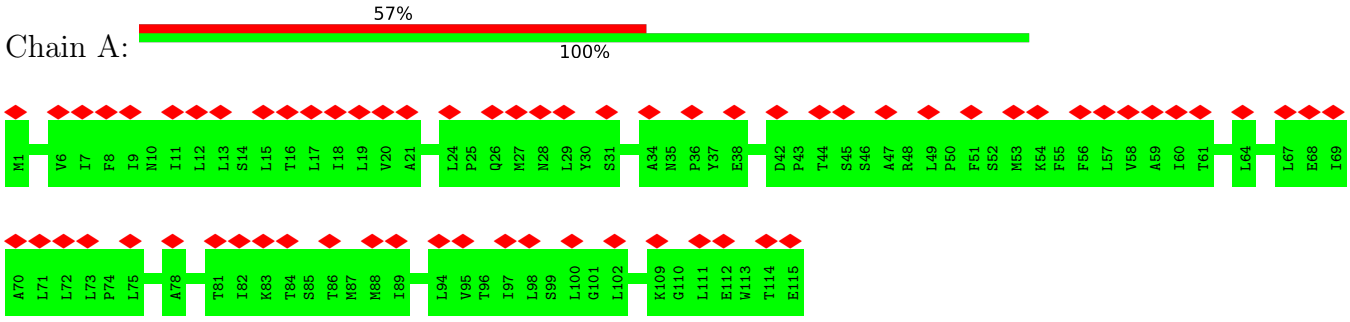


Mol	Chain	Residues	Atoms							AltConf
55	T	1	Total	C	H	N	O	P	S	0
			84	25	47	2	8	1	1	
55	U	1	Total	C	H	N	O	P	S	0
			84	25	47	2	8	1	1	

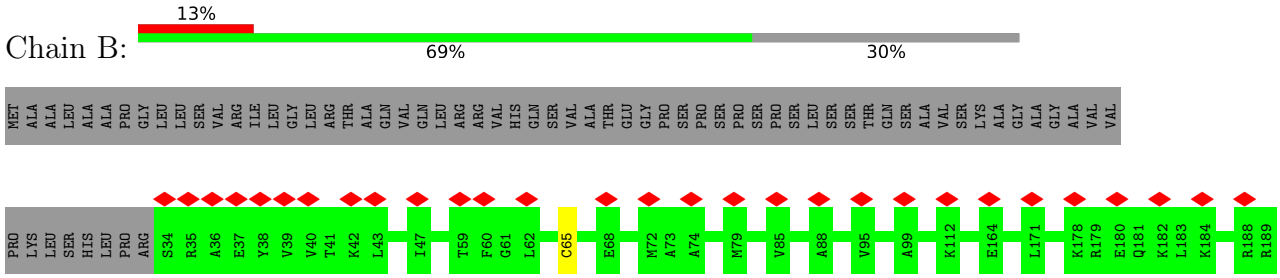
3 Residue-property plots (i)

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.

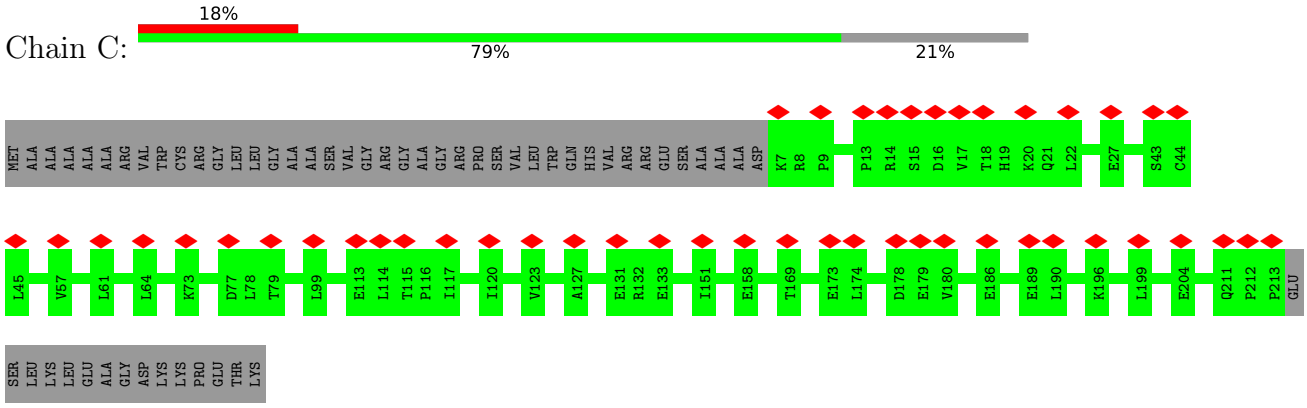
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3



• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

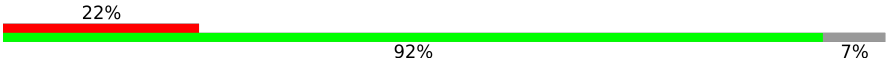


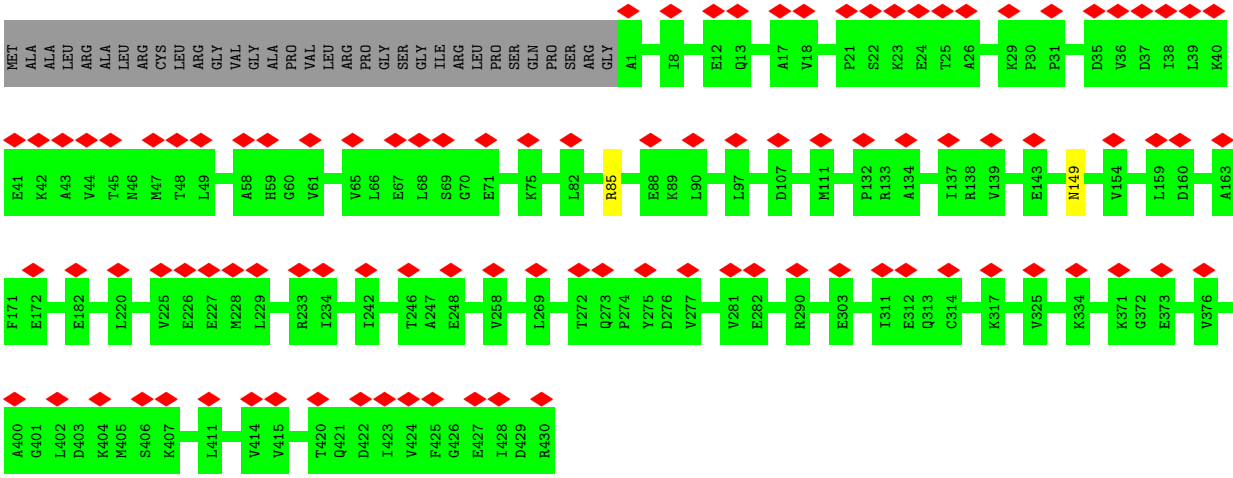
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

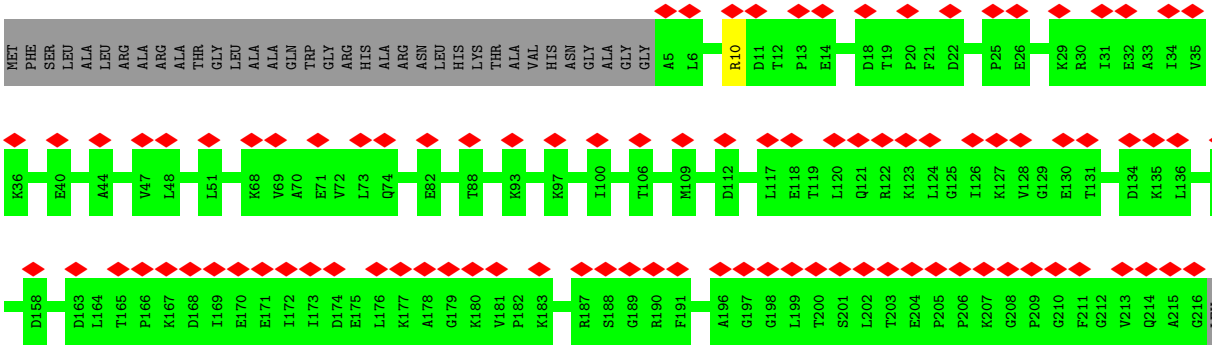
Chain D:





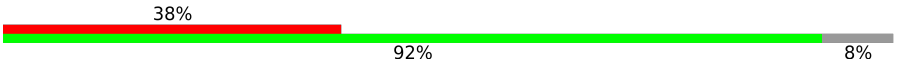
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

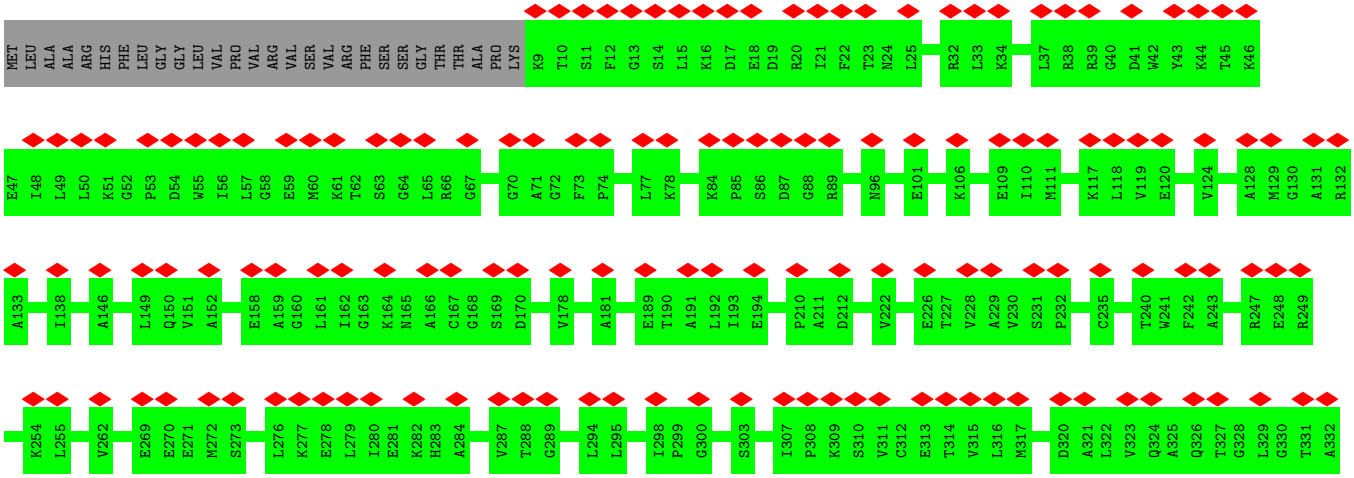
Chain E:

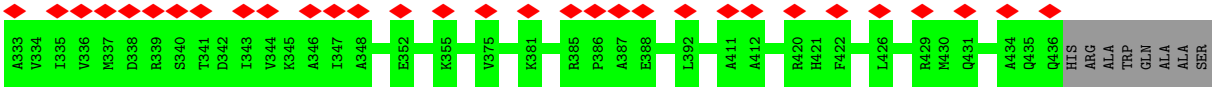


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:

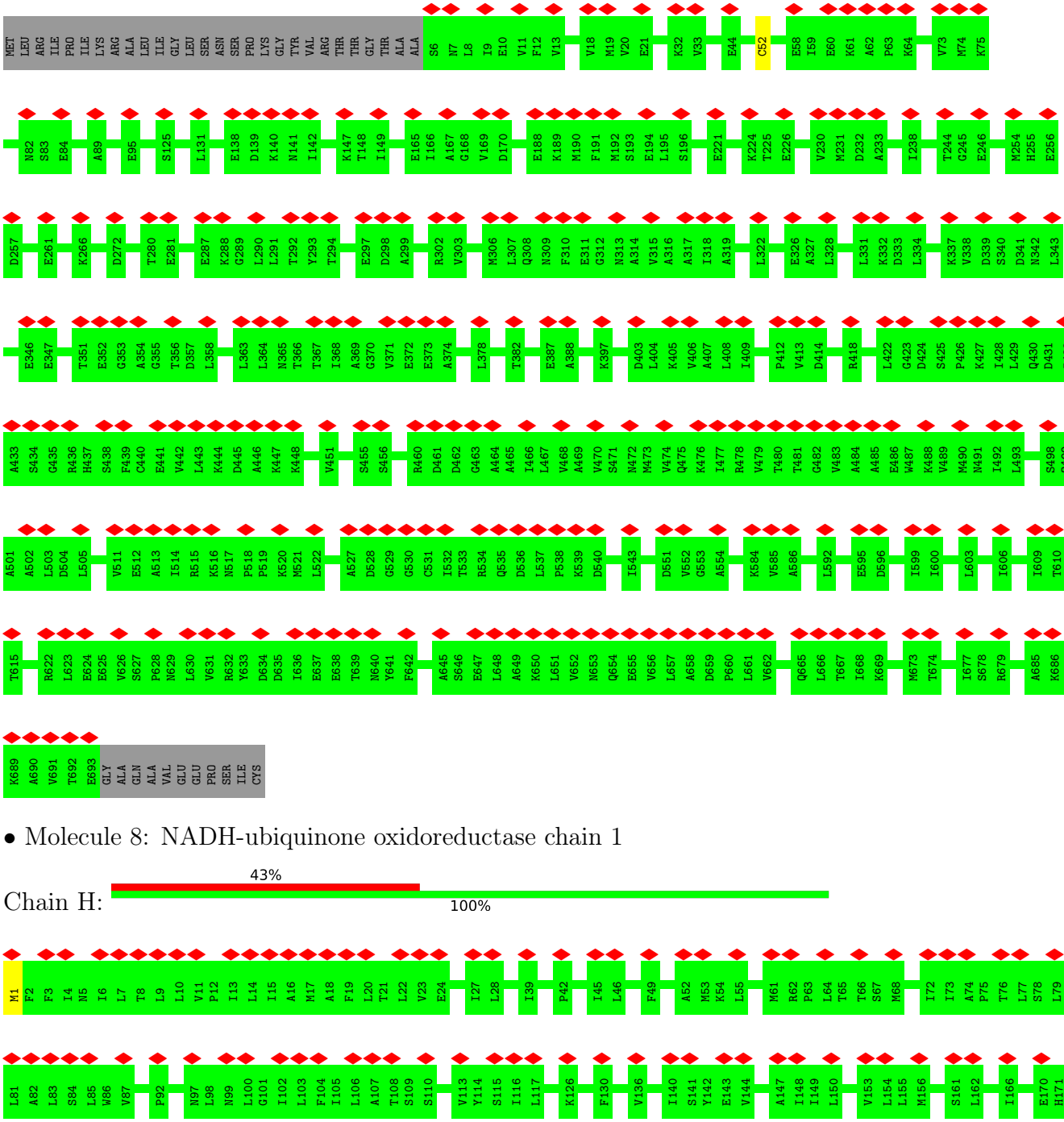






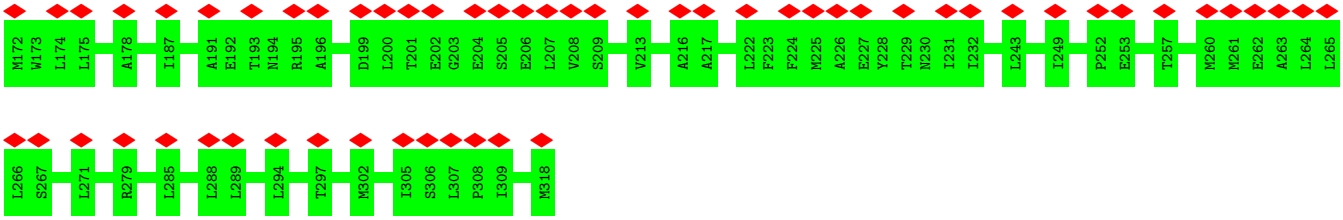
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:

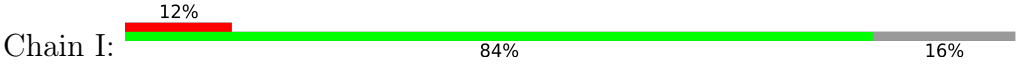


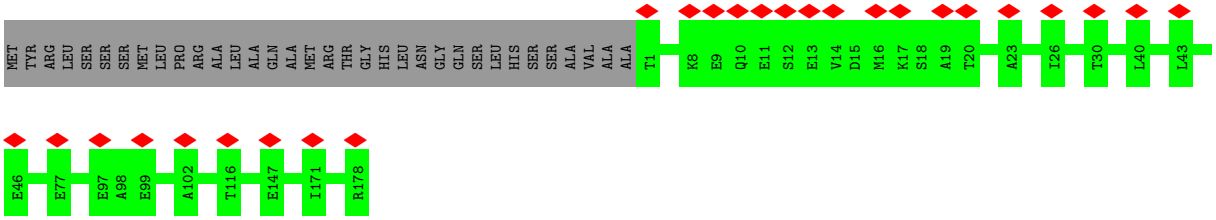
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:

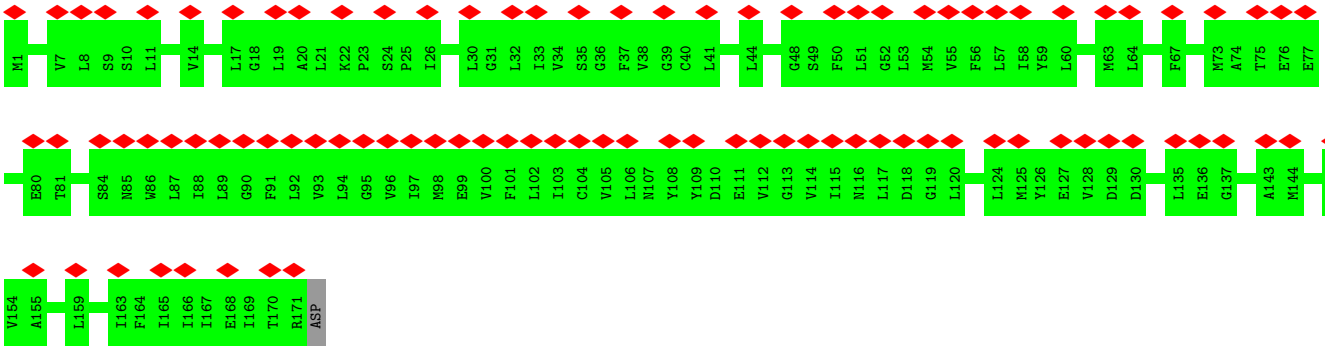


• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

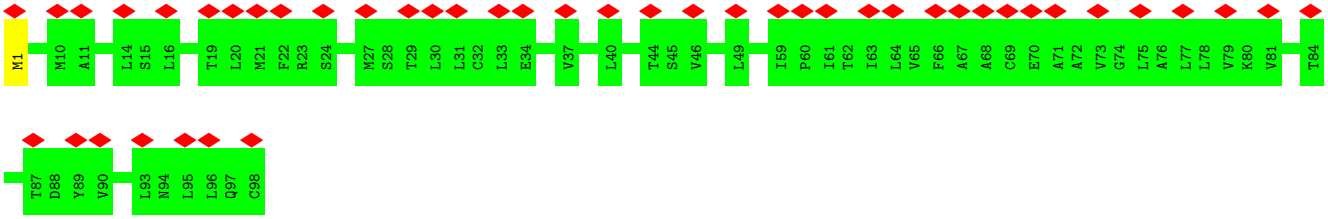




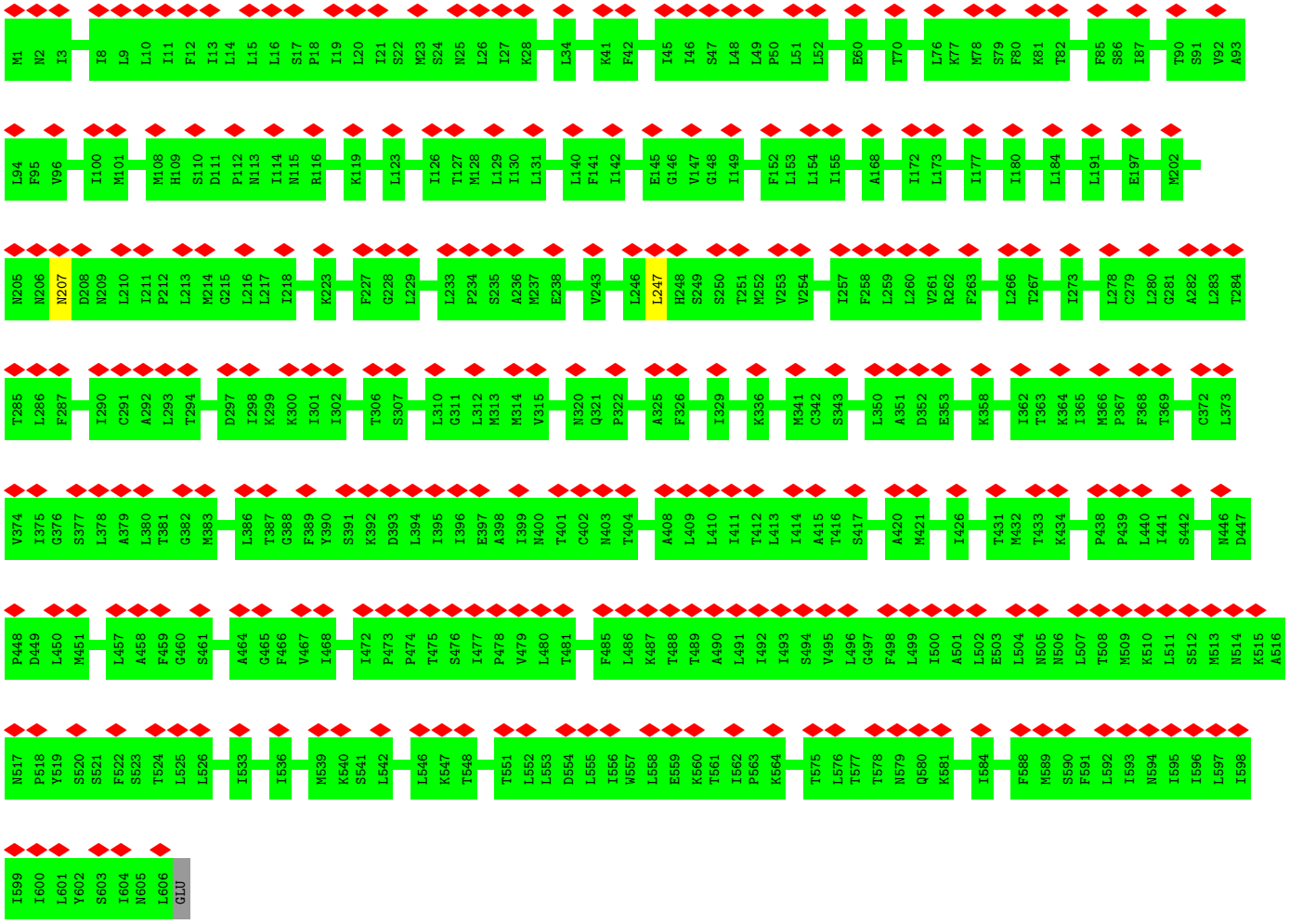
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6



• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

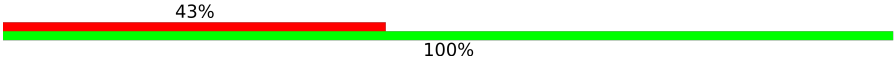


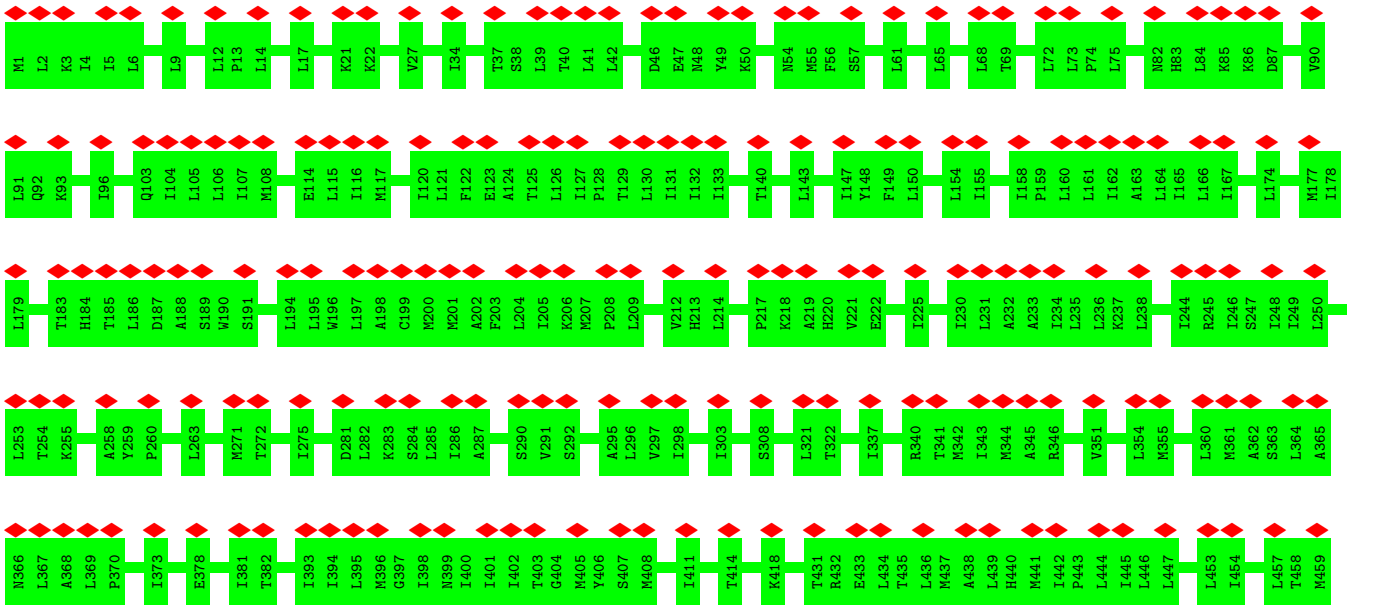
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5



• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

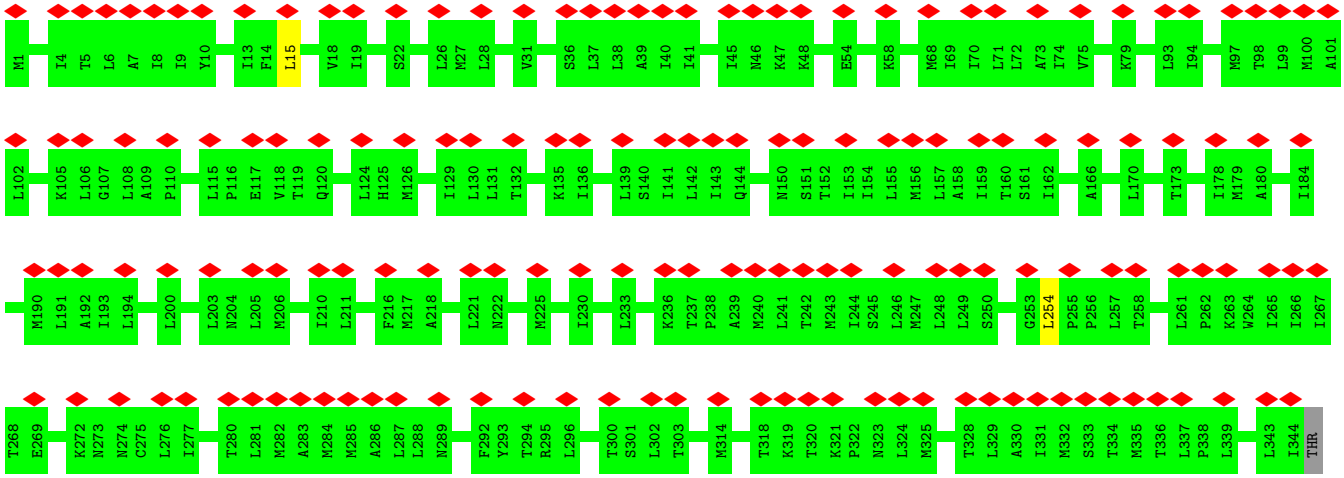
Chain M:





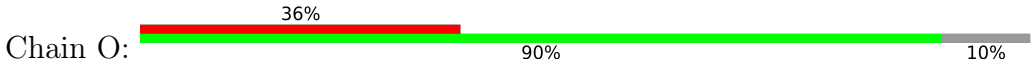
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

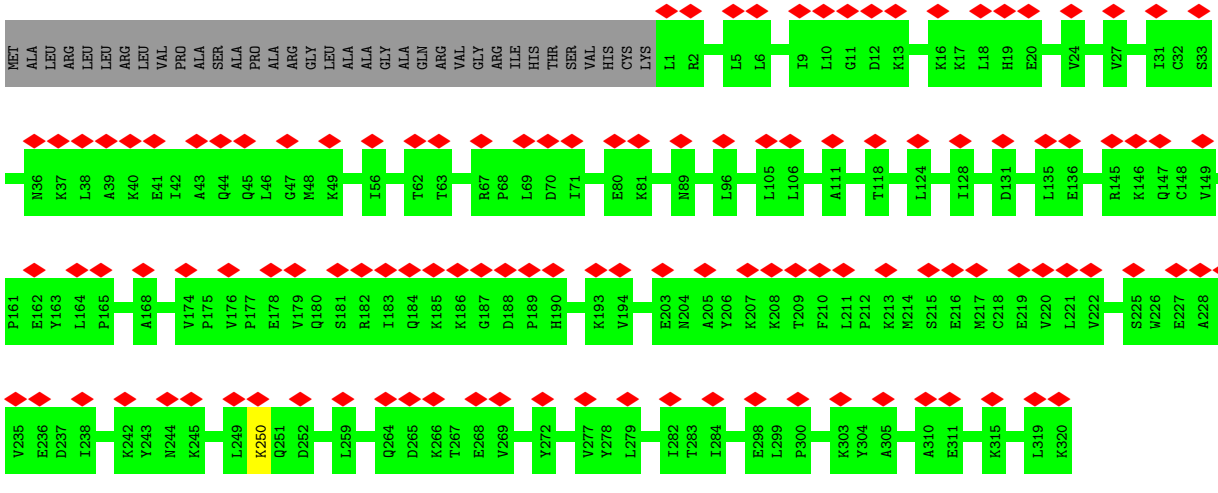
Chain N:



• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

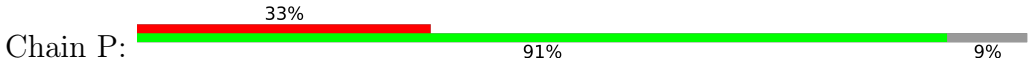
Chain O:

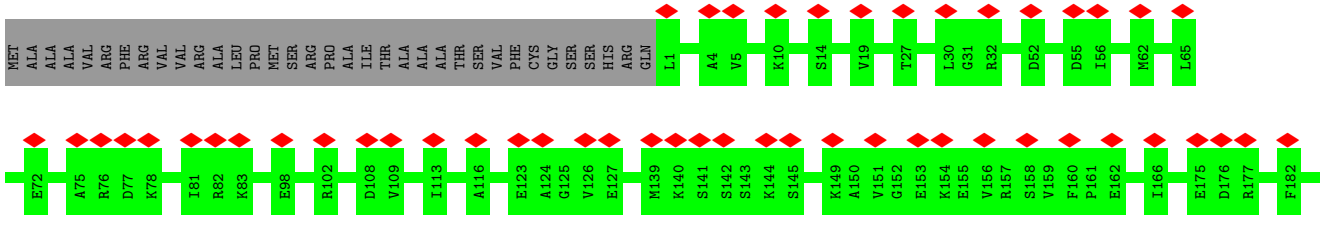


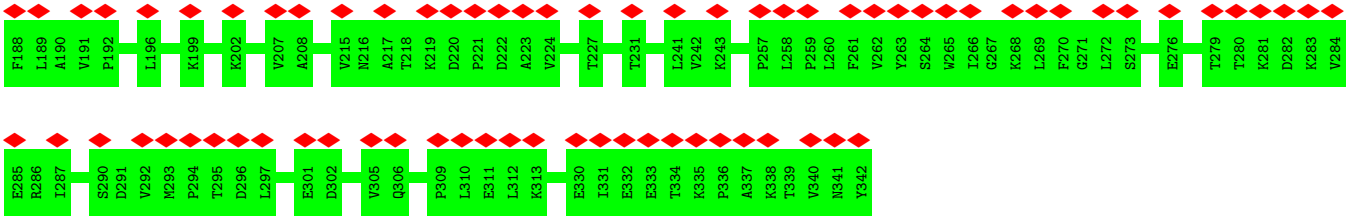


• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

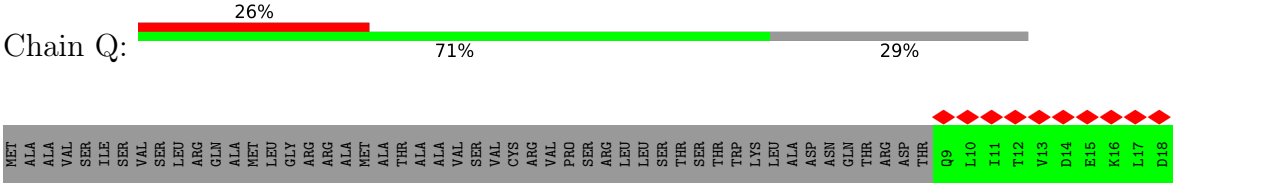
Chain P:



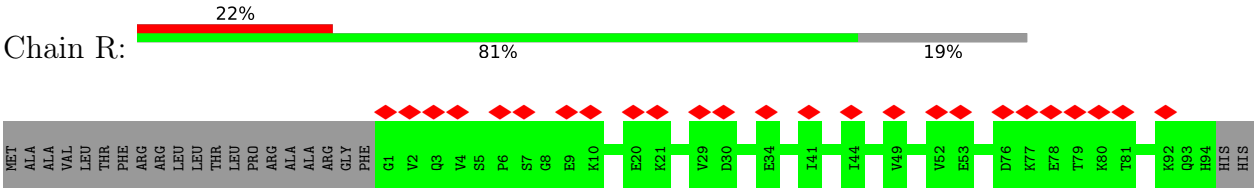




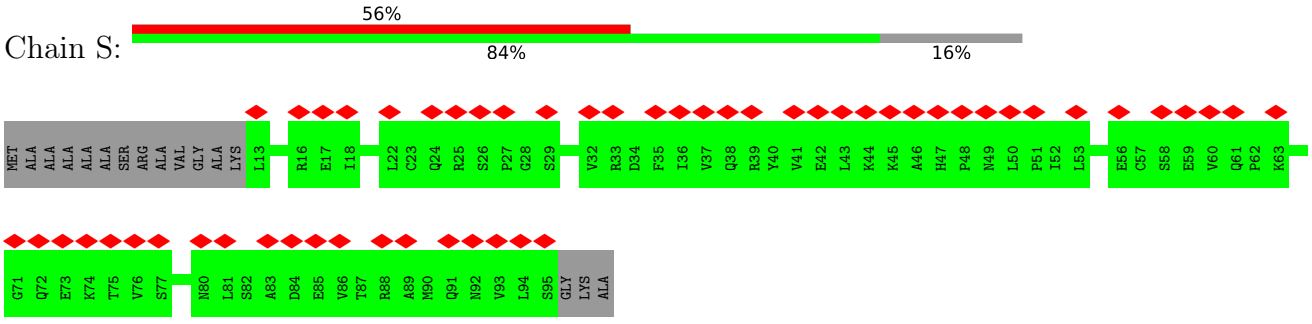
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



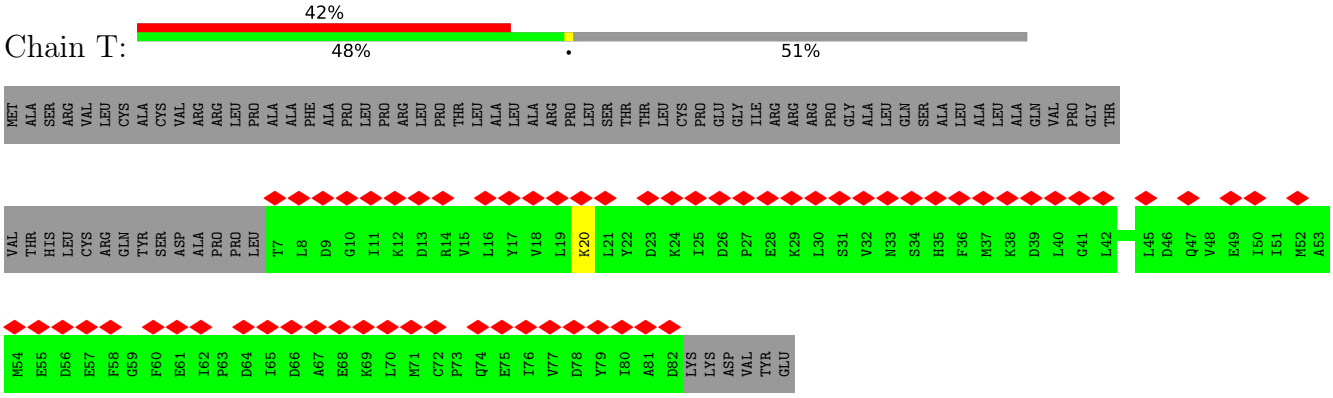
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

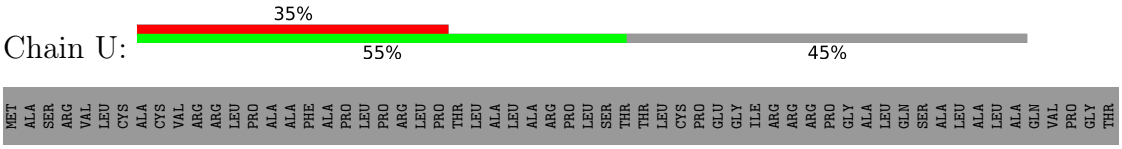


• Molecule 20: Acyl carrier protein, mitochondrial



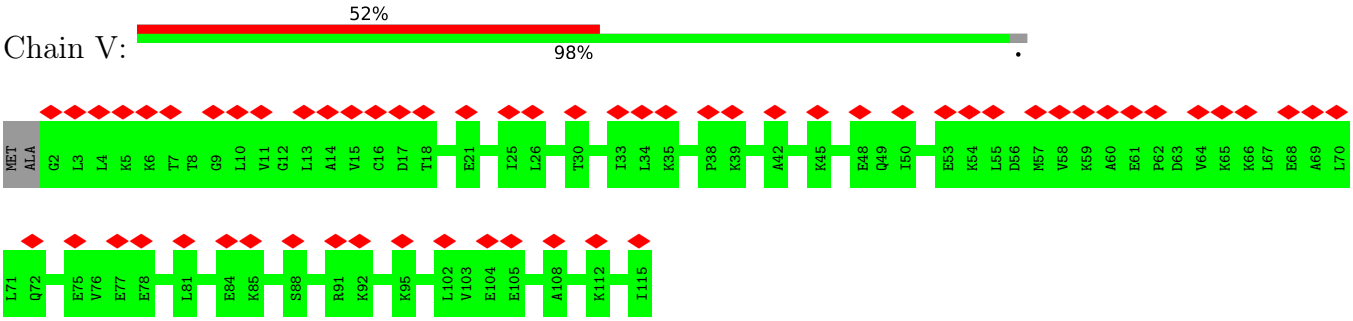
• Molecule 20: Acyl carrier protein, mitochondrial

Chain U:



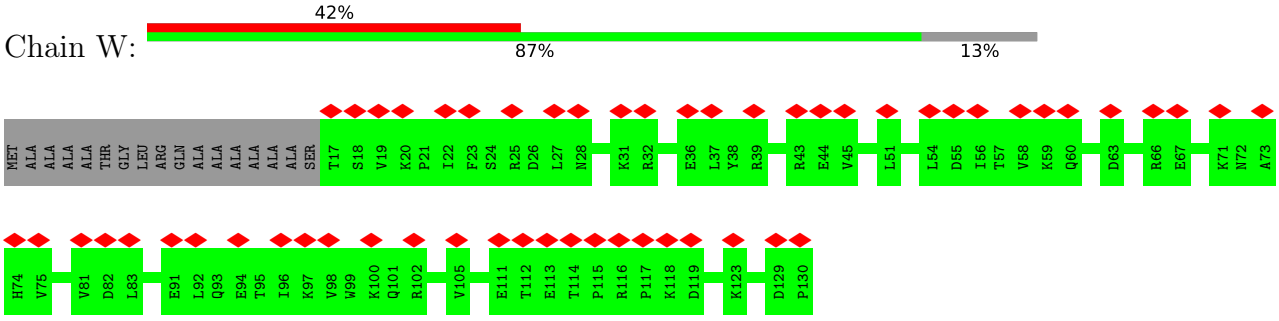
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:



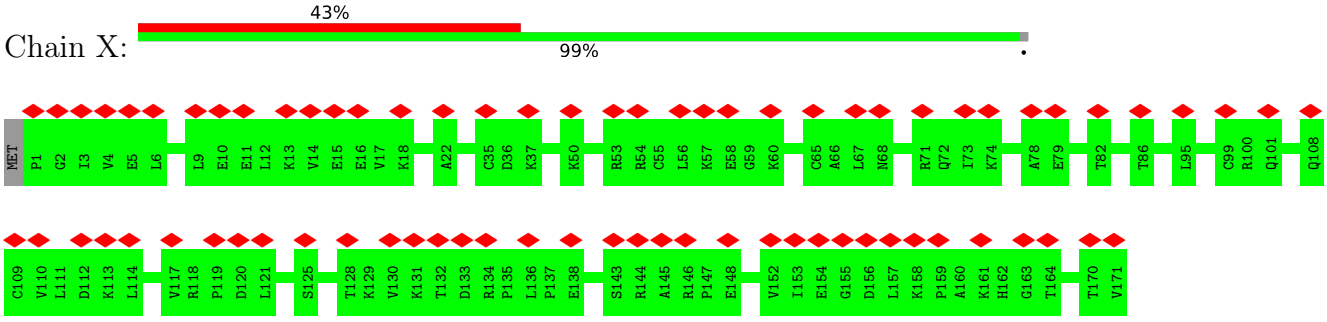
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:



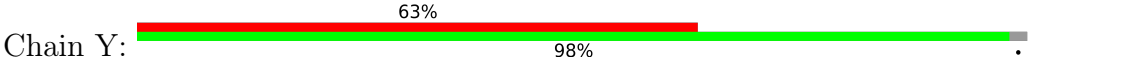
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

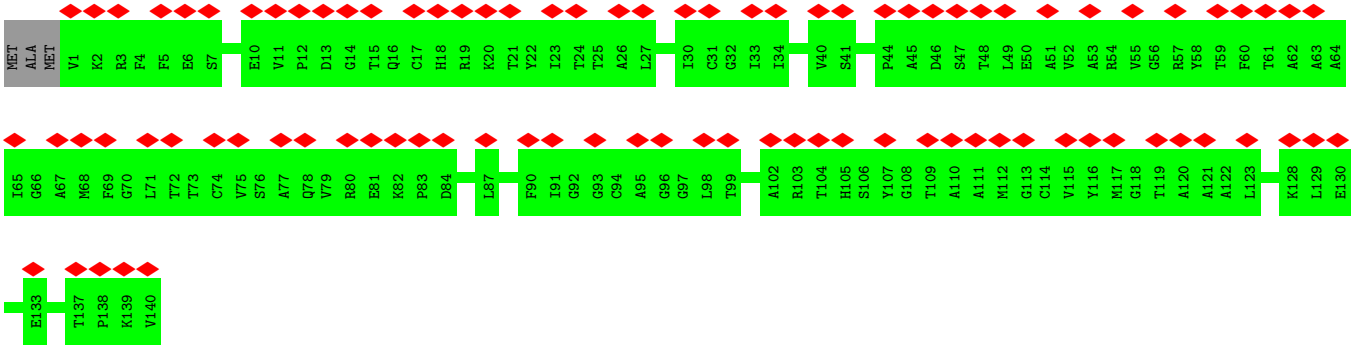
Chain X:



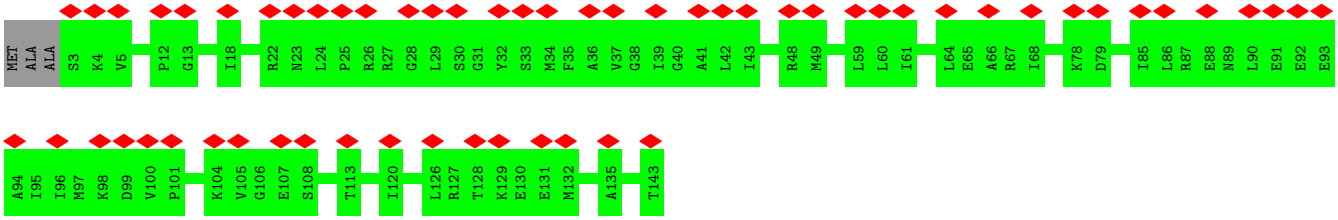
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:

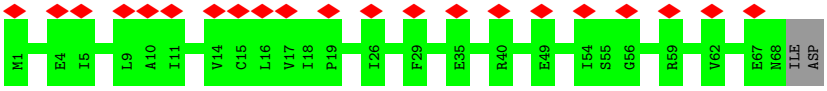




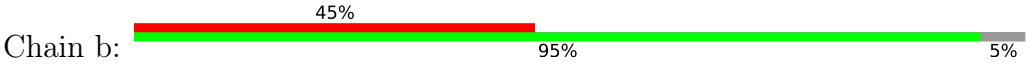
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

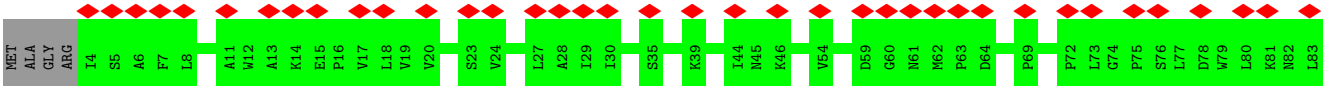


• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

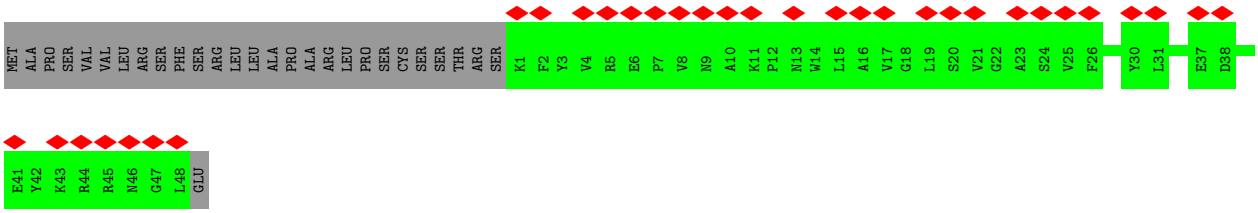


• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



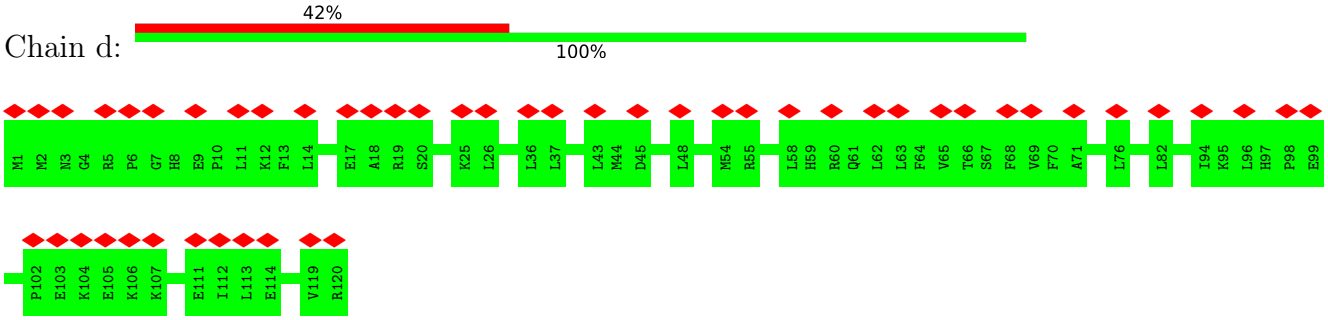


• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



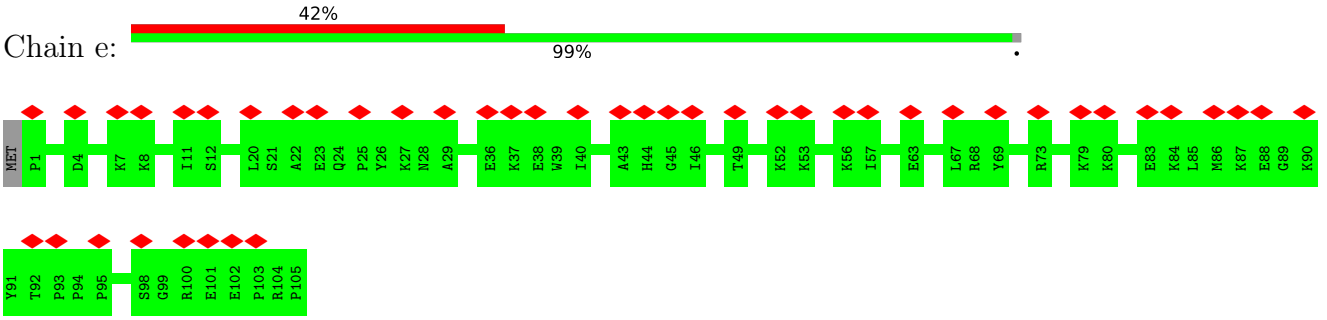
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:



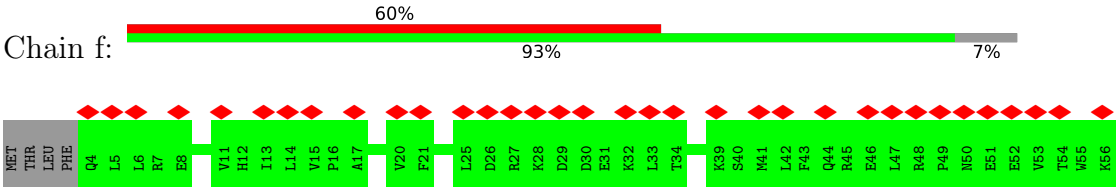
• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:



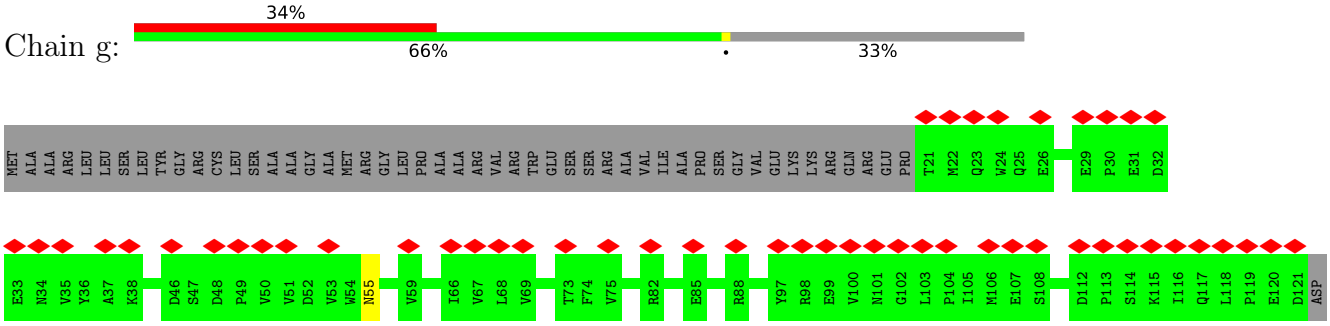
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:



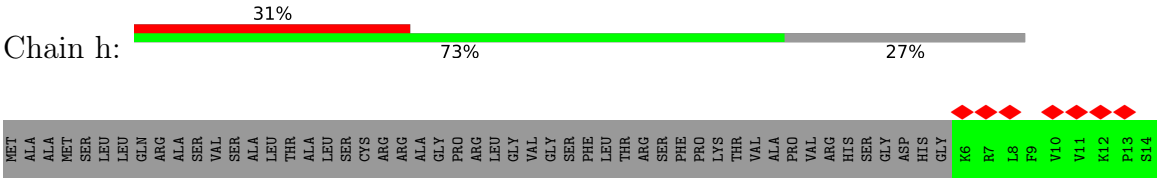
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:

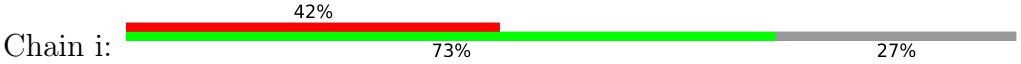


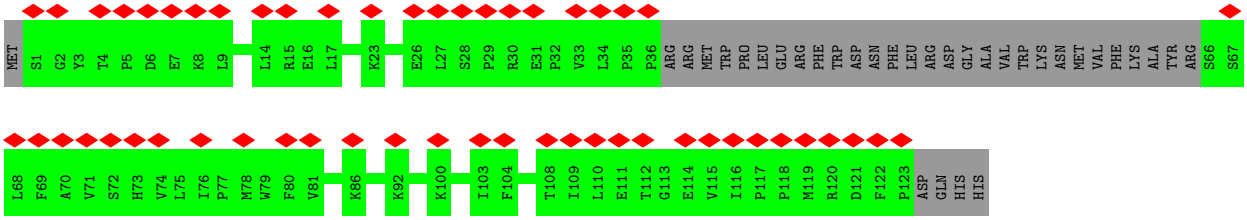
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:

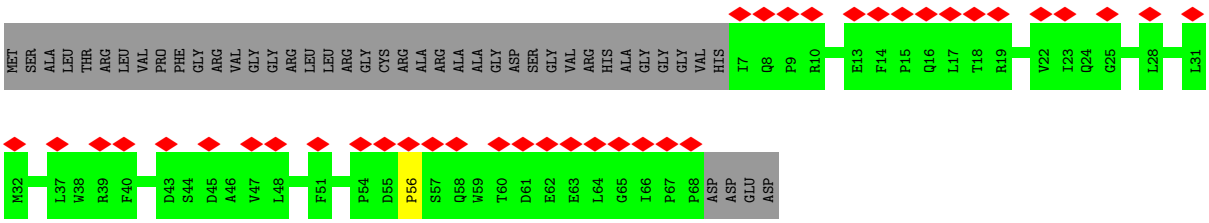


• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

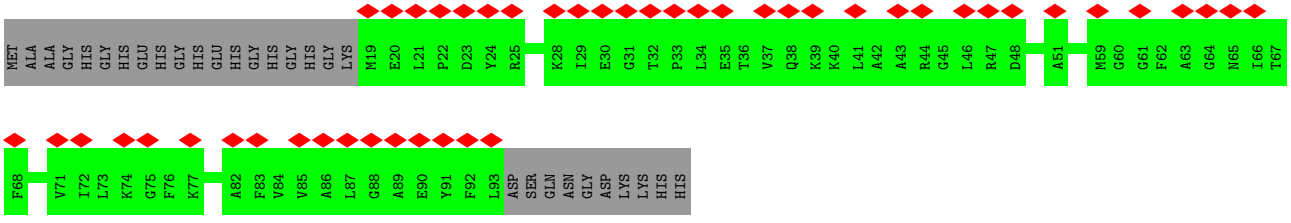




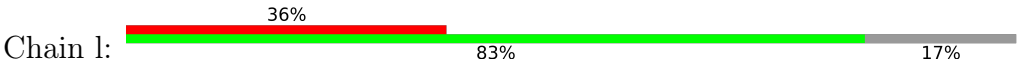
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

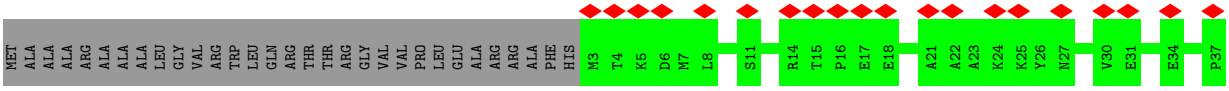


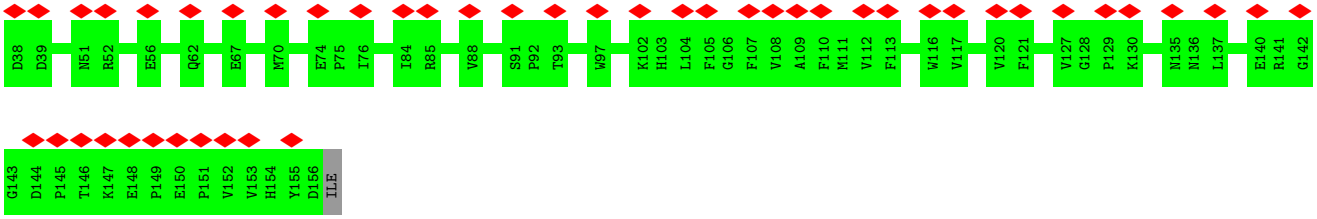
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



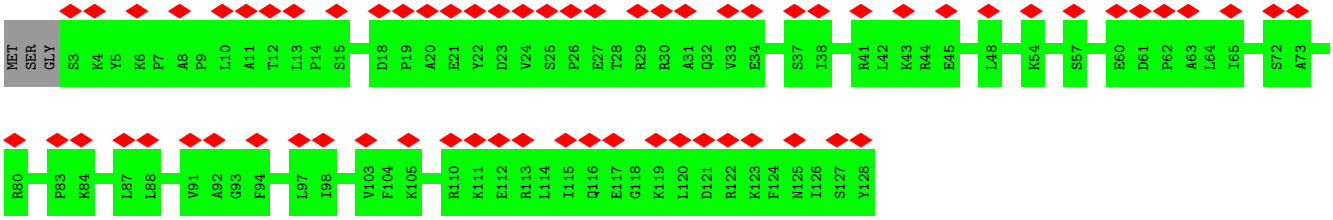
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



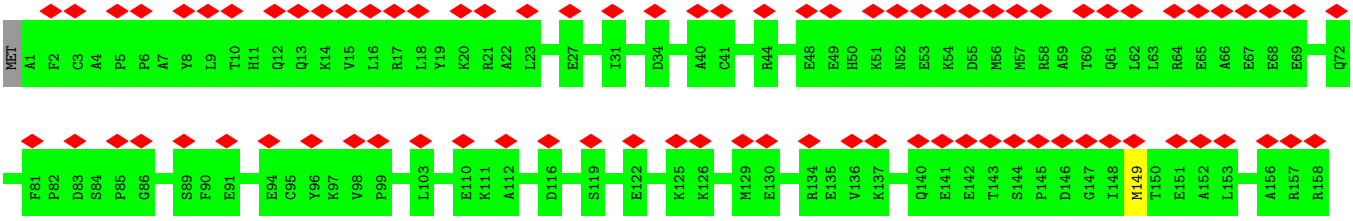




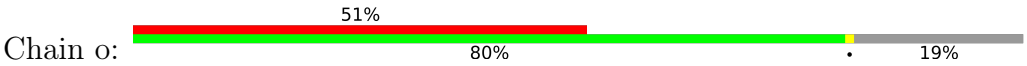
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

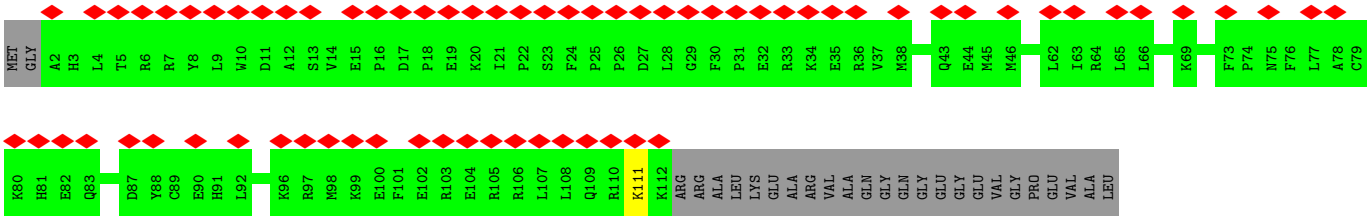


• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

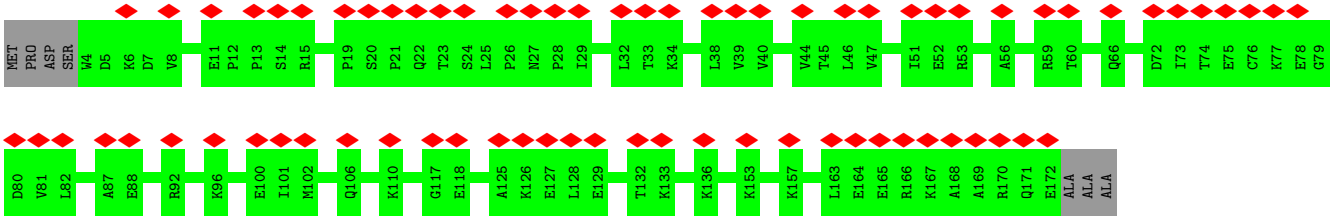


• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

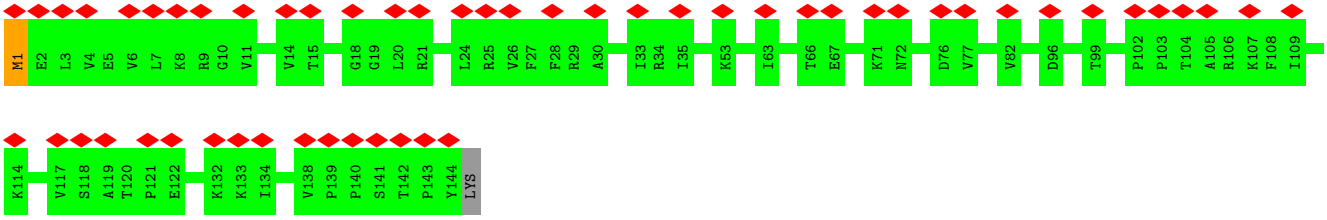




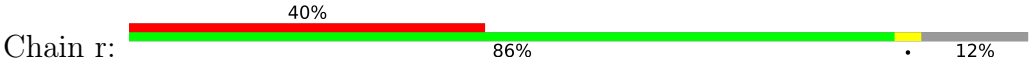
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

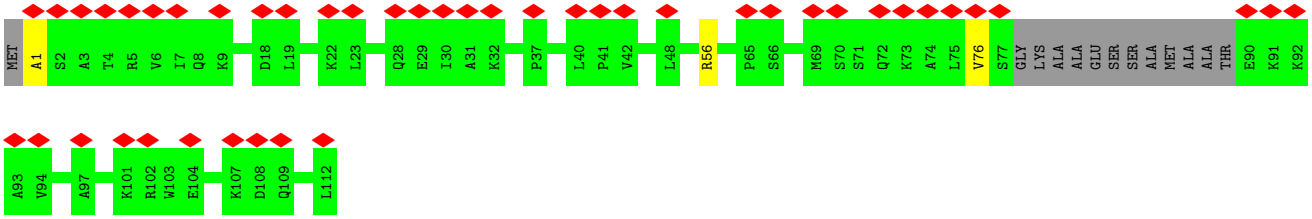


• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

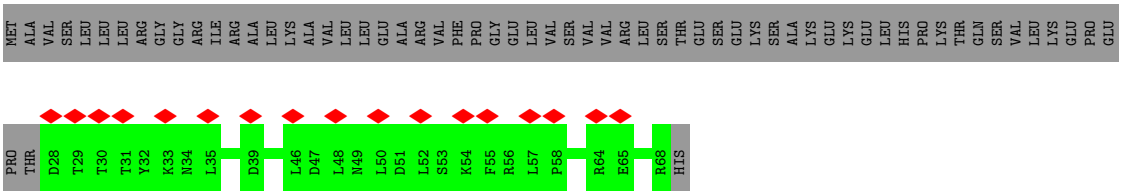


• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7





• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15754	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.265	Depositor
Minimum map value	-0.084	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	469.35, 469.35, 469.35	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.043, 1.043, 1.043	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 88I, 3PE, ZN, EHZ, 2MR, CDL, AYA, SF4, AME, FME, FES, FMN, NDP, PC1, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.32	0/949	0.46	0/1297
2	B	0.43	0/1278	0.58	1/1730 (0.1%)
3	C	0.40	0/1771	0.56	0/2412
4	D	0.38	0/3540	0.53	0/4795
5	E	0.32	0/1688	0.51	0/2300
6	F	0.33	0/3374	0.54	0/4557
7	G	0.34	1/5383 (0.0%)	0.53	0/7293
8	H	0.34	0/2607	0.48	0/3564
9	I	0.42	0/1461	0.56	0/1974
10	J	0.33	0/1322	0.46	0/1799
11	K	0.30	0/738	0.48	0/1002
12	L	0.31	0/4913	0.48	2/6686 (0.0%)
13	M	0.31	0/3709	0.48	0/5052
14	N	0.31	0/2748	0.50	3/3741 (0.1%)
15	O	0.34	0/2674	0.48	0/3626
16	P	0.33	0/2823	0.53	0/3828
17	Q	0.32	0/1038	0.53	0/1401
18	R	0.37	0/751	0.53	0/1011
19	S	0.29	0/678	0.57	0/915
20	T	0.26	0/620	0.45	0/836
20	U	0.31	0/704	0.46	0/951
21	V	0.30	0/949	0.47	0/1286
22	W	0.32	0/993	0.54	0/1335
23	X	0.31	0/1434	0.53	0/1937
24	Y	0.29	0/1061	0.47	0/1439
25	Z	0.32	0/1198	0.57	0/1616
26	a	0.33	0/569	0.53	0/766
27	b	0.31	0/651	0.44	0/895
28	c	0.29	0/409	0.46	0/555
29	d	0.35	0/1028	0.51	0/1387
30	e	0.31	0/900	0.50	0/1199
31	f	0.29	0/468	0.51	0/630

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	g	0.34	0/878	0.48	0/1196
33	h	0.36	0/1197	0.50	0/1621
34	i	0.32	0/810	0.50	0/1102
35	j	0.32	0/561	0.53	1/768 (0.1%)
36	k	0.29	0/629	0.49	0/851
37	l	0.34	0/1348	0.51	0/1840
38	m	0.32	0/1079	0.55	0/1463
39	n	0.31	0/1589	0.51	0/2152
40	o	0.31	0/982	0.54	0/1320
41	p	0.33	0/1466	0.53	0/1981
42	q	0.38	0/1234	0.53	0/1681
43	r	0.33	0/812	0.62	1/1098 (0.1%)
44	s	0.31	0/353	0.50	0/479
All	All	0.33	1/67367 (0.0%)	0.51	8/91367 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
42	q	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	52	CYS	CB-SG	-5.68	1.72	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	247	LEU	CB-CG-CD2	7.43	123.63	111.00
14	N	254	LEU	CB-CG-CD2	6.87	122.67	111.00
2	B	65	CYS	CA-CB-SG	6.77	126.19	114.00
43	r	76	VAL	CG1-CB-CG2	6.73	121.66	110.90
14	N	15	LEU	CB-CG-CD2	5.76	120.80	111.00
35	j	56	PRO	CA-N-CD	-5.25	104.15	111.50
14	N	254	LEU	CB-CG-CD1	5.24	119.91	111.00
12	L	247	LEU	CB-CG-CD1	5.17	119.78	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
42	q	1	AME	Mainchain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
2	B	154/224 (69%)	142 (92%)	12 (8%)	0	100	100
3	C	205/263 (78%)	191 (93%)	14 (7%)	0	100	100
4	D	427/463 (92%)	398 (93%)	29 (7%)	0	100	100
5	E	210/248 (85%)	191 (91%)	19 (9%)	0	100	100
6	F	426/464 (92%)	392 (92%)	34 (8%)	0	100	100
7	G	686/727 (94%)	629 (92%)	57 (8%)	0	100	100
8	H	316/318 (99%)	296 (94%)	20 (6%)	0	100	100
9	I	176/212 (83%)	164 (93%)	12 (7%)	0	100	100
10	J	169/172 (98%)	158 (94%)	11 (6%)	0	100	100
11	K	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
12	L	604/607 (100%)	559 (92%)	45 (8%)	0	100	100
13	M	457/459 (100%)	440 (96%)	17 (4%)	0	100	100
14	N	342/345 (99%)	324 (95%)	18 (5%)	0	100	100
15	O	318/355 (90%)	306 (96%)	12 (4%)	0	100	100
16	P	340/377 (90%)	302 (89%)	38 (11%)	0	100	100
17	Q	123/175 (70%)	116 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	R	92/116 (79%)	90 (98%)	2 (2%)	0	100	100
19	S	81/99 (82%)	68 (84%)	13 (16%)	0	100	100
20	T	74/156 (47%)	69 (93%)	5 (7%)	0	100	100
20	U	84/156 (54%)	78 (93%)	6 (7%)	0	100	100
21	V	112/116 (97%)	103 (92%)	9 (8%)	0	100	100
22	W	112/131 (86%)	107 (96%)	5 (4%)	0	100	100
23	X	169/172 (98%)	159 (94%)	10 (6%)	0	100	100
24	Y	138/143 (96%)	132 (96%)	6 (4%)	0	100	100
25	Z	139/144 (96%)	132 (95%)	7 (5%)	0	100	100
26	a	66/70 (94%)	65 (98%)	1 (2%)	0	100	100
27	b	78/84 (93%)	73 (94%)	5 (6%)	0	100	100
28	c	46/76 (60%)	43 (94%)	3 (6%)	0	100	100
29	d	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
30	e	103/106 (97%)	95 (92%)	8 (8%)	0	100	100
31	f	51/57 (90%)	48 (94%)	3 (6%)	0	100	100
32	g	99/151 (66%)	91 (92%)	8 (8%)	0	100	100
33	h	136/189 (72%)	129 (95%)	7 (5%)	0	100	100
34	i	90/128 (70%)	84 (93%)	6 (7%)	0	100	100
35	j	60/105 (57%)	58 (97%)	2 (3%)	0	100	100
36	k	73/104 (70%)	72 (99%)	1 (1%)	0	100	100
37	l	152/186 (82%)	133 (88%)	19 (12%)	0	100	100
38	m	124/129 (96%)	115 (93%)	9 (7%)	0	100	100
39	n	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
40	o	109/137 (80%)	97 (89%)	12 (11%)	0	100	100
41	p	167/176 (95%)	157 (94%)	10 (6%)	0	100	100
42	q	142/145 (98%)	136 (96%)	6 (4%)	0	100	100
43	r	96/113 (85%)	86 (90%)	10 (10%)	0	100	100
44	s	39/104 (38%)	36 (92%)	3 (8%)	0	100	100
All	All	8087/9214 (88%)	7538 (93%)	549 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	A	103/103 (100%)	103 (100%)	0	100 100
2	B	132/185 (71%)	132 (100%)	0	100 100
3	C	189/227 (83%)	189 (100%)	0	100 100
4	D	370/394 (94%)	369 (100%)	1 (0%)	92 97
5	E	183/206 (89%)	182 (100%)	1 (0%)	88 94
6	F	343/370 (93%)	343 (100%)	0	100 100
7	G	580/610 (95%)	580 (100%)	0	100 100
8	H	279/279 (100%)	279 (100%)	0	100 100
9	I	152/178 (85%)	152 (100%)	0	100 100
10	J	136/137 (99%)	136 (100%)	0	100 100
11	K	87/87 (100%)	87 (100%)	0	100 100
12	L	548/549 (100%)	547 (100%)	1 (0%)	93 98
13	M	414/414 (100%)	414 (100%)	0	100 100
14	N	306/307 (100%)	306 (100%)	0	100 100
15	O	284/309 (92%)	283 (100%)	1 (0%)	91 95
16	P	299/325 (92%)	299 (100%)	0	100 100
17	Q	112/153 (73%)	112 (100%)	0	100 100
18	R	79/96 (82%)	79 (100%)	0	100 100
19	S	74/80 (92%)	74 (100%)	0	100 100
20	T	70/135 (52%)	69 (99%)	1 (1%)	67 83
20	U	79/135 (58%)	79 (100%)	0	100 100
21	V	101/102 (99%)	101 (100%)	0	100 100
22	W	108/114 (95%)	108 (100%)	0	100 100
23	X	153/154 (99%)	153 (100%)	0	100 100
24	Y	105/107 (98%)	105 (100%)	0	100 100
25	Z	122/123 (99%)	122 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	a	58/60 (97%)	58 (100%)	0	100	100
27	b	71/73 (97%)	71 (100%)	0	100	100
28	c	42/67 (63%)	42 (100%)	0	100	100
29	d	107/107 (100%)	107 (100%)	0	100	100
30	e	93/94 (99%)	93 (100%)	0	100	100
31	f	49/53 (92%)	49 (100%)	0	100	100
32	g	92/129 (71%)	91 (99%)	1 (1%)	73	86
33	h	123/162 (76%)	123 (100%)	0	100	100
34	i	89/120 (74%)	89 (100%)	0	100	100
35	j	58/87 (67%)	58 (100%)	0	100	100
36	k	58/78 (74%)	58 (100%)	0	100	100
37	l	139/161 (86%)	139 (100%)	0	100	100
38	m	112/114 (98%)	112 (100%)	0	100	100
39	n	162/164 (99%)	161 (99%)	1 (1%)	86	94
40	o	104/121 (86%)	103 (99%)	1 (1%)	76	88
41	p	154/158 (98%)	154 (100%)	0	100	100
42	q	129/130 (99%)	129 (100%)	0	100	100
43	r	89/96 (93%)	88 (99%)	1 (1%)	73	86
44	s	40/95 (42%)	40 (100%)	0	100	100
All	All	7177/7948 (90%)	7168 (100%)	9 (0%)	93	98

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	149	ASN
5	E	10	ARG
12	L	207	ASN
15	O	250	LYS
20	T	20	LYS
32	g	55	ASN
39	n	149	MET
40	o	111	LYS
43	r	56	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	27	ASN
7	G	259	ASN
12	L	226	GLN
13	M	48	ASN
30	e	96	HIS
33	h	44	ASN
33	h	86	ASN
42	q	123	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
43	AYA	r	1	43	6,7,8	1.79	2 (33%)	5,8,10	1.34	1 (20%)
12	FME	L	1	12	8,9,10	0.94	0	7,9,11	0.75	0
13	FME	M	1	13	8,9,10	0.97	0	7,9,11	0.82	0
14	FME	N	1	14	8,9,10	0.95	0	7,9,11	0.77	0
11	FME	K	1	11	8,9,10	0.96	0	7,9,11	1.42	1 (14%)
8	FME	H	1	8	8,9,10	0.84	0	7,9,11	1.42	1 (14%)
1	FME	A	1	1	8,9,10	0.96	0	7,9,11	0.96	0
42	AME	q	1	42	9,10,11	1.48	1 (11%)	9,11,13	1.56	3 (33%)
10	FME	J	1	10	8,9,10	0.88	0	7,9,11	0.92	0
4	2MR	D	85	4	10,12,13	2.37	2 (20%)	5,13,15	1.25	1 (20%)

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
43	AYA	r	1	43	-	0/4/6/8	-
12	FME	L	1	12	-	5/7/9/11	-
13	FME	M	1	13	-	2/7/9/11	-
14	FME	N	1	14	-	1/7/9/11	-
11	FME	K	1	11	-	4/7/9/11	-
8	FME	H	1	8	-	4/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
42	AME	q	1	42	-	3/9/10/12	-
10	FME	J	1	10	-	2/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NE	5.02	1.45	1.34
4	D	85	2MR	CZ-NH2	4.75	1.43	1.33
42	q	1	AME	CT1-N	3.34	1.45	1.34
43	r	1	AYA	CT-N	3.17	1.45	1.34
43	r	1	AYA	OT-CT	-2.02	1.18	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	1	FME	C-CA-N	3.17	115.45	109.73
11	K	1	FME	C-CA-N	2.86	114.89	109.73
42	q	1	AME	CE-SD-CG	2.63	109.45	100.40
4	D	85	2MR	CD-NE-CZ	2.62	128.31	123.41
42	q	1	AME	O-C-CA	-2.32	118.70	124.78
42	q	1	AME	CT2-CT1-N	2.19	119.80	116.10
43	r	1	AYA	CM-CT-N	2.09	119.64	116.10

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
8	H	1	FME	CB-CA-N-CN
8	H	1	FME	N-CA-CB-CG
8	H	1	FME	C-CA-CB-CG
10	J	1	FME	CA-CB-CG-SD

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Mol	Chain	Res	Type	Atoms
12	L	1	FME	CB-CA-N-CN
12	L	1	FME	N-CA-CB-CG
12	L	1	FME	O-C-CA-CB
13	M	1	FME	CB-CA-N-CN
42	q	1	AME	O-C-CA-CB
14	N	1	FME	CA-CB-CG-SD
10	J	1	FME	N-CA-CB-CG
13	M	1	FME	N-CA-CB-CG
1	A	1	FME	CB-CG-SD-CE
8	H	1	FME	CB-CG-SD-CE
12	L	1	FME	CB-CG-SD-CE
42	q	1	AME	CB-CG-SD-CE
11	K	1	FME	CA-CB-CG-SD
42	q	1	AME	CA-CB-CG-SD
11	K	1	FME	N-CA-CB-CG
11	K	1	FME	CB-CG-SD-CE
12	L	1	FME	C-CA-CB-CG
11	K	1	FME	CB-CA-N-CN

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 35 ligands modelled in this entry, 1 is monoatomic - leaving 34 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	$\#\|Z\| > 2$
51	CDL	r	201	-	56,56,99	1.15	8 (14%)	62,68,111	1.17	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
51	CDL	d	202	-	62,62,99	1.08	8 (12%)	68,74,111	1.15	4 (5%)
55	EHZ	T	201	20	29,36,37	1.66	5 (17%)	35,44,47	1.41	3 (8%)
49	3PE	K	201	-	32,32,50	1.06	4 (12%)	35,37,55	1.20	2 (5%)
46	PC1	B	203	-	42,42,53	1.04	4 (9%)	48,50,61	1.05	2 (4%)
49	3PE	Y	401	-	40,40,50	0.96	4 (10%)	43,45,55	1.05	2 (4%)
46	PC1	B	202	-	34,34,53	1.15	4 (11%)	40,42,61	1.06	2 (5%)
45	SF4	F	501	6	0,12,12	-	-	-		
49	3PE	H	401	-	50,50,50	0.86	4 (8%)	53,55,55	1.07	2 (3%)
52	ATP	O	401	-	26,33,33	0.62	0	31,52,52	1.06	3 (9%)
49	3PE	H	403	-	43,43,50	0.91	4 (9%)	46,48,55	1.14	2 (4%)
51	CDL	X	201	-	66,66,99	1.05	8 (12%)	72,78,111	1.15	4 (5%)
46	PC1	Z	201	-	44,44,53	1.04	4 (9%)	50,52,61	1.03	2 (4%)
46	PC1	J	201	-	41,41,53	1.05	4 (9%)	47,49,61	1.06	2 (4%)
51	CDL	N	401	-	64,64,99	1.08	7 (10%)	70,76,111	1.14	4 (5%)
47	FES	E	301	5	0,4,4	-	-	-		
45	SF4	I	201	9	0,12,12	-	-	-		
48	FMN	F	502	-	31,33,33	1.36	5 (16%)	40,50,50	1.57	6 (15%)
49	3PE	M	501	-	36,36,50	1.01	3 (8%)	39,41,55	1.12	2 (5%)
45	SF4	G	803	7	0,12,12	-	-	-		
50	88I	H	402	-	45,45,45	1.93	9 (20%)	56,56,56	1.70	13 (23%)
55	EHZ	U	201	20	29,36,37	1.68	5 (17%)	35,44,47	1.65	8 (22%)
45	SF4	B	201	2	0,12,12	-	-	-		
49	3PE	L	702	-	41,41,50	0.95	4 (9%)	44,46,55	1.15	2 (4%)
45	SF4	G	801	7	0,12,12	-	-	-		
49	3PE	M	502	-	41,41,50	0.94	3 (7%)	44,46,55	1.10	2 (4%)
51	CDL	i	201	-	69,69,99	1.02	7 (10%)	75,81,111	1.17	5 (6%)
49	3PE	L	704	-	48,48,50	0.88	3 (6%)	51,53,55	1.06	2 (3%)
47	FES	G	802	7	0,4,4	-	-	-		
51	CDL	L	703	-	73,73,99	1.00	8 (10%)	79,85,111	1.13	4 (5%)
53	NDP	P	501	-	45,52,52	2.09	4 (8%)	53,80,80	1.76	12 (22%)
49	3PE	L	701	-	48,48,50	0.88	4 (8%)	51,53,55	1.11	2 (3%)
51	CDL	d	201	-	58,58,99	1.02	6 (10%)	63,69,111	1.05	3 (4%)
45	SF4	I	202	9	0,12,12	-	-	-		

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
51	CDL	r	201	-	-	27/67/67/110	-
51	CDL	d	202	-	-	31/73/73/110	-
55	EHZ	T	201	20	1/1/9/9	17/42/44/45	-
49	3PE	K	201	-	-	15/36/36/54	-
46	PC1	B	203	-	-	13/46/46/57	-
49	3PE	Y	401	-	-	14/44/44/54	-
46	PC1	B	202	-	-	14/38/38/57	-
45	SF4	F	501	6	-	-	0/6/5/5
49	3PE	H	401	-	-	20/54/54/54	-
52	ATP	O	401	-	-	6/18/38/38	0/3/3/3
49	3PE	H	403	-	-	20/47/47/54	-
51	CDL	X	201	-	-	36/77/77/110	-
46	PC1	Z	201	-	-	18/48/48/57	-
46	PC1	J	201	-	-	16/45/45/57	-
51	CDL	N	401	-	-	37/75/75/110	-
47	FES	E	301	5	-	-	0/1/1/1
48	FMN	F	502	-	-	11/18/18/18	0/3/3/3
49	3PE	M	501	-	-	15/40/40/54	-
45	SF4	I	201	9	-	-	0/6/5/5
45	SF4	G	803	7	-	-	0/6/5/5
50	88I	H	402	-	-	17/37/67/67	0/3/3/3
55	EHZ	U	201	20	1/1/9/9	15/42/44/45	-
45	SF4	B	201	2	-	-	0/6/5/5
49	3PE	L	702	-	-	16/45/45/54	-
45	SF4	G	801	7	-	-	0/6/5/5
49	3PE	M	502	-	-	13/45/45/54	-
51	CDL	i	201	-	-	32/80/80/110	-
49	3PE	L	704	-	-	24/52/52/54	-
47	FES	G	802	7	-	-	0/1/1/1
51	CDL	L	703	-	-	33/84/84/110	-
53	NDP	P	501	-	-	8/30/77/77	0/5/5/5
49	3PE	L	701	-	-	16/52/52/54	-
51	CDL	d	201	-	-	30/67/67/110	-
45	SF4	I	202	9	-	-	0/6/5/5

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	P	501	NDP	P2B-O2B	11.26	1.80	1.59
50	H	402	88I	C4-C5	-9.71	1.32	1.54
55	U	201	EHZ	C15-N2	5.48	1.45	1.33
55	T	201	EHZ	C15-N2	5.33	1.45	1.33
55	U	201	EHZ	C12-N1	5.18	1.45	1.33
55	T	201	EHZ	C12-N1	5.11	1.45	1.33
53	P	501	NDP	PN-O5D	3.84	1.74	1.59
48	F	502	FMN	C10-N1	3.42	1.37	1.33
48	F	502	FMN	C1'-N10	3.36	1.51	1.48
50	H	402	88I	O4'-C4'	-3.11	1.38	1.45
50	H	402	88I	O3-C16	3.10	1.39	1.35
53	P	501	NDP	O2B-C2B	-3.09	1.32	1.44
49	M	501	3PE	O21-C2	-2.63	1.40	1.46
51	d	202	CDL	OB6-CB4	-2.63	1.40	1.46
51	i	201	CDL	OA6-CA4	-2.62	1.40	1.46
49	M	502	3PE	O21-C2	-2.62	1.40	1.46
51	i	201	CDL	OB6-CB4	-2.61	1.40	1.46
51	L	703	CDL	OB6-CB4	-2.60	1.40	1.46
49	L	701	3PE	O21-C2	-2.58	1.40	1.46
49	H	401	3PE	O21-C2	-2.55	1.40	1.46
46	B	203	PC1	O21-C2	-2.55	1.40	1.46
49	L	704	3PE	O31-C31	2.54	1.40	1.33
51	N	401	CDL	OA8-CA7	2.54	1.40	1.33
51	N	401	CDL	OB6-CB4	-2.54	1.40	1.46
51	r	201	CDL	OB6-CB4	-2.54	1.40	1.46
51	N	401	CDL	OA6-CA4	-2.53	1.40	1.46
50	H	402	88I	O4'-C1'	-2.49	1.39	1.45
46	J	201	PC1	O21-C2	-2.49	1.40	1.46
49	L	702	3PE	O21-C2	-2.48	1.40	1.46
51	X	201	CDL	OA6-CA4	-2.48	1.40	1.46
51	X	201	CDL	OB8-CB7	2.46	1.40	1.33
46	Z	201	PC1	O31-C31	2.45	1.40	1.33
49	Y	401	3PE	O21-C2	-2.44	1.40	1.46
51	r	201	CDL	OA8-CA7	2.44	1.40	1.33
51	L	703	CDL	OB8-CB7	2.43	1.40	1.33
49	H	403	3PE	O31-C31	2.43	1.40	1.33
51	L	703	CDL	OA8-CA7	2.42	1.40	1.33
46	B	202	PC1	O31-C31	2.41	1.40	1.33
51	d	202	CDL	OB8-CB7	2.41	1.40	1.33
51	d	201	CDL	OB8-CB7	2.40	1.40	1.33
51	r	201	CDL	OB8-CB7	2.40	1.40	1.33
51	N	401	CDL	OB8-CB7	2.40	1.40	1.33
50	H	402	88I	CAD-C1	2.39	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	d	202	CDL	OA8-CA7	2.39	1.40	1.33
55	U	201	EHZ	O4-C15	-2.39	1.18	1.23
46	Z	201	PC1	O21-C2	-2.39	1.40	1.46
51	r	201	CDL	OA6-CA4	-2.37	1.40	1.46
46	B	202	PC1	O21-C2	-2.37	1.40	1.46
51	X	201	CDL	OB6-CB4	-2.37	1.40	1.46
49	H	401	3PE	O31-C3	-2.37	1.39	1.45
46	B	203	PC1	O31-C31	2.37	1.40	1.33
49	L	704	3PE	O21-C2	-2.36	1.40	1.46
51	i	201	CDL	OB8-CB6	-2.36	1.39	1.45
51	d	202	CDL	OA6-CA4	-2.36	1.40	1.46
51	i	201	CDL	OA8-CA7	2.35	1.40	1.33
49	K	201	3PE	O21-C2	-2.35	1.40	1.46
48	F	502	FMN	C4-N3	2.35	1.37	1.33
49	M	501	3PE	O31-C31	2.34	1.40	1.33
49	L	701	3PE	O31-C31	2.34	1.40	1.33
49	Y	401	3PE	O31-C31	2.34	1.40	1.33
51	d	201	CDL	OA8-CA7	2.33	1.40	1.33
49	L	702	3PE	O31-C31	2.32	1.40	1.33
51	X	201	CDL	OA8-CA6	-2.31	1.39	1.45
46	B	202	PC1	O21-C21	2.30	1.40	1.34
49	Y	401	3PE	O31-C3	-2.30	1.39	1.45
49	K	201	3PE	O31-C31	2.30	1.40	1.33
49	M	501	3PE	O31-C3	-2.29	1.39	1.45
51	i	201	CDL	OB8-CB7	2.29	1.40	1.33
46	Z	201	PC1	O21-C21	2.29	1.40	1.34
49	M	502	3PE	O31-C31	2.29	1.40	1.33
46	J	201	PC1	O31-C31	2.28	1.40	1.33
50	H	402	88I	OP3-CAD	-2.28	1.38	1.43
48	F	502	FMN	C4A-N5	2.28	1.36	1.33
55	U	201	EHZ	C9-S1	2.28	1.81	1.76
55	T	201	EHZ	O4-C15	-2.27	1.18	1.23
55	T	201	EHZ	O3-C12	-2.27	1.18	1.23
49	L	702	3PE	O31-C3	-2.26	1.40	1.45
51	d	201	CDL	OA8-CA6	-2.26	1.40	1.45
51	r	201	CDL	OB6-CB5	2.26	1.40	1.34
49	H	403	3PE	O31-C3	-2.24	1.40	1.45
49	L	702	3PE	O21-C21	2.24	1.40	1.34
51	X	201	CDL	OA8-CA7	2.23	1.39	1.33
51	d	201	CDL	OB8-CB6	-2.23	1.40	1.45
50	H	402	88I	C5-C16	2.23	1.54	1.51
51	L	703	CDL	OA6-CA4	-2.23	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	i	201	CDL	OA8-CA6	-2.23	1.40	1.45
51	d	202	CDL	OB8-CB6	-2.22	1.40	1.45
49	H	403	3PE	O21-C2	-2.22	1.41	1.46
55	U	201	EHZ	O3-C12	-2.21	1.18	1.23
51	X	201	CDL	OA6-CA5	2.21	1.40	1.34
51	d	201	CDL	OB6-CB5	2.21	1.40	1.34
53	P	501	NDP	O5D-C5D	-2.19	1.36	1.44
51	r	201	CDL	OB8-CB6	-2.18	1.40	1.45
51	r	201	CDL	OA6-CA5	2.18	1.40	1.34
51	N	401	CDL	OB8-CB6	-2.18	1.40	1.45
49	L	704	3PE	O21-C21	2.17	1.40	1.34
49	H	401	3PE	O31-C31	2.17	1.39	1.33
49	K	201	3PE	O31-C3	-2.16	1.40	1.45
46	B	203	PC1	O21-C21	2.16	1.40	1.34
49	K	201	3PE	O21-C21	2.16	1.40	1.34
46	J	201	PC1	O31-C3	-2.16	1.40	1.45
49	M	502	3PE	O31-C3	-2.16	1.40	1.45
51	X	201	CDL	OB6-CB5	2.15	1.40	1.34
51	d	201	CDL	OB6-CB4	-2.15	1.41	1.46
51	L	703	CDL	OA8-CA6	-2.13	1.40	1.45
49	H	401	3PE	O21-C21	2.12	1.40	1.34
51	d	202	CDL	OA6-CA5	2.12	1.40	1.34
51	d	202	CDL	OA8-CA6	-2.12	1.40	1.45
55	T	201	EHZ	C9-S1	2.12	1.81	1.76
48	F	502	FMN	C6-C5A	-2.11	1.38	1.41
51	N	401	CDL	OA6-CA5	2.11	1.40	1.34
51	L	703	CDL	OA6-CA5	2.11	1.40	1.34
51	L	703	CDL	OB8-CB6	-2.11	1.40	1.45
49	L	701	3PE	O31-C3	-2.09	1.40	1.45
51	X	201	CDL	OB8-CB6	-2.08	1.40	1.45
51	N	401	CDL	OB6-CB5	2.07	1.40	1.34
46	J	201	PC1	O21-C21	2.07	1.40	1.34
46	B	202	PC1	O31-C3	-2.06	1.40	1.45
49	L	701	3PE	O21-C21	2.06	1.40	1.34
51	i	201	CDL	OA6-CA5	2.06	1.40	1.34
51	L	703	CDL	OB6-CB5	2.06	1.40	1.34
49	Y	401	3PE	O21-C21	2.06	1.40	1.34
46	B	203	PC1	O31-C3	-2.06	1.40	1.45
49	H	403	3PE	O21-C21	2.03	1.40	1.34
46	Z	201	PC1	O31-C3	-2.02	1.40	1.45
51	d	202	CDL	OB6-CB5	2.02	1.40	1.34
51	r	201	CDL	OA8-CA6	-2.01	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	H	402	88I	O2'-C2'	-2.01	1.40	1.45
50	H	402	88I	O2'-C1	-2.00	1.40	1.45

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	P	501	NDP	PN-O3-PA	-7.43	107.34	132.83
55	T	201	EHZ	C8-C9-S1	6.07	121.14	113.63
48	F	502	FMN	C1'-N10-C9A	5.52	122.64	118.29
55	U	201	EHZ	C8-C9-S1	5.46	120.38	113.63
50	H	402	88I	C29-C28-C5'	-5.42	105.27	114.18
49	L	701	3PE	O21-C21-C22	4.53	121.25	111.50
48	F	502	FMN	C2-N3-C4	4.51	118.95	115.14
49	K	201	3PE	O21-C21-C22	4.48	121.17	111.50
49	L	702	3PE	O21-C21-C22	4.47	121.13	111.50
51	i	201	CDL	OB6-CB5-C51	4.26	120.68	111.50
46	B	202	PC1	O21-C21-C22	4.22	120.59	111.50
51	N	401	CDL	OA6-CA5-C11	4.20	120.56	111.50
49	M	502	3PE	O21-C21-C22	4.18	120.51	111.50
51	X	201	CDL	OA6-CA5-C11	4.18	120.50	111.50
51	r	201	CDL	OA6-CA5-C11	4.15	120.44	111.50
49	H	403	3PE	O21-C21-C22	4.12	120.39	111.50
51	L	703	CDL	OA6-CA5-C11	4.10	120.34	111.50
51	L	703	CDL	OB6-CB5-C51	4.10	120.34	111.50
46	Z	201	PC1	O21-C21-C22	4.06	120.25	111.50
51	X	201	CDL	OB6-CB5-C51	4.03	120.20	111.50
46	B	203	PC1	O21-C21-C22	4.00	120.12	111.50
51	r	201	CDL	OB6-CB5-C51	3.96	120.03	111.50
51	d	201	CDL	OB6-CB5-C51	3.91	119.92	111.50
49	M	501	3PE	O21-C21-C22	3.86	119.81	111.50
51	d	202	CDL	OB6-CB5-C51	3.85	119.81	111.50
49	H	401	3PE	O21-C21-C22	3.85	119.80	111.50
51	N	401	CDL	OB6-CB5-C51	3.85	119.79	111.50
51	d	202	CDL	OA6-CA5-C11	3.85	119.79	111.50
51	i	201	CDL	OA6-CA5-C11	3.84	119.78	111.50
49	Y	401	3PE	O21-C21-C22	3.84	119.78	111.50
46	J	201	PC1	O21-C21-C22	3.84	119.77	111.50
49	L	704	3PE	O21-C21-C22	3.80	119.69	111.50
53	P	501	NDP	O2B-P2B-O1X	-3.47	96.00	109.39
50	H	402	88I	O3-C16-O3'	3.45	125.63	121.29
50	H	402	88I	O3-C17-C4	3.24	109.92	103.56
55	U	201	EHZ	C13-C12-N1	3.21	121.83	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	U	201	EHZ	C16-C15-N2	3.19	122.92	116.58
49	H	403	3PE	O31-C31-C32	3.18	121.89	111.91
50	H	402	88I	O4'-C1'-C24	3.06	109.61	104.36
50	H	402	88I	C6-C5-C16	2.96	121.55	112.06
46	J	201	PC1	O31-C31-C32	2.96	121.19	111.91
55	T	201	EHZ	O2-C9-S1	-2.90	118.85	122.61
51	d	202	CDL	OA8-CA7-C31	2.86	120.90	111.91
51	N	401	CDL	OA8-CA7-C31	2.83	120.79	111.91
50	H	402	88I	C25-C24-C1'	-2.83	97.64	103.08
51	r	201	CDL	OA8-CA7-C31	2.83	120.78	111.91
51	X	201	CDL	OB8-CB7-C71	2.78	120.64	111.91
53	P	501	NDP	PA-O5B-C5B	-2.75	105.53	121.68
49	M	501	3PE	O31-C31-C32	2.75	120.53	111.91
48	F	502	FMN	C4A-N5-C5A	2.74	119.51	116.77
49	L	702	3PE	O31-C31-C32	2.73	120.47	111.91
49	L	704	3PE	O31-C31-C32	2.71	120.42	111.91
49	H	401	3PE	O31-C31-C32	2.71	120.42	111.91
50	H	402	88I	O5'-C5'-C4'	2.70	115.80	109.98
51	L	703	CDL	OB8-CB7-C71	2.69	120.35	111.91
46	B	203	PC1	O31-C31-C32	2.68	120.33	111.91
48	F	502	FMN	C9A-N10-C10	-2.66	118.42	121.91
50	H	402	88I	C18-C17-C4	-2.65	110.01	115.98
46	Z	201	PC1	O31-C31-C32	2.64	120.20	111.91
51	d	201	CDL	OA8-CA7-C31	2.62	120.13	111.91
53	P	501	NDP	PN-O5D-C5D	-2.61	106.35	121.68
49	K	201	3PE	O31-C31-C32	2.61	120.10	111.91
49	L	701	3PE	O31-C31-C32	2.61	120.09	111.91
51	d	202	CDL	OB8-CB7-C71	2.60	120.07	111.91
46	B	202	PC1	O31-C31-C32	2.60	120.05	111.91
53	P	501	NDP	C2A-N1A-C6A	-2.57	114.35	118.75
53	P	501	NDP	O3X-P2B-O2X	2.57	117.45	107.64
51	i	201	CDL	OA8-CA7-C31	2.56	119.94	111.91
51	d	201	CDL	OB8-CB7-C71	2.54	119.88	111.91
51	r	201	CDL	OB8-CB7-C71	2.54	119.87	111.91
48	F	502	FMN	C5A-C9A-N10	2.53	119.55	117.72
51	i	201	CDL	OB8-CB7-C71	2.53	119.85	111.91
51	L	703	CDL	OA8-CA7-C31	2.52	119.82	111.91
50	H	402	88I	C4-C5-C16	2.46	105.81	102.49
55	U	201	EHZ	C19-C17-C16	2.46	113.08	108.82
49	Y	401	3PE	O31-C31-C32	2.44	119.57	111.91
51	X	201	CDL	OA8-CA7-C31	2.43	119.54	111.91
55	T	201	EHZ	C10-C11-N1	-2.38	107.41	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	N	401	CDL	OB8-CB7-C71	2.38	119.36	111.91
50	H	402	88I	O3-C16-C5	-2.35	107.16	110.09
50	H	402	88I	C8-CAD-C1	2.31	117.61	111.95
53	P	501	NDP	O2N-PN-O1N	2.30	123.63	112.24
55	U	201	EHZ	O4-C15-N2	-2.28	118.09	122.99
55	U	201	EHZ	C11-N1-C12	-2.25	118.65	122.84
49	M	502	3PE	O31-C31-C32	2.25	118.98	111.91
52	O	401	ATP	C5-C6-N6	2.25	123.77	120.35
53	P	501	NDP	O4B-C4B-C3B	2.24	109.56	105.11
55	U	201	EHZ	O2-C9-S1	-2.21	119.75	122.61
48	F	502	FMN	C4A-C4-N3	-2.20	120.42	123.43
50	H	402	88I	O2'-C2'-C21	2.20	108.13	104.36
53	P	501	NDP	O5D-PN-O1N	-2.18	100.55	109.07
50	H	402	88I	O2'-C1-C20	2.17	108.09	104.36
51	i	201	CDL	CB4-OB6-CB5	-2.15	112.51	117.79
53	P	501	NDP	C5B-C4B-C3B	-2.12	107.24	115.18
53	P	501	NDP	C3N-C2N-N1N	-2.12	120.07	123.10
52	O	401	ATP	O2'-C2'-C1'	-2.04	103.31	110.85
55	U	201	EHZ	C10-S1-C9	2.04	108.21	101.87
53	P	501	NDP	N3A-C2A-N1A	2.00	131.81	128.68
52	O	401	ATP	PB-O3B-PG	2.00	139.69	132.83

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
55	T	201	EHZ	C16
55	U	201	EHZ	C16

All (514) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	B	202	PC1	C11-O13-P-O12
46	B	202	PC1	C11-O13-P-O14
46	B	202	PC1	C1-O11-P-O13
46	B	202	PC1	O13-C11-C12-N
46	B	203	PC1	O13-C11-C12-N
46	B	203	PC1	O22-C21-O21-C2
46	B	203	PC1	C22-C21-O21-C2
46	J	201	PC1	C11-O13-P-O12
46	J	201	PC1	O21-C2-C3-O31
46	Z	201	PC1	C11-O13-P-O12
46	Z	201	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
46	Z	201	PC1	C11-O13-P-O11
46	Z	201	PC1	O13-C11-C12-N
48	F	502	FMN	N10-C1'-C2'-O2'
48	F	502	FMN	C1'-C2'-C3'-O3'
48	F	502	FMN	C1'-C2'-C3'-C4'
48	F	502	FMN	C3'-C4'-C5'-O5'
48	F	502	FMN	O4'-C4'-C5'-O5'
48	F	502	FMN	C5'-O5'-P-O2P
48	F	502	FMN	C5'-O5'-P-O3P
49	H	401	3PE	C11-O13-P-O11
49	H	401	3PE	C11-O13-P-O14
49	H	401	3PE	C12-C11-O13-P
49	H	403	3PE	C1-O11-P-O12
49	H	403	3PE	C1-O11-P-O14
49	H	403	3PE	O13-C11-C12-N
49	K	201	3PE	O32-C31-O31-C3
49	L	701	3PE	C1-O11-P-O12
49	L	701	3PE	C1-O11-P-O13
49	L	701	3PE	C1-O11-P-O14
49	L	701	3PE	O22-C21-O21-C2
49	L	702	3PE	C11-O13-P-O12
49	L	702	3PE	C11-O13-P-O14
49	L	702	3PE	C22-C21-O21-C2
49	L	704	3PE	C1-O11-P-O12
49	L	704	3PE	C12-C11-O13-P
49	M	501	3PE	C11-O13-P-O14
49	M	501	3PE	C22-C21-O21-C2
49	M	502	3PE	O22-C21-O21-C2
49	M	502	3PE	C22-C21-O21-C2
50	H	402	88I	C25-C4'-C5'-C28
50	H	402	88I	C25-C4'-C5'-O5'
50	H	402	88I	O4'-C4'-C5'-C28
50	H	402	88I	O4'-C4'-C5'-O5'
50	H	402	88I	C16-C5-C6-C13
50	H	402	88I	C4-C5-C6-C13
50	H	402	88I	CAC-C8-CAD-C1
51	L	703	CDL	CB3-OB5-PB2-OB3
51	L	703	CDL	CB3-OB5-PB2-OB4
51	L	703	CDL	OB7-CB5-OB6-CB4
51	N	401	CDL	CA3-OA5-PA1-OA2
51	N	401	CDL	CA3-OA5-PA1-OA3
51	N	401	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
51	N	401	CDL	CB2-OB2-PB2-OB3
51	N	401	CDL	CB2-OB2-PB2-OB4
51	X	201	CDL	O1-C1-CA2-OA2
51	X	201	CDL	CB2-C1-CA2-OA2
51	X	201	CDL	C1-CA2-OA2-PA1
51	X	201	CDL	CA2-OA2-PA1-OA3
51	X	201	CDL	CA2-OA2-PA1-OA4
51	X	201	CDL	CA3-OA5-PA1-OA2
51	X	201	CDL	CA3-OA5-PA1-OA3
51	X	201	CDL	CA3-OA5-PA1-OA4
51	X	201	CDL	CB2-OB2-PB2-OB3
51	X	201	CDL	CB3-OB5-PB2-OB3
51	X	201	CDL	CB3-OB5-PB2-OB4
51	X	201	CDL	C51-CB5-OB6-CB4
51	d	201	CDL	O1-C1-CB2-OB2
51	d	201	CDL	CB2-OB2-PB2-OB5
51	d	201	CDL	CB3-OB5-PB2-OB2
51	d	201	CDL	CB3-OB5-PB2-OB3
51	d	201	CDL	CB3-OB5-PB2-OB4
51	d	201	CDL	C51-CB5-OB6-CB4
51	d	202	CDL	CB2-C1-CA2-OA2
51	d	202	CDL	CB2-OB2-PB2-OB3
51	i	201	CDL	C1-CA2-OA2-PA1
51	i	201	CDL	CA2-OA2-PA1-OA3
51	i	201	CDL	CB2-OB2-PB2-OB5
51	i	201	CDL	CB3-OB5-PB2-OB3
51	i	201	CDL	OB6-CB4-CB6-OB8
51	r	201	CDL	CA3-OA5-PA1-OA3
51	r	201	CDL	CA3-OA5-PA1-OA4
51	r	201	CDL	CB2-OB2-PB2-OB4
51	r	201	CDL	OB6-CB4-CB6-OB8
52	O	401	ATP	PB-O3B-PG-O2G
52	O	401	ATP	C5'-O5'-PA-O2A
53	P	501	NDP	C5B-O5B-PA-O1A
53	P	501	NDP	C5B-O5B-PA-O2A
53	P	501	NDP	O4D-C4D-C5D-O5D
55	T	201	EHZ	C7-C8-C9-S1
55	T	201	EHZ	C11-C10-S1-C9
55	T	201	EHZ	C12-C13-C14-N2
55	T	201	EHZ	N2-C15-C16-C17
55	T	201	EHZ	N2-C15-C16-O5
55	T	201	EHZ	O4-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
55	T	201	EHZ	C16-C17-C20-O6
55	U	201	EHZ	C16-C15-N2-C14
55	U	201	EHZ	C15-C16-C17-C18
55	U	201	EHZ	C15-C16-C17-C19
55	U	201	EHZ	C15-C16-C17-C20
55	U	201	EHZ	O5-C16-C17-C18
55	U	201	EHZ	O5-C16-C17-C19
55	U	201	EHZ	O5-C16-C17-C20
46	J	201	PC1	O32-C31-O31-C3
49	H	403	3PE	O32-C31-O31-C3
49	L	704	3PE	O32-C31-O31-C3
51	X	201	CDL	OA9-CA7-OA8-CA6
49	H	403	3PE	C32-C31-O31-C3
49	L	704	3PE	C32-C31-O31-C3
49	M	501	3PE	O32-C31-O31-C3
51	d	202	CDL	OA9-CA7-OA8-CA6
51	d	202	CDL	OB9-CB7-OB8-CB6
51	i	201	CDL	OB9-CB7-OB8-CB6
51	r	201	CDL	OA9-CA7-OA8-CA6
51	X	201	CDL	OB7-CB5-OB6-CB4
51	i	201	CDL	OA7-CA5-OA6-CA4
51	i	201	CDL	OB7-CB5-OB6-CB4
46	J	201	PC1	C32-C31-O31-C3
49	H	401	3PE	C32-C31-O31-C3
49	K	201	3PE	C32-C31-O31-C3
49	M	501	3PE	C32-C31-O31-C3
51	X	201	CDL	C31-CA7-OA8-CA6
51	d	202	CDL	C71-CB7-OB8-CB6
51	r	201	CDL	C31-CA7-OA8-CA6
49	L	701	3PE	C22-C21-O21-C2
51	L	703	CDL	C51-CB5-OB6-CB4
51	i	201	CDL	C51-CB5-OB6-CB4
51	d	202	CDL	C31-CA7-OA8-CA6
51	i	201	CDL	C71-CB7-OB8-CB6
49	L	702	3PE	O22-C21-O21-C2
49	M	501	3PE	O22-C21-O21-C2
51	d	201	CDL	OB7-CB5-OB6-CB4
49	H	401	3PE	O32-C31-O31-C3
49	Y	401	3PE	O32-C31-O31-C3
51	N	401	CDL	OB9-CB7-OB8-CB6
51	L	703	CDL	O1-C1-CB2-OB2
51	d	202	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
51	L	703	CDL	C71-CB7-OB8-CB6
51	L	703	CDL	OB9-CB7-OB8-CB6
55	U	201	EHZ	O4-C15-N2-C14
49	H	403	3PE	C22-C21-O21-C2
51	i	201	CDL	C11-CA5-OA6-CA4
53	P	501	NDP	O4B-C4B-C5B-O5B
53	P	501	NDP	C3B-C4B-C5B-O5B
53	P	501	NDP	C3D-C4D-C5D-O5D
49	Y	401	3PE	C32-C31-O31-C3
51	N	401	CDL	C71-CB7-OB8-CB6
51	d	201	CDL	CB4-CB3-OB5-PB2
49	H	403	3PE	O22-C21-O21-C2
46	B	203	PC1	C32-C31-O31-C3
51	N	401	CDL	C31-CA7-OA8-CA6
51	X	201	CDL	C71-CB7-OB8-CB6
51	d	201	CDL	C31-CA7-OA8-CA6
51	d	201	CDL	C71-CB7-OB8-CB6
53	P	501	NDP	O4D-C1D-N1N-C6N
51	d	201	CDL	OA5-CA3-CA4-OA6
46	Z	201	PC1	O21-C2-C3-O31
49	L	704	3PE	O21-C2-C3-O31
49	L	701	3PE	C21-C22-C23-C24
46	B	203	PC1	O32-C31-O31-C3
51	N	401	CDL	OA9-CA7-OA8-CA6
46	J	201	PC1	C21-C22-C23-C24
51	X	201	CDL	OB9-CB7-OB8-CB6
51	d	201	CDL	OB9-CB7-OB8-CB6
51	X	201	CDL	CA5-C11-C12-C13
51	r	201	CDL	C71-CB7-OB8-CB6
51	i	201	CDL	CA5-C11-C12-C13
51	d	201	CDL	OA9-CA7-OA8-CA6
51	N	401	CDL	C51-CB5-OB6-CB4
46	B	202	PC1	C11-O13-P-O11
46	J	201	PC1	C11-O13-P-O11
46	J	201	PC1	C1-O11-P-O13
49	H	403	3PE	C1-O11-P-O13
49	H	403	3PE	C11-O13-P-O11
49	K	201	3PE	C11-O13-P-O11
49	L	702	3PE	C11-O13-P-O11
49	L	704	3PE	C1-O11-P-O13
49	L	704	3PE	C11-O13-P-O11
49	M	501	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
49	M	502	3PE	C11-O13-P-O11
49	Y	401	3PE	C11-O13-P-O11
51	L	703	CDL	CB3-OB5-PB2-OB2
51	N	401	CDL	CB2-OB2-PB2-OB5
51	X	201	CDL	CA2-OA2-PA1-OA5
51	X	201	CDL	CB3-OB5-PB2-OB2
51	d	201	CDL	CA2-OA2-PA1-OA5
51	i	201	CDL	CB3-OB5-PB2-OB2
51	r	201	CDL	CA3-OA5-PA1-OA2
51	r	201	CDL	CB2-OB2-PB2-OB5
51	d	201	CDL	CA2-C1-CB2-OB2
51	d	201	CDL	OA5-CA3-CA4-CA6
51	N	401	CDL	OB7-CB5-OB6-CB4
49	K	201	3PE	C25-C26-C27-C28
49	L	702	3PE	C23-C24-C25-C26
49	L	704	3PE	C38-C39-C3A-C3B
49	L	704	3PE	C22-C21-O21-C2
46	J	201	PC1	C33-C34-C35-C36
50	H	402	88I	C10-C11-C12-C13
50	H	402	88I	C29-C30-C31-C32
49	L	701	3PE	C32-C31-O31-C3
49	M	502	3PE	C3A-C3B-C3C-C3D
51	L	703	CDL	C74-C75-C76-C77
46	B	202	PC1	C2-C1-O11-P
51	r	201	CDL	OB9-CB7-OB8-CB6
51	L	703	CDL	OA5-CA3-CA4-OA6
49	L	701	3PE	C22-C23-C24-C25
49	L	704	3PE	C31-C32-C33-C34
51	L	703	CDL	OB6-CB4-CB6-OB8
49	H	401	3PE	C25-C26-C27-C28
49	L	701	3PE	C35-C36-C37-C38
51	L	703	CDL	C11-C12-C13-C14
51	N	401	CDL	C31-C32-C33-C34
49	H	403	3PE	C34-C35-C36-C37
49	L	702	3PE	C26-C27-C28-C29
49	L	702	3PE	C2A-C2B-C2C-C2D
51	i	201	CDL	C18-C19-C20-C21
49	L	704	3PE	O22-C21-O21-C2
51	r	201	CDL	C51-CB5-OB6-CB4
51	i	201	CDL	CB7-C71-C72-C73
49	L	701	3PE	C27-C28-C29-C2A
51	r	201	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
49	M	502	3PE	C3D-C3E-C3F-C3G
51	L	703	CDL	C35-C36-C37-C38
49	M	502	3PE	C36-C37-C38-C39
51	X	201	CDL	C33-C34-C35-C36
51	L	703	CDL	C11-CA5-OA6-CA4
46	Z	201	PC1	C29-C2A-C2B-C2C
51	N	401	CDL	C51-C52-C53-C54
49	L	701	3PE	O32-C31-O31-C3
49	Y	401	3PE	C32-C33-C34-C35
51	L	703	CDL	CA2-C1-CB2-OB2
51	d	201	CDL	C58-C59-C60-C61
51	L	703	CDL	OA7-CA5-OA6-CA4
51	r	201	CDL	OB7-CB5-OB6-CB4
50	H	402	88I	CAA-C7-CAB-C2
49	L	704	3PE	C23-C24-C25-C26
51	L	703	CDL	CB5-C51-C52-C53
51	i	201	CDL	C31-C32-C33-C34
49	H	403	3PE	C39-C3A-C3B-C3C
49	H	401	3PE	O22-C21-O21-C2
51	N	401	CDL	OA7-CA5-OA6-CA4
46	B	203	PC1	C37-C38-C39-C3A
51	L	703	CDL	C76-C77-C78-C79
55	U	201	EHZ	C5-C6-C7-C8
49	Y	401	3PE	C35-C36-C37-C38
49	L	702	3PE	C32-C33-C34-C35
49	M	502	3PE	C32-C33-C34-C35
55	U	201	EHZ	C12-C13-C14-N2
46	B	202	PC1	C22-C21-O21-C2
49	H	401	3PE	C22-C21-O21-C2
51	N	401	CDL	C11-CA5-OA6-CA4
51	d	202	CDL	C51-CB5-OB6-CB4
46	B	202	PC1	O22-C21-O21-C2
51	L	703	CDL	C16-C17-C18-C19
49	M	502	3PE	O21-C2-C3-O31
49	Y	401	3PE	O21-C2-C3-O31
50	H	402	88I	CAB-C2-CAC-C8
51	N	401	CDL	C78-C79-C80-C81
51	N	401	CDL	C74-C75-C76-C77
51	d	202	CDL	OB7-CB5-OB6-CB4
48	F	502	FMN	O2'-C2'-C3'-C4'
49	L	701	3PE	C11-O13-P-O11
51	d	202	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
51	i	201	CDL	CA2-OA2-PA1-OA5
51	N	401	CDL	C1-CA2-OA2-PA1
49	L	704	3PE	C28-C29-C2A-C2B
50	H	402	88I	C31-C32-C33-C34
51	i	201	CDL	C22-C23-C24-C25
50	H	402	88I	CAC-C8-CAD-OP3
51	N	401	CDL	C77-C78-C79-C80
46	B	203	PC1	C1-C2-C3-O31
46	J	201	PC1	C1-C2-C3-O31
46	Z	201	PC1	C1-C2-C3-O31
49	H	401	3PE	C32-C33-C34-C35
49	L	704	3PE	C1-C2-C3-O31
51	N	401	CDL	CB3-CB4-CB6-OB8
51	i	201	CDL	CA3-CA4-CA6-OA8
51	r	201	CDL	CB3-CB4-CB6-OB8
51	i	201	CDL	C23-C24-C25-C26
55	T	201	EHZ	O4-C15-C16-O5
49	Y	401	3PE	C34-C35-C36-C37
51	N	401	CDL	CA5-C11-C12-C13
55	U	201	EHZ	C5-C6-C7-O1
55	T	201	EHZ	C18-C17-C20-O6
51	d	202	CDL	CA5-C11-C12-C13
51	L	703	CDL	C52-C53-C54-C55
51	N	401	CDL	C55-C56-C57-C58
49	H	403	3PE	C3-C2-O21-C21
51	L	703	CDL	CA6-CA4-OA6-CA5
51	d	202	CDL	C79-C80-C81-C82
48	F	502	FMN	C5'-O5'-P-O1P
49	M	502	3PE	C24-C25-C26-C27
49	L	702	3PE	C33-C34-C35-C36
50	H	402	88I	C12-C13-C6-C5
50	H	402	88I	C11-C10-C9-CAA
49	H	401	3PE	C29-C2A-C2B-C2C
51	L	703	CDL	CB2-C1-CA2-OA2
51	d	202	CDL	C11-CA5-OA6-CA4
46	B	203	PC1	C35-C36-C37-C38
51	L	703	CDL	C51-C52-C53-C54
51	N	401	CDL	OA5-CA3-CA4-CA6
51	d	202	CDL	OA5-CA3-CA4-CA6
49	H	401	3PE	C21-C22-C23-C24
46	Z	201	PC1	C32-C33-C34-C35
49	K	201	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
51	X	201	CDL	C71-C72-C73-C74
49	M	501	3PE	C1-C2-C3-O31
49	Y	401	3PE	C1-C2-C3-O31
51	L	703	CDL	CB3-CB4-CB6-OB8
49	Y	401	3PE	C26-C27-C28-C29
55	U	201	EHZ	C1-C2-C3-C4
55	T	201	EHZ	C7-C8-C9-O2
49	L	702	3PE	C2D-C2E-C2F-C2G
51	X	201	CDL	CB2-OB2-PB2-OB5
49	H	403	3PE	C32-C33-C34-C35
49	K	201	3PE	O11-C1-C2-O21
51	N	401	CDL	OA5-CA3-CA4-OA6
51	d	202	CDL	OA7-CA5-OA6-CA4
48	F	502	FMN	O2'-C2'-C3'-O3'
51	i	201	CDL	C31-CA7-OA8-CA6
49	L	701	3PE	C29-C2A-C2B-C2C
51	L	703	CDL	C31-C32-C33-C34
49	H	403	3PE	C36-C37-C38-C39
51	L	703	CDL	C1-CA2-OA2-PA1
51	d	202	CDL	C1-CA2-OA2-PA1
51	d	202	CDL	C76-C77-C78-C79
51	N	401	CDL	C76-C77-C78-C79
49	K	201	3PE	O11-C1-C2-C3
51	L	703	CDL	OA5-CA3-CA4-CA6
51	L	703	CDL	O1-C1-CA2-OA2
51	d	201	CDL	C72-C73-C74-C75
55	T	201	EHZ	C19-C17-C20-O6
51	r	201	CDL	CA3-CA4-OA6-CA5
51	X	201	CDL	C56-C57-C58-C59
46	B	202	PC1	C21-C22-C23-C24
51	r	201	CDL	C1-CA2-OA2-PA1
51	i	201	CDL	OA9-CA7-OA8-CA6
55	T	201	EHZ	O1-C7-C8-C9
46	Z	201	PC1	C34-C35-C36-C37
51	X	201	CDL	C32-C33-C34-C35
49	H	401	3PE	O21-C2-C3-O31
51	d	201	CDL	C75-C76-C77-C78
52	O	401	ATP	C5'-O5'-PA-O3A
51	r	201	CDL	C11-C12-C13-C14
55	U	201	EHZ	C3-C4-C5-C6
46	B	203	PC1	C11-O13-P-O11
46	Z	201	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
51	N	401	CDL	CB3-OB5-PB2-OB2
51	d	202	CDL	CB3-OB5-PB2-OB2
51	i	201	CDL	CA3-OA5-PA1-OA2
51	r	201	CDL	CA4-CA3-OA5-PA1
46	B	203	PC1	C11-O13-P-O14
46	J	201	PC1	C11-O13-P-O14
46	J	201	PC1	C1-O11-P-O12
46	Z	201	PC1	C1-O11-P-O14
49	H	403	3PE	C11-O13-P-O12
49	K	201	3PE	C11-O13-P-O14
49	L	704	3PE	C1-O11-P-O14
49	L	704	3PE	C11-O13-P-O12
49	M	501	3PE	C11-O13-P-O12
49	M	502	3PE	C11-O13-P-O12
49	Y	401	3PE	C11-O13-P-O12
51	d	201	CDL	CA2-OA2-PA1-OA3
51	i	201	CDL	CA2-OA2-PA1-OA4
51	r	201	CDL	CB2-OB2-PB2-OB3
52	O	401	ATP	C5'-O5'-PA-O1A
55	T	201	EHZ	C6-C7-C8-C9
49	Y	401	3PE	C21-C22-C23-C24
51	d	201	CDL	C72-C71-CB7-OB8
55	T	201	EHZ	C1-C2-C3-C4
49	L	701	3PE	C39-C3A-C3B-C3C
46	B	202	PC1	C12-C11-O13-P
49	L	701	3PE	C12-C11-O13-P
49	L	702	3PE	C12-C11-O13-P
49	H	403	3PE	C31-C32-C33-C34
51	r	201	CDL	CA5-C11-C12-C13
49	Y	401	3PE	C33-C34-C35-C36
51	N	401	CDL	OB5-CB3-CB4-OB6
51	r	201	CDL	OA5-CA3-CA4-OA6
46	J	201	PC1	O13-C11-C12-N
48	F	502	FMN	N10-C1'-C2'-C3'
51	d	202	CDL	C33-C34-C35-C36
51	i	201	CDL	CB3-CB4-CB6-OB8
49	M	501	3PE	O21-C2-C3-O31
51	N	401	CDL	OB6-CB4-CB6-OB8
51	X	201	CDL	OA6-CA4-CA6-OA8
51	i	201	CDL	OA6-CA4-CA6-OA8
51	N	401	CDL	CA4-CA3-OA5-PA1
51	L	703	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
51	d	202	CDL	C32-C33-C34-C35
51	i	201	CDL	C16-C17-C18-C19
49	L	704	3PE	C2A-C2B-C2C-C2D
46	B	203	PC1	C32-C33-C34-C35
51	d	201	CDL	C31-C32-C33-C34
49	L	702	3PE	C3-C2-O21-C21
51	X	201	CDL	CB3-CB4-OB6-CB5
51	d	201	CDL	CB6-CB4-OB6-CB5
51	d	202	CDL	CA6-CA4-OA6-CA5
51	r	201	CDL	OA7-CA5-OA6-CA4
51	d	201	CDL	C52-C53-C54-C55
49	M	501	3PE	C31-C32-C33-C34
49	L	704	3PE	C2-C1-O11-P
46	B	203	PC1	O21-C2-C3-O31
51	L	703	CDL	CA3-OA5-PA1-OA2
49	L	702	3PE	O21-C21-C22-C23
49	M	502	3PE	C1-C2-C3-O31
49	K	201	3PE	C27-C28-C29-C2A
51	N	401	CDL	C83-C84-C85-C86
51	d	202	CDL	CA4-CA3-OA5-PA1
51	d	202	CDL	C72-C73-C74-C75
51	X	201	CDL	C52-C53-C54-C55
49	L	702	3PE	C34-C35-C36-C37
46	B	202	PC1	C34-C35-C36-C37
51	X	201	CDL	C61-C62-C63-C64
49	M	501	3PE	C25-C26-C27-C28
51	i	201	CDL	C14-C15-C16-C17
51	X	201	CDL	C13-C14-C15-C16
46	J	201	PC1	C38-C39-C3A-C3B
51	N	401	CDL	C80-C81-C82-C83
51	d	202	CDL	C75-C76-C77-C78
51	d	201	CDL	OB5-CB3-CB4-CB6
51	r	201	CDL	OA5-CA3-CA4-CA6
46	Z	201	PC1	C2C-C2D-C2E-C2F
51	r	201	CDL	C71-C72-C73-C74
52	O	401	ATP	O4'-C4'-C5'-O5'
46	Z	201	PC1	C36-C37-C38-C39
55	U	201	EHZ	C11-C10-S1-C9
46	J	201	PC1	C26-C27-C28-C29
49	M	502	3PE	C23-C24-C25-C26
55	T	201	EHZ	C21-C22-C23-C24
55	T	201	EHZ	C13-C14-N2-C15

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Mol	Chain	Res	Type	Atoms
49	H	401	3PE	C2D-C2E-C2F-C2G
51	N	401	CDL	C84-C85-C86-C87
49	M	502	3PE	C35-C36-C37-C38
51	X	201	CDL	C59-C60-C61-C62
49	H	401	3PE	C22-C23-C24-C25
49	H	401	3PE	C36-C37-C38-C39
51	d	202	CDL	OA5-CA3-CA4-OA6
51	X	201	CDL	C63-C64-C65-C66
49	M	501	3PE	C34-C35-C36-C37
51	N	401	CDL	OB5-CB3-CB4-CB6
51	r	201	CDL	C11-CA5-OA6-CA4
51	d	202	CDL	C31-C32-C33-C34
49	K	201	3PE	O21-C21-C22-C23
49	L	701	3PE	C26-C27-C28-C29
49	M	501	3PE	C2-C1-O11-P
51	i	201	CDL	C11-C12-C13-C14
51	d	202	CDL	OA6-CA4-CA6-OA8
49	M	501	3PE	C39-C3A-C3B-C3C
49	H	403	3PE	C3C-C3D-C3E-C3F
50	H	402	88I	C28-C29-C30-C31
51	d	202	CDL	C73-C74-C75-C76
52	O	401	ATP	PB-O3B-PG-O1G
51	L	703	CDL	C12-C11-CA5-OA6
46	B	202	PC1	O21-C21-C22-C23
55	T	201	EHZ	C10-C11-N1-C12
49	H	401	3PE	C35-C36-C37-C38
49	K	201	3PE	O31-C31-C32-C33
49	L	704	3PE	O21-C21-C22-C23
50	H	402	88I	C10-C9-CAA-C7
51	X	201	CDL	CA3-CA4-CA6-OA8
49	H	403	3PE	O21-C21-C22-C23
46	Z	201	PC1	C11-C12-N-C14
46	J	201	PC1	C35-C36-C37-C38
49	Y	401	3PE	O31-C31-C32-C33
46	J	201	PC1	C3A-C3B-C3C-C3D
53	P	501	NDP	C5B-O5B-PA-O3
46	B	203	PC1	C3C-C3D-C3E-C3F
49	H	401	3PE	C28-C29-C2A-C2B
51	X	201	CDL	C62-C63-C64-C65
49	H	401	3PE	C2-C1-O11-P
49	K	201	3PE	C2-C1-O11-P
46	Z	201	PC1	O21-C21-C22-C23

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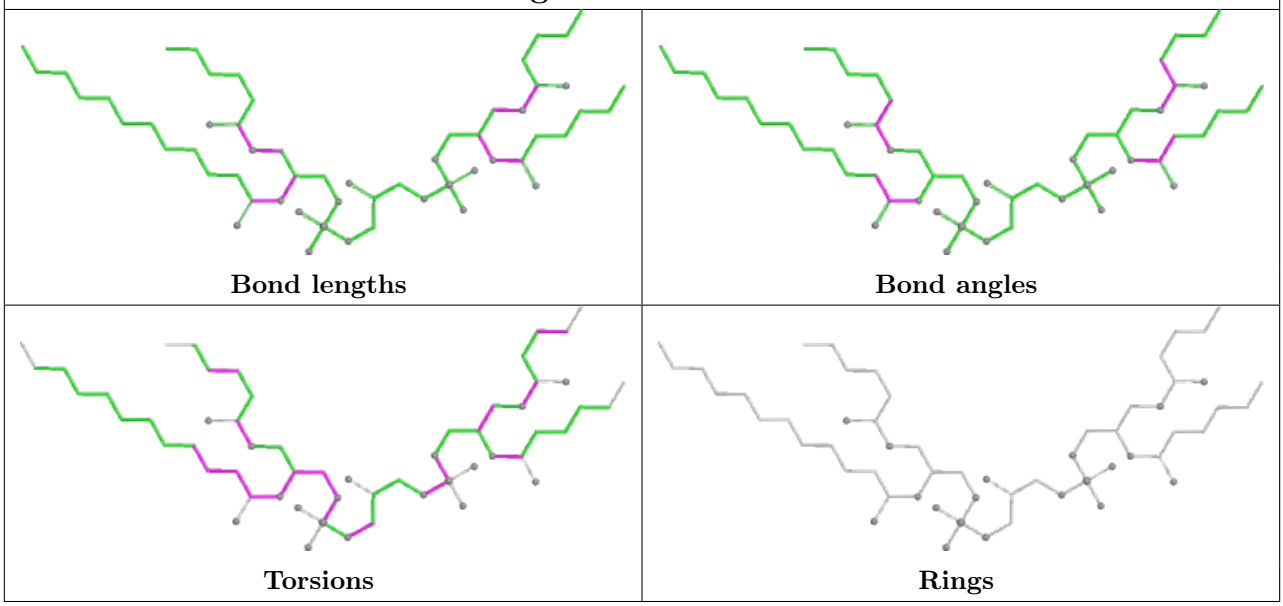
Mol	Chain	Res	Type	Atoms
49	L	704	3PE	O31-C31-C32-C33
51	d	202	CDL	C12-C11-CA5-OA6
46	Z	201	PC1	C28-C29-C2A-C2B
46	B	202	PC1	O22-C21-C22-C23
49	L	704	3PE	C2B-C2C-C2D-C2E
51	d	201	CDL	C56-C57-C58-C59
49	L	704	3PE	O32-C31-C32-C33
49	K	201	3PE	O22-C21-C22-C23
49	L	704	3PE	O22-C21-C22-C23
51	L	703	CDL	C12-C11-CA5-OA7
51	i	201	CDL	C72-C71-CB7-OB8
49	K	201	3PE	O32-C31-C32-C33
51	d	202	CDL	C12-C11-CA5-OA7
51	X	201	CDL	C55-C56-C57-C58
46	Z	201	PC1	C11-C12-N-C13
51	L	703	CDL	CA3-OA5-PA1-OA3
51	d	202	CDL	CA2-OA2-PA1-OA4
51	i	201	CDL	CB3-OB5-PB2-OB4
51	r	201	CDL	CB3-OB5-PB2-OB3
46	B	202	PC1	C24-C25-C26-C27
49	H	401	3PE	C3E-C3F-C3G-C3H
49	L	704	3PE	O13-C11-C12-N
49	H	403	3PE	O22-C21-C22-C23
51	X	201	CDL	C31-C32-C33-C34
55	U	201	EHZ	C2-C3-C4-C5
49	K	201	3PE	C12-C11-O13-P
49	M	501	3PE	C12-C11-O13-P
49	Y	401	3PE	O32-C31-C32-C33
46	Z	201	PC1	C2A-C2B-C2C-C2D
51	d	201	CDL	C32-C31-CA7-OA8
49	H	403	3PE	C24-C25-C26-C27
51	N	401	CDL	C52-C51-CB5-OB6
49	H	401	3PE	C3C-C3D-C3E-C3F
51	d	201	CDL	C52-C51-CB5-OB6
49	L	702	3PE	C24-C25-C26-C27
51	d	201	CDL	C71-C72-C73-C74
51	N	401	CDL	C52-C51-CB5-OB7
51	d	201	CDL	C32-C31-CA7-OA9
51	i	201	CDL	C72-C71-CB7-OB9
51	N	401	CDL	C32-C31-CA7-OA8
51	r	201	CDL	C12-C11-CA5-OA6

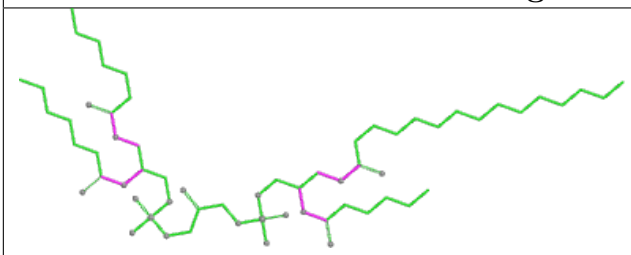
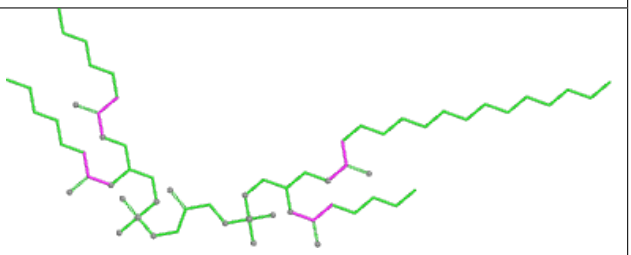
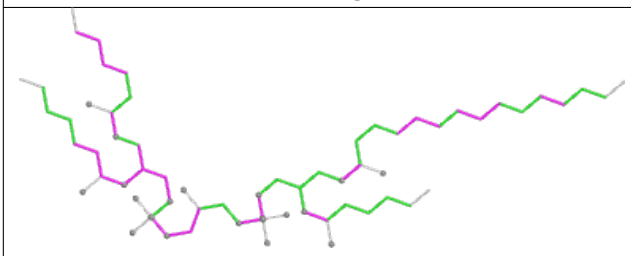
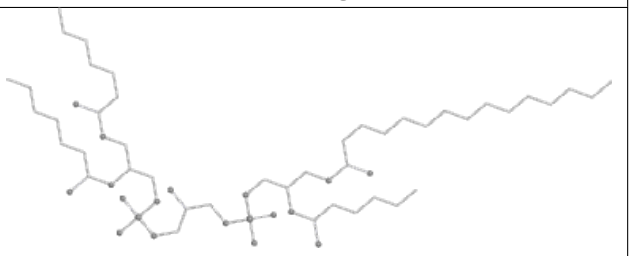
There are no ring outliers.

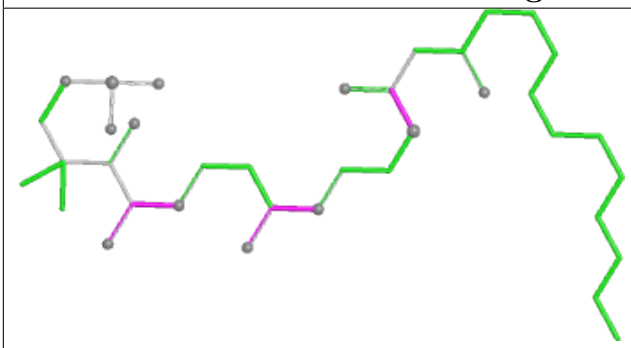
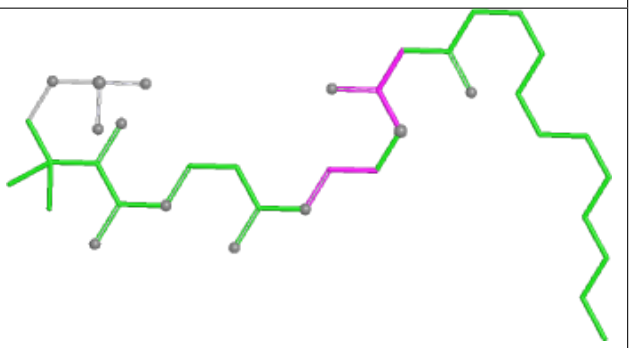
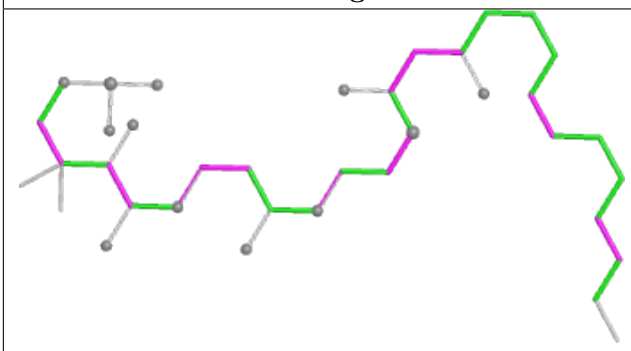
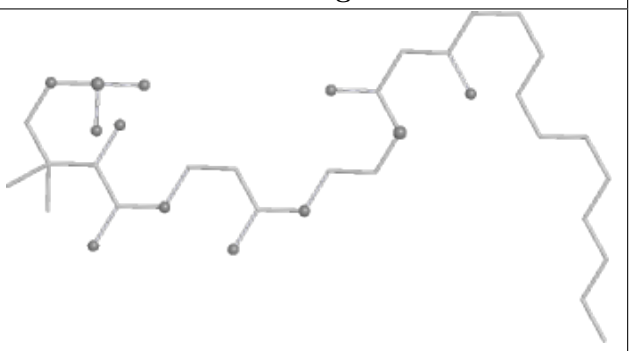
No monomer is involved in short contacts.

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

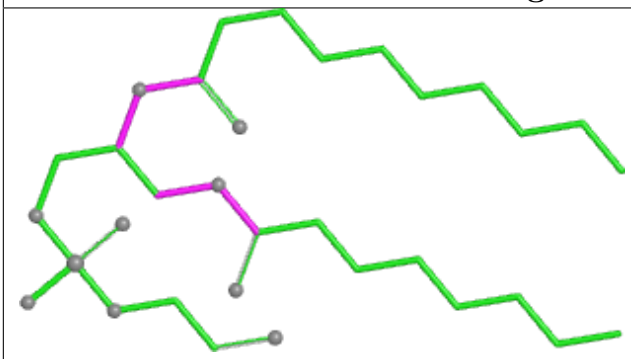
Ligand CDL r 201



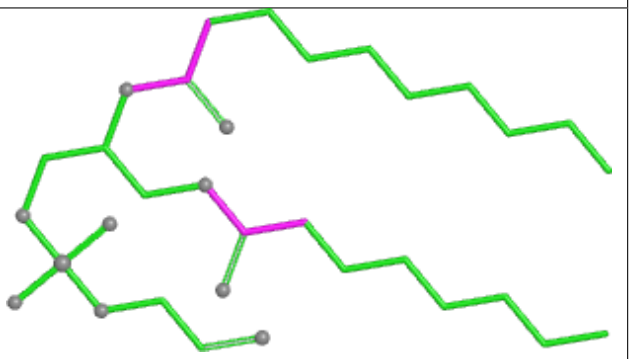
Ligand CDL d 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand EHZ T 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

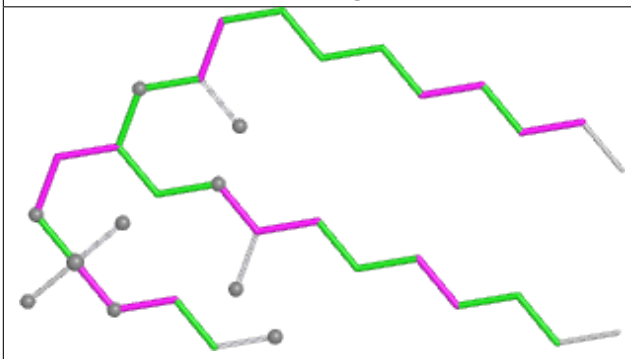
Ligand 3PE K 201



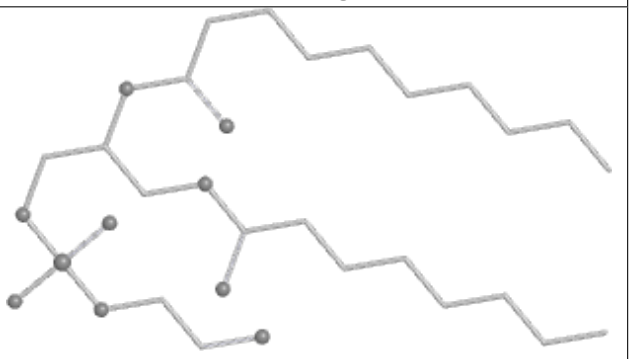
Bond lengths



Bond angles

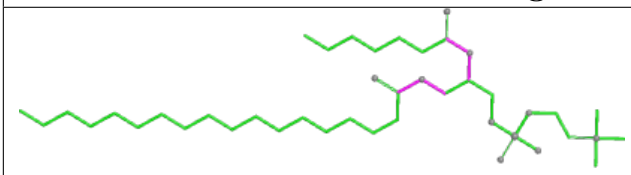


Torsions



Rings

Ligand PC1 B 203



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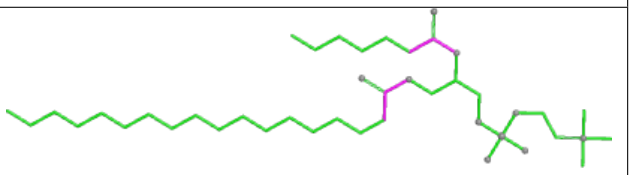
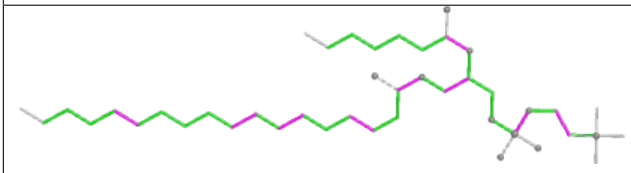
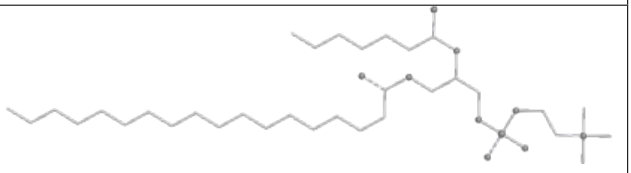


Bond angles

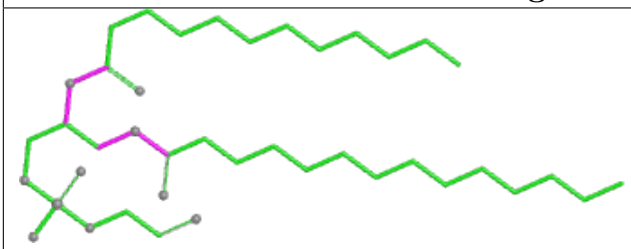


Torsions

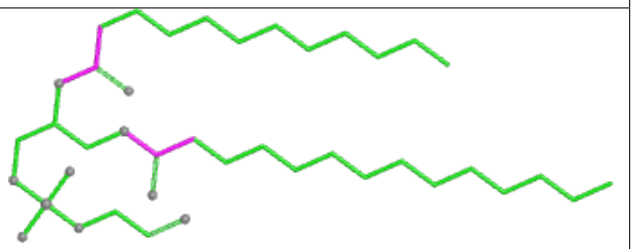


Rings

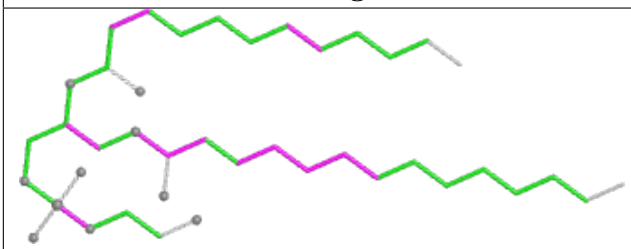
Ligand 3PE Y 401



Bond lengths



Bond angles



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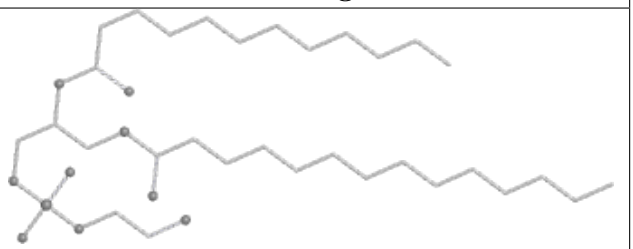
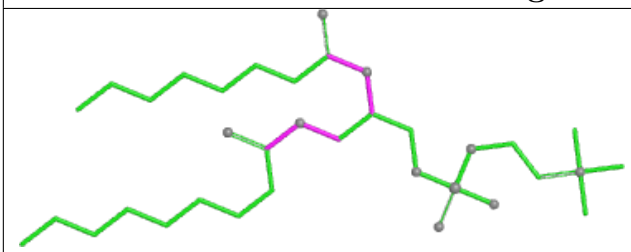


Rings

Ligand PC1 B 202



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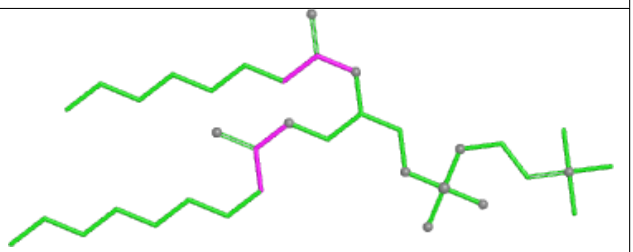
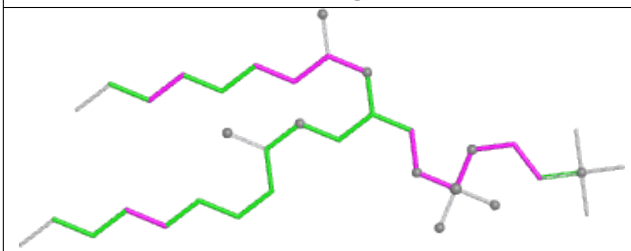


Bond angles



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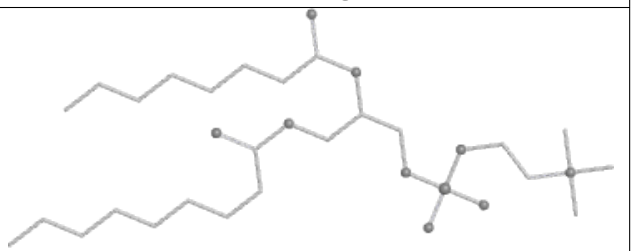
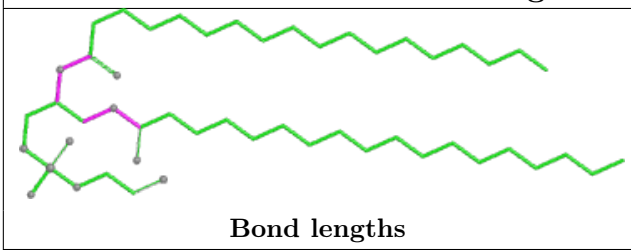


Rings

Ligand 3PE H 401



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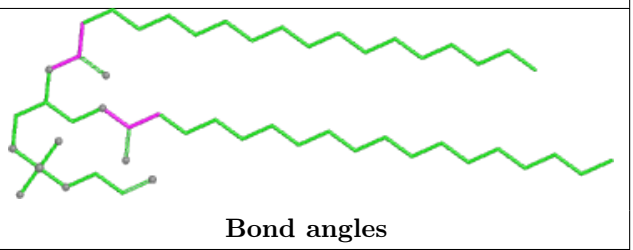

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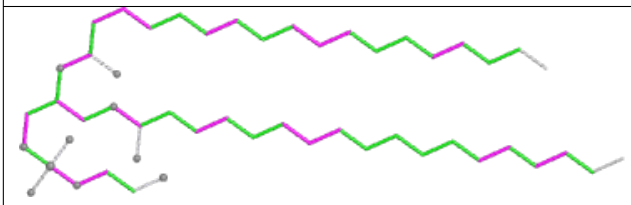

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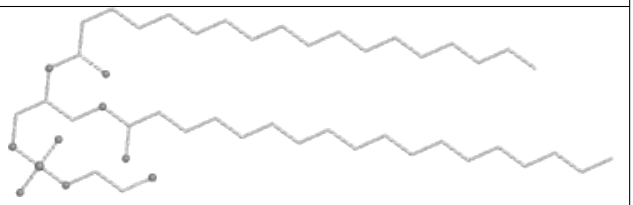
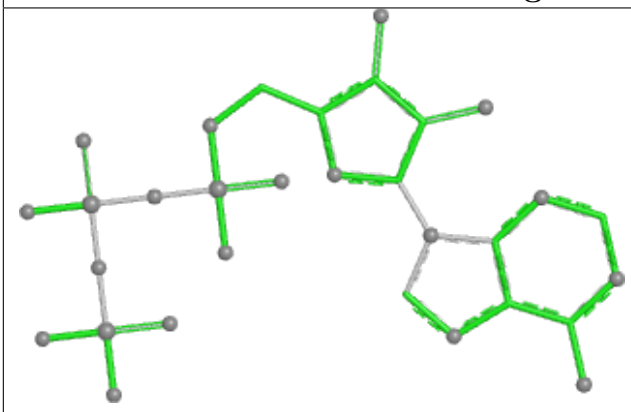
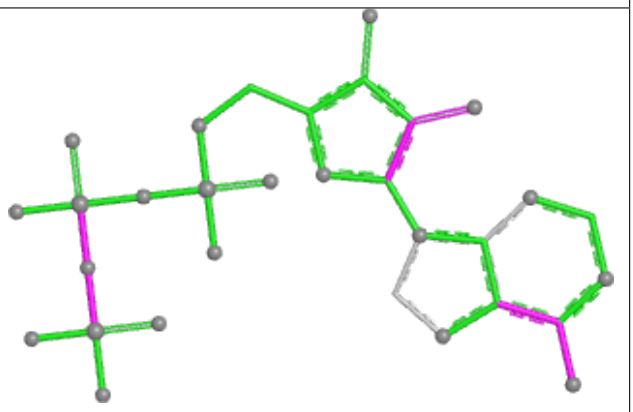
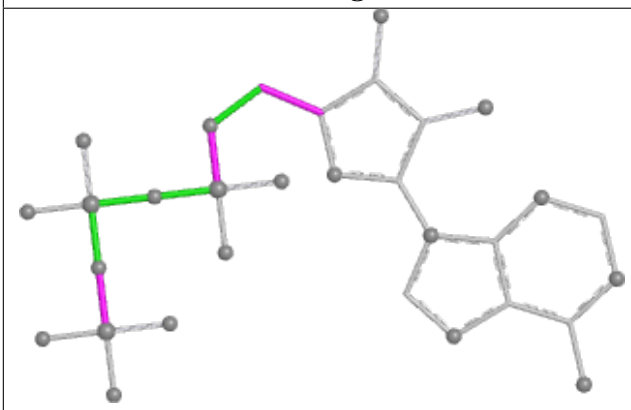
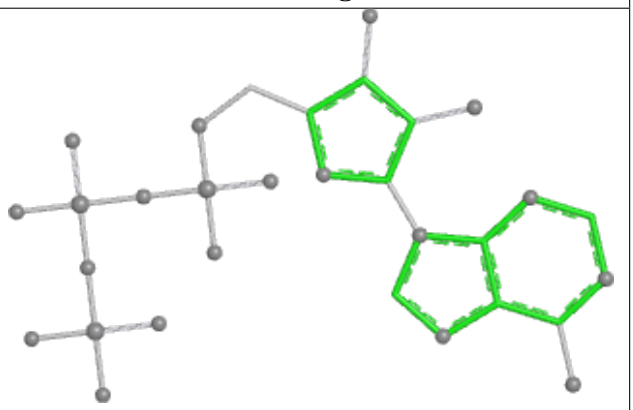


Rings

Ligand ATP O 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

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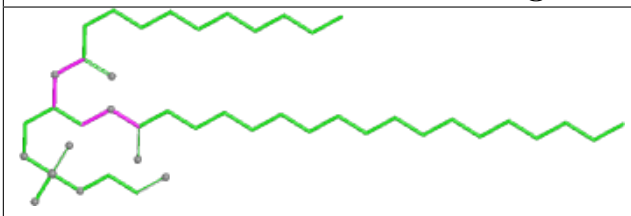
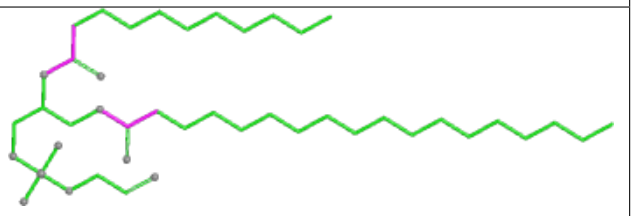
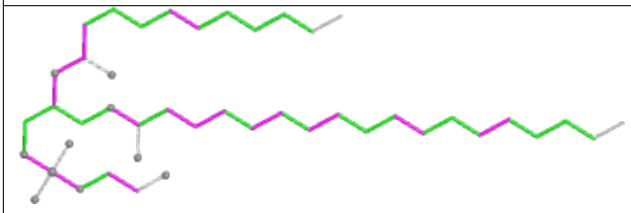
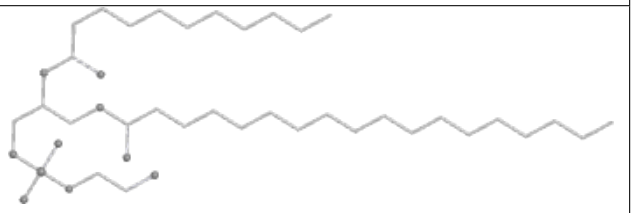
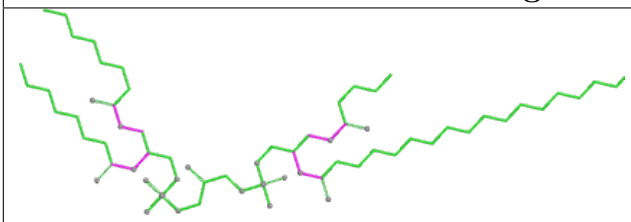
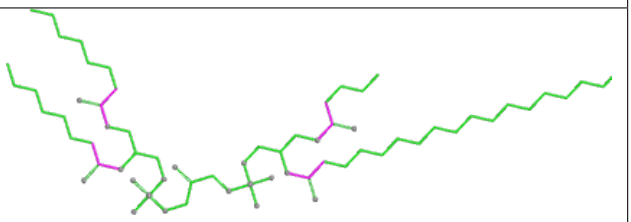
 Bond lengths	 Bond angles
 Torsions	 Rings

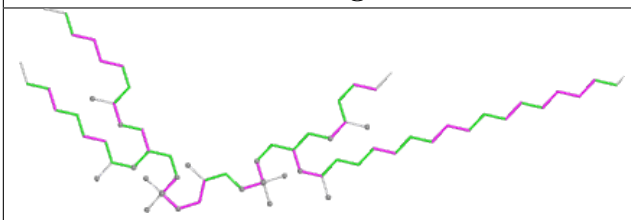
Ligand CDL X 201



Bond lengths



Bond angles



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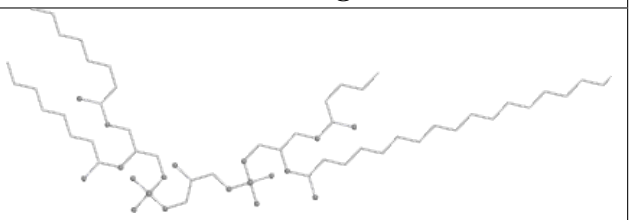
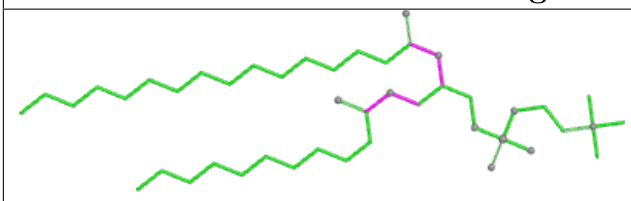
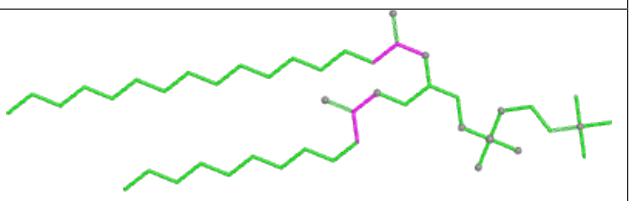


Rings

Ligand PC1 Z 201



Bond lengths



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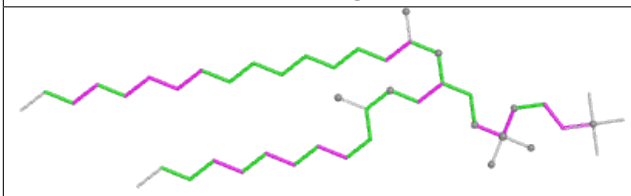

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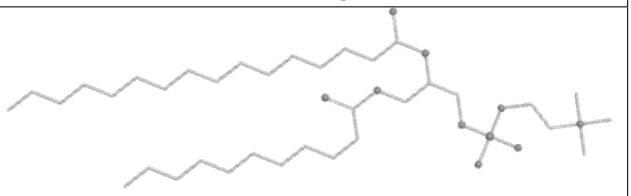
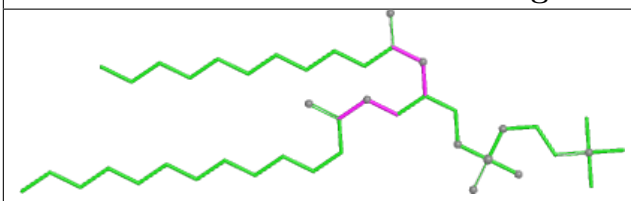
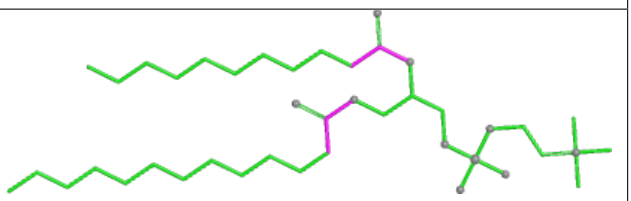


Rings

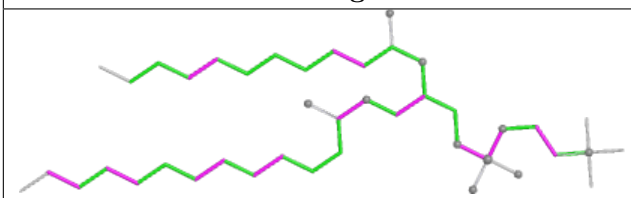
Ligand PC1 J 201



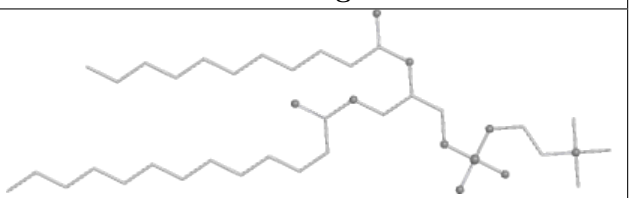
Bond lengths



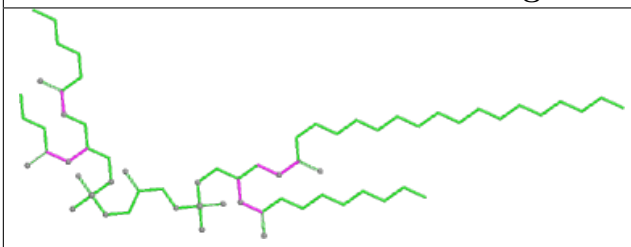
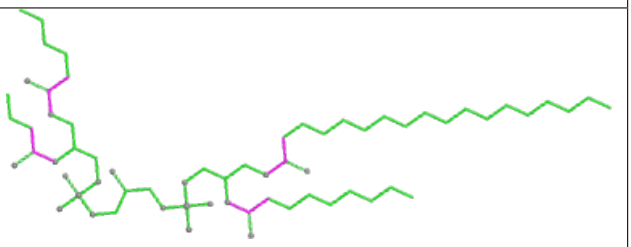
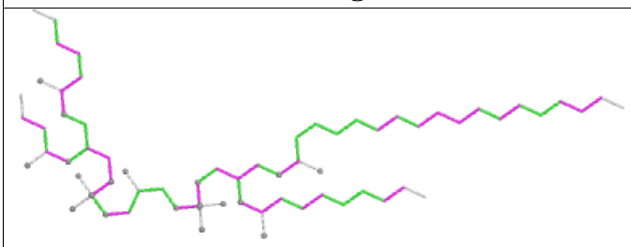
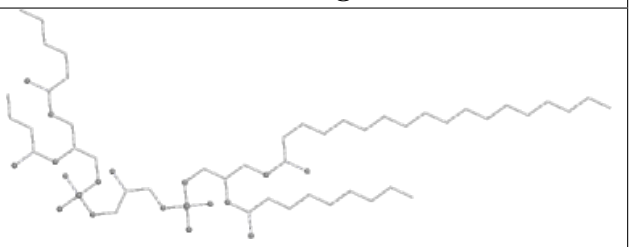
Bond angles



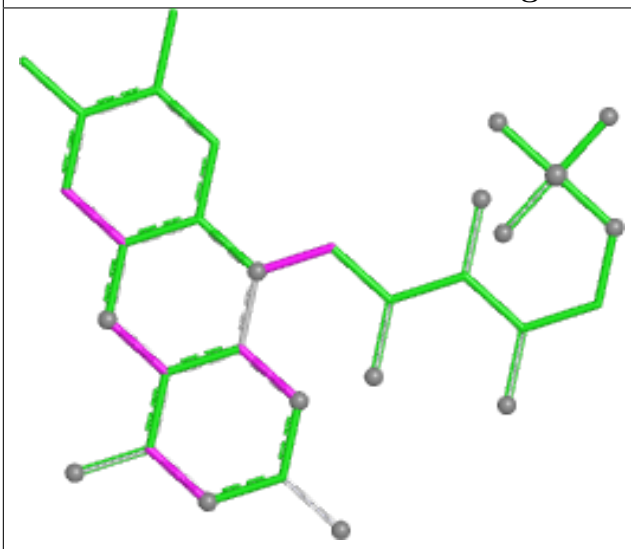
Torsions



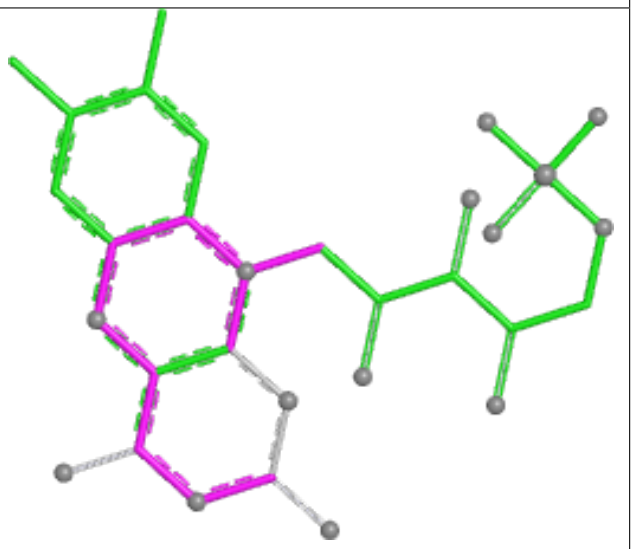
Rings

Ligand CDL N 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

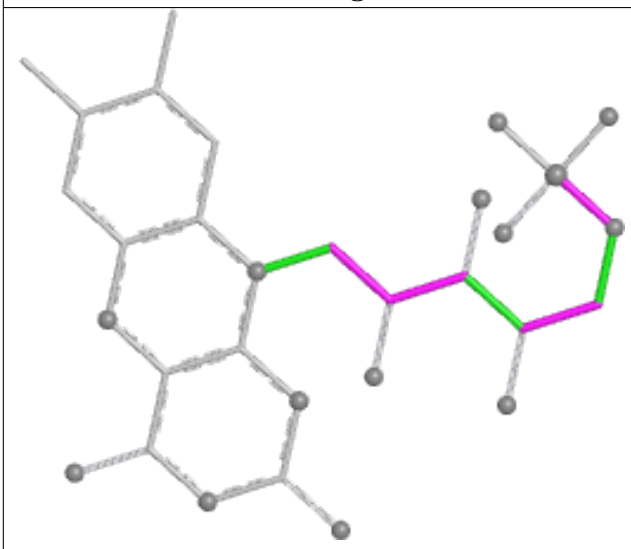
Ligand FMN F 502



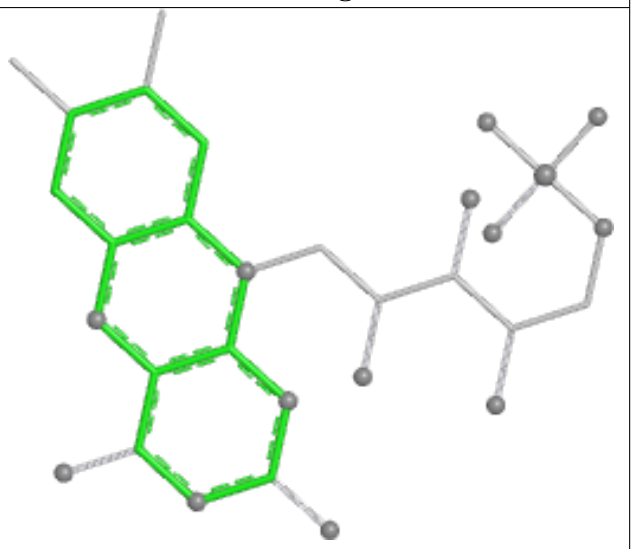
Bond lengths



Bond angles

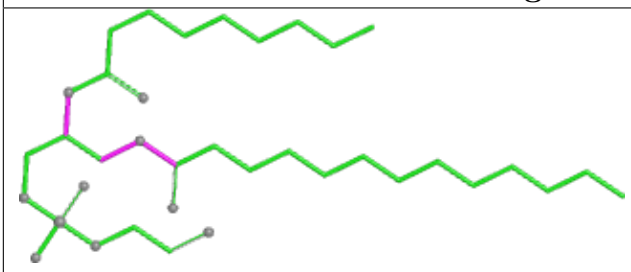


Torsions

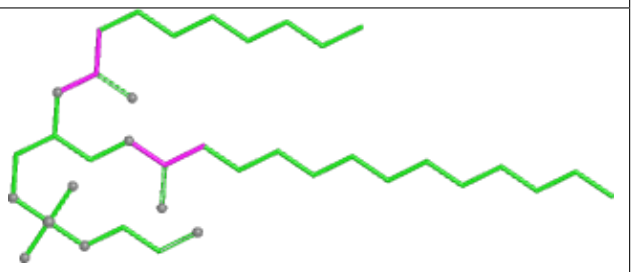


Rings

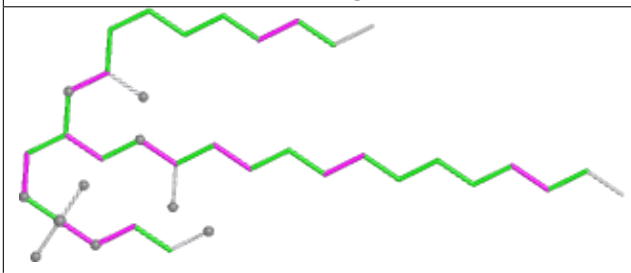
Ligand 3PE M 501



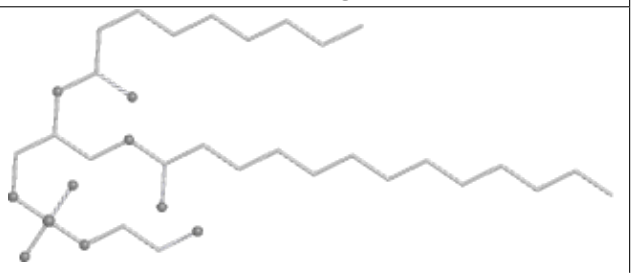
Bond lengths



Bond angles

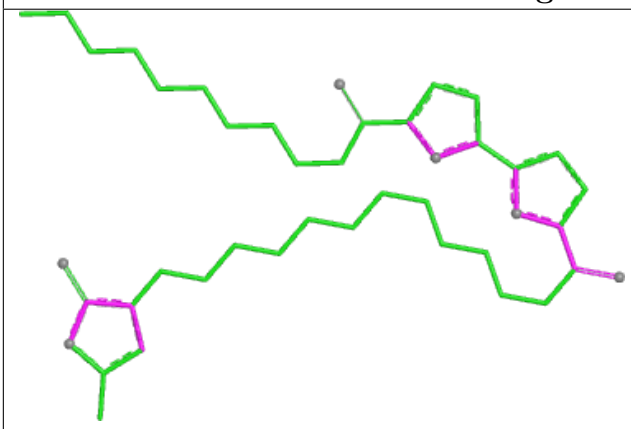


Torsions

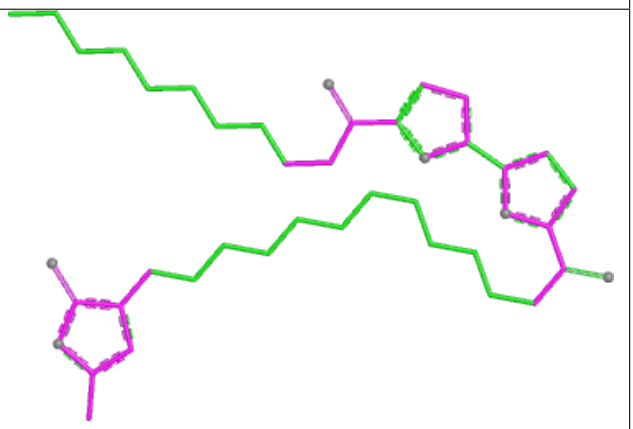


Rings

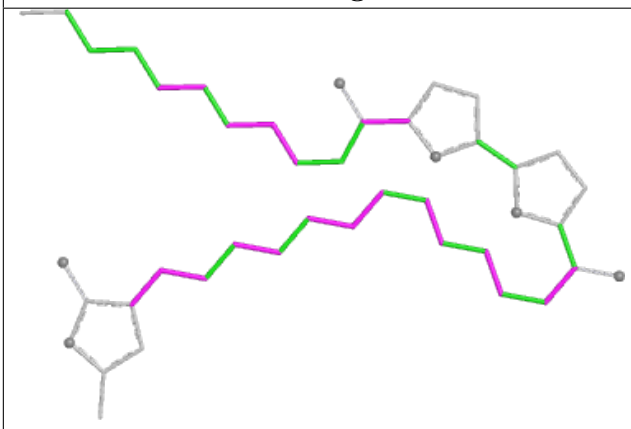
Ligand 88I H 402



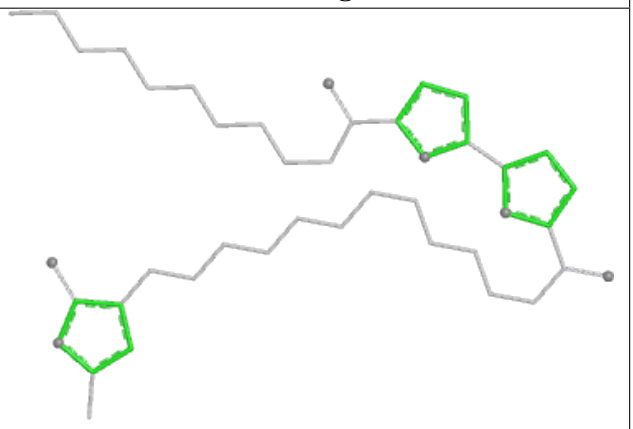
Bond lengths



Bond angles

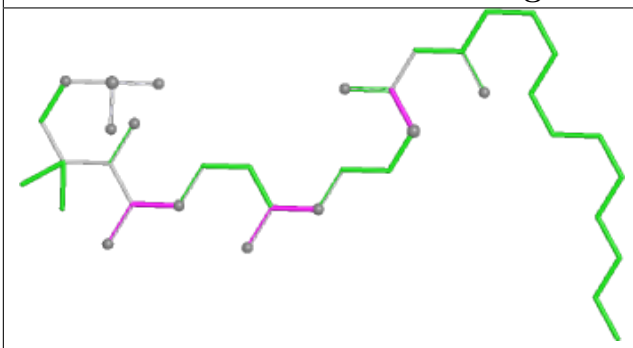


Torsions



Rings

Ligand EHZ U 201



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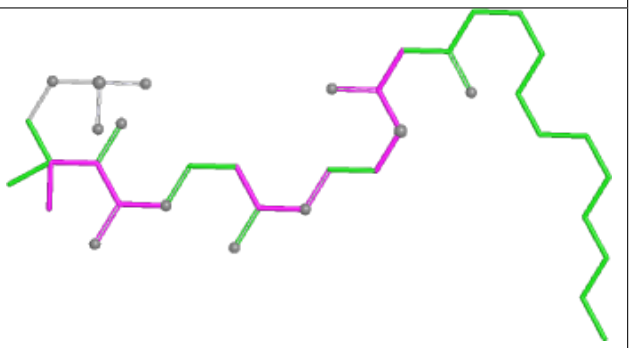
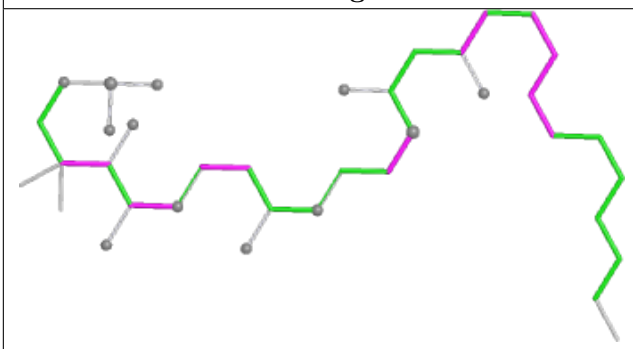
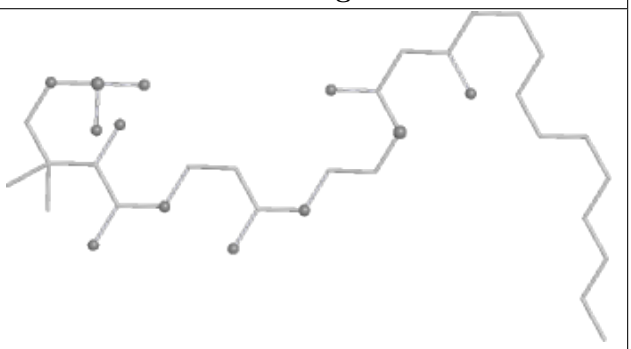


Bond angles

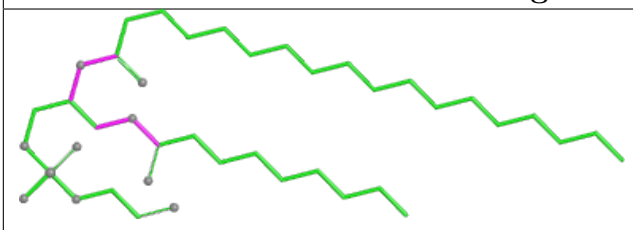


Torsions

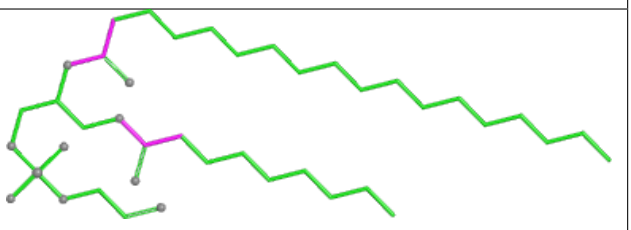


Rings

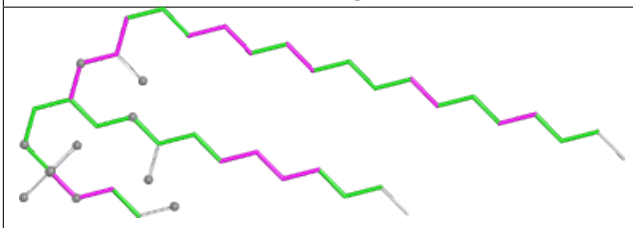
Ligand 3PE L 702



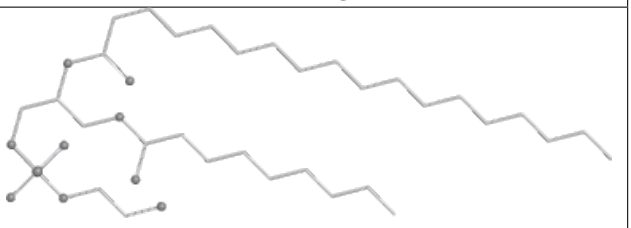
Bond lengths



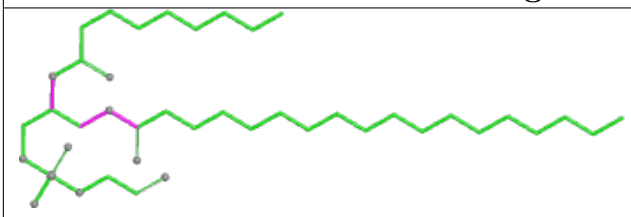
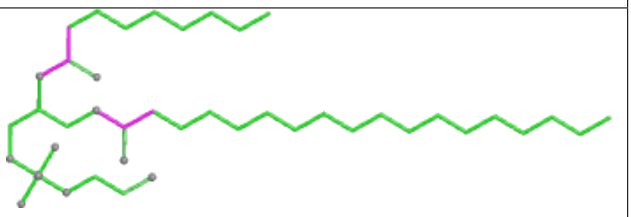
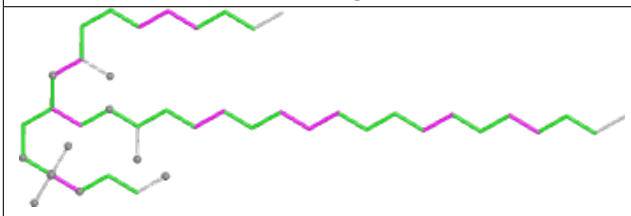
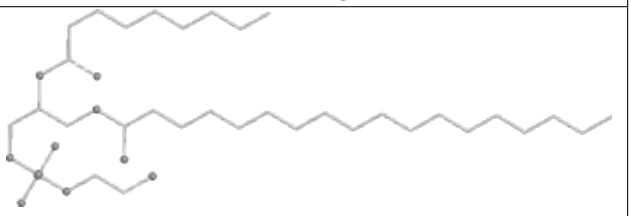
Bond angles

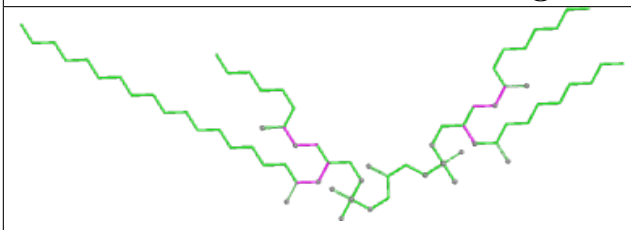
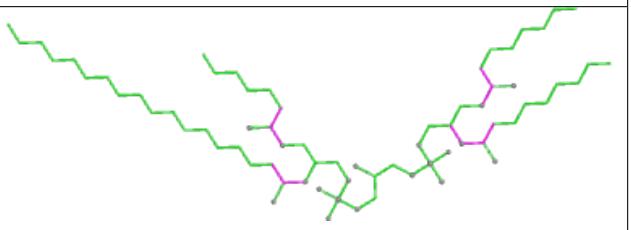
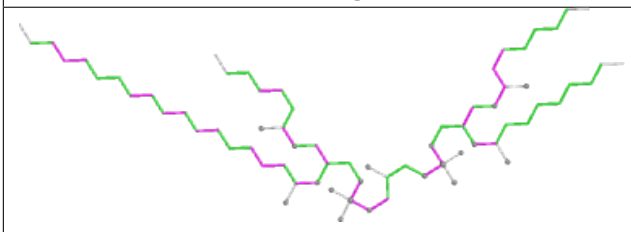
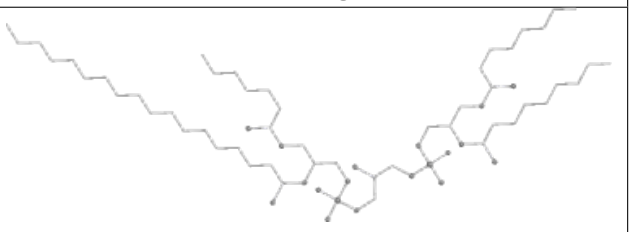


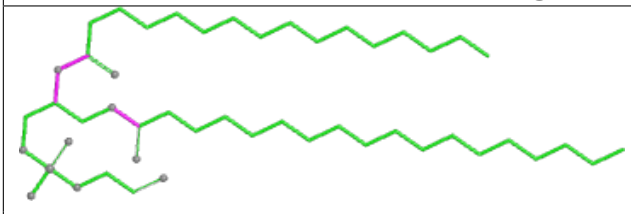
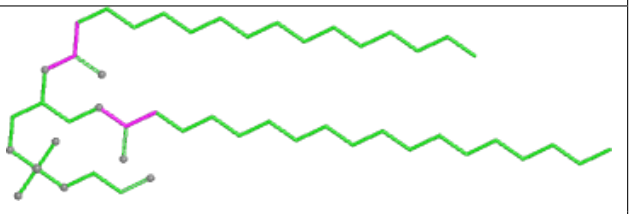
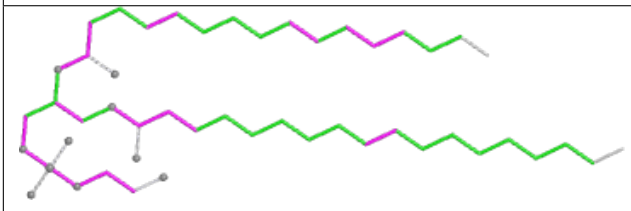
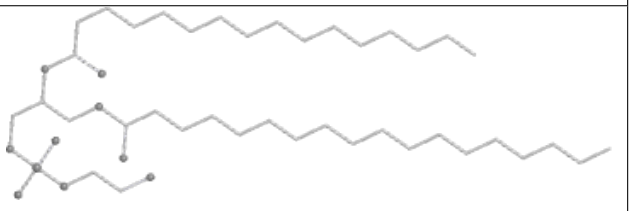
Torsions

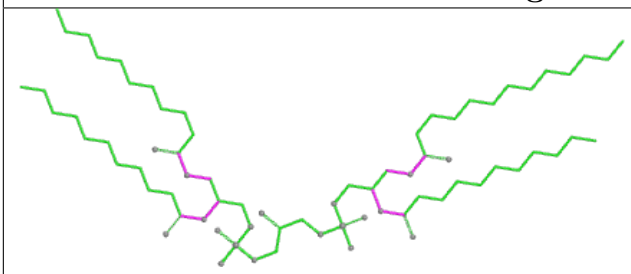
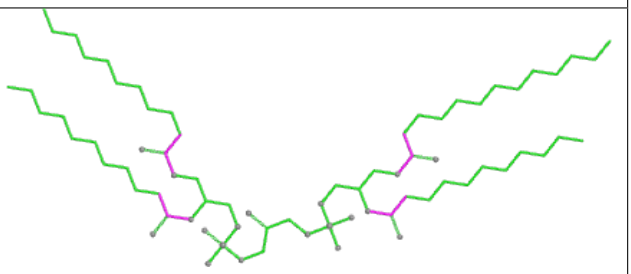
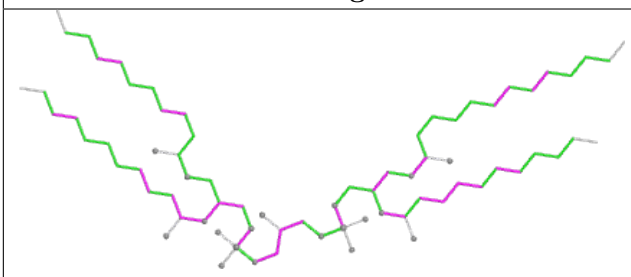
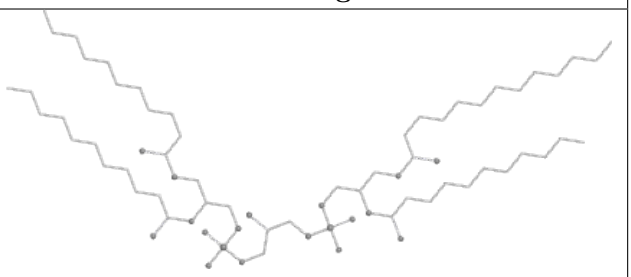


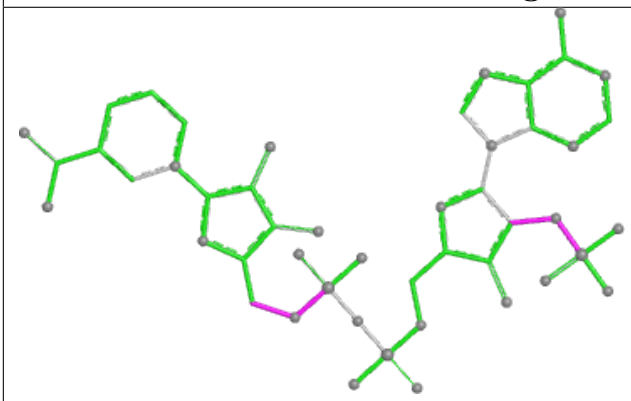
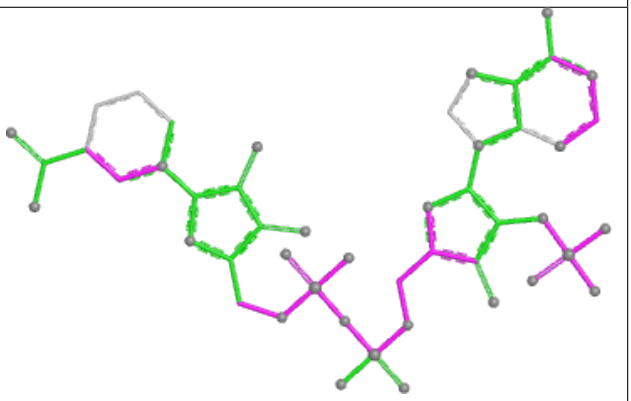
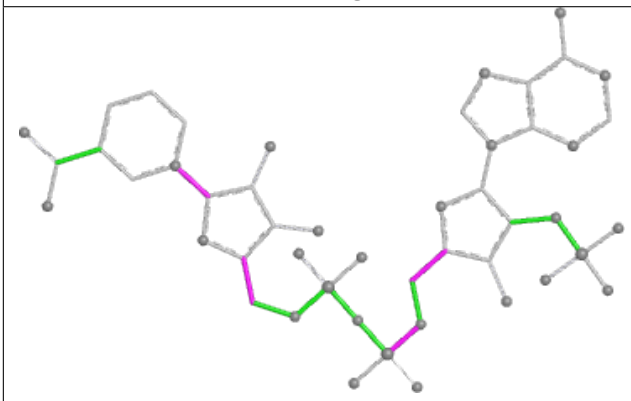
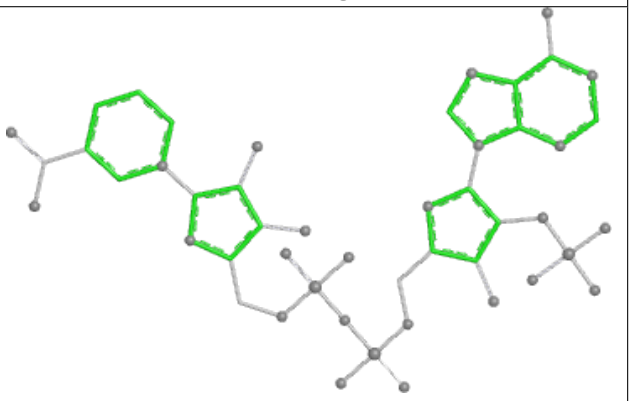
Rings

Ligand 3PE M 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

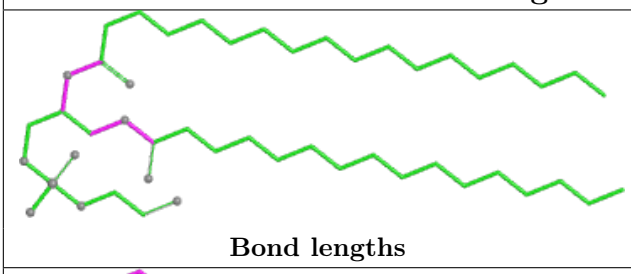
Ligand CDL i 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE L 704	
 Bond lengths	 Bond angles
 Torsions	 Rings

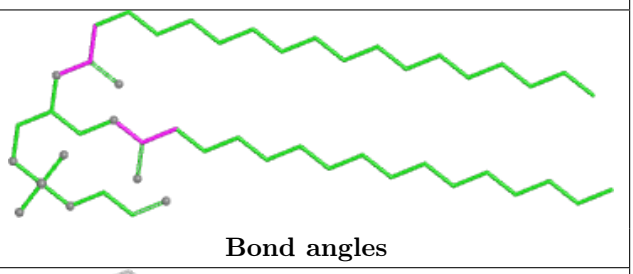
Ligand CDL L 703	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NDP P 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

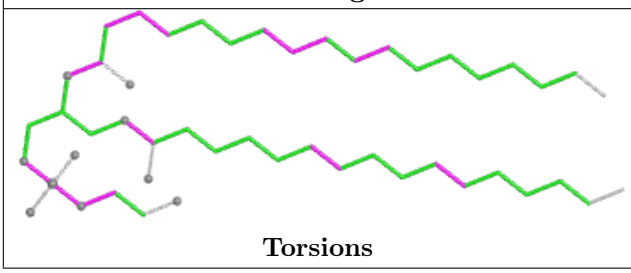
Ligand 3PE L 701



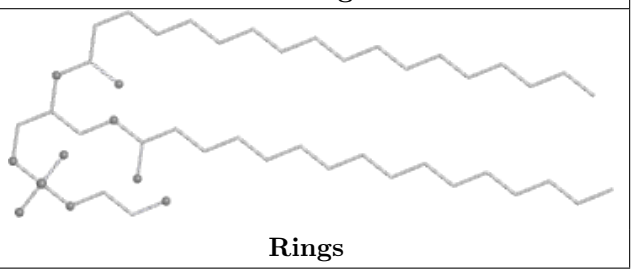
Bond lengths



Bond angles

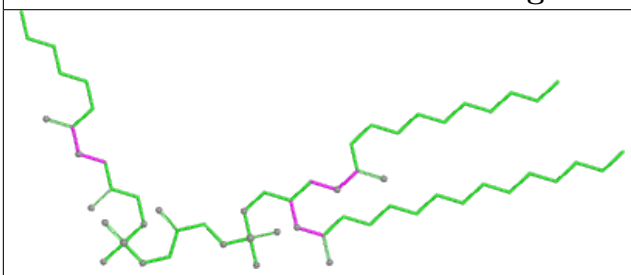


Torsions

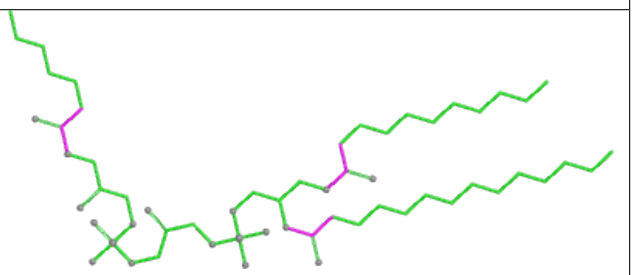


Rings

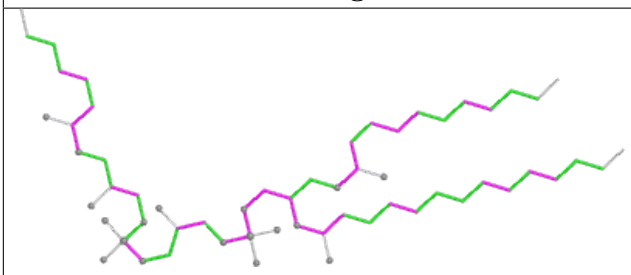
Ligand CDL d 201



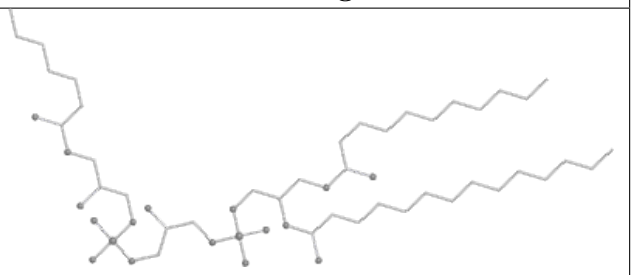
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

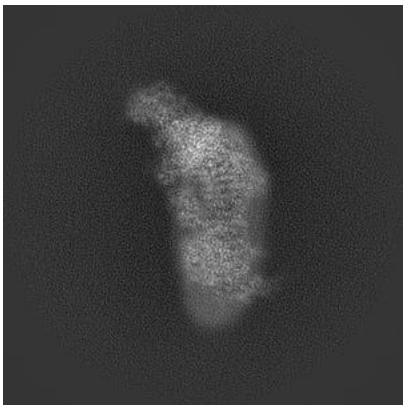
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13611. These allow visual inspection of the internal detail of the map and identification of artifacts.

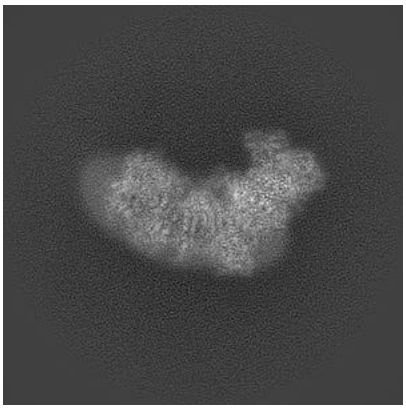
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

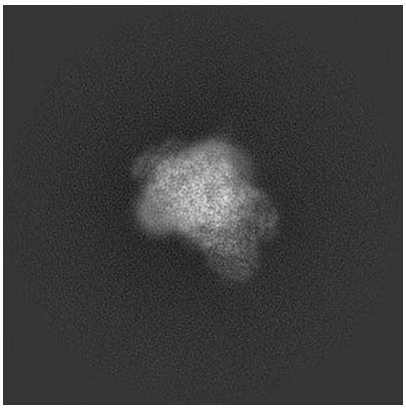
6.1.1 Primary map



X

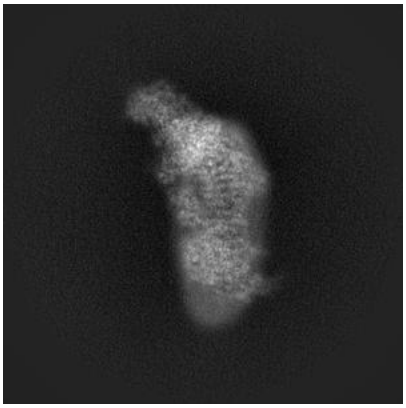


Y

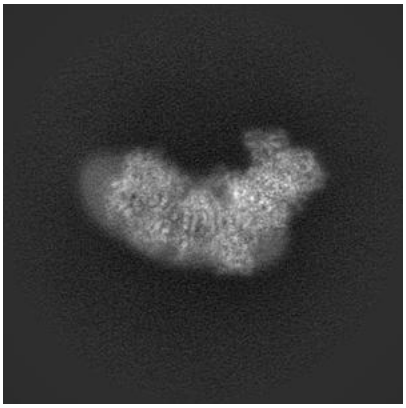


Z

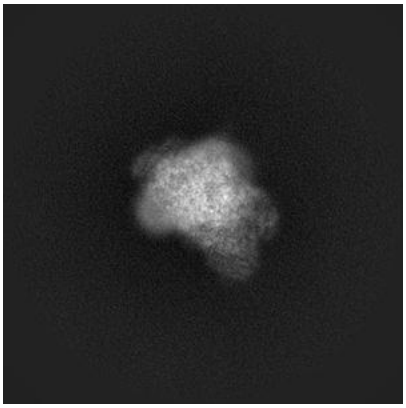
6.1.2 Raw map



X



Y

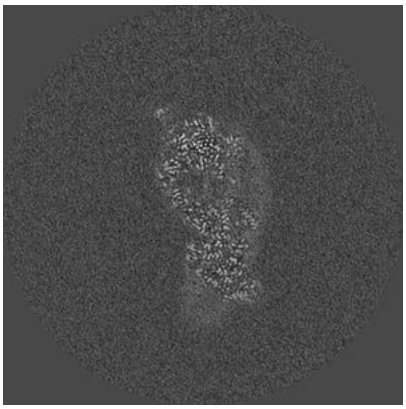


Z

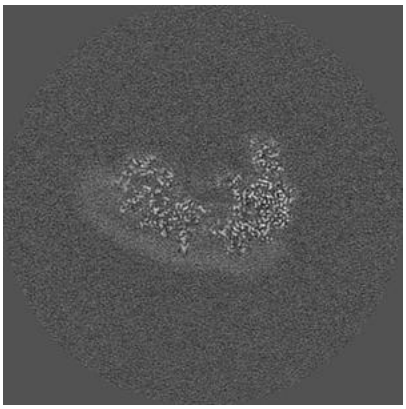
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

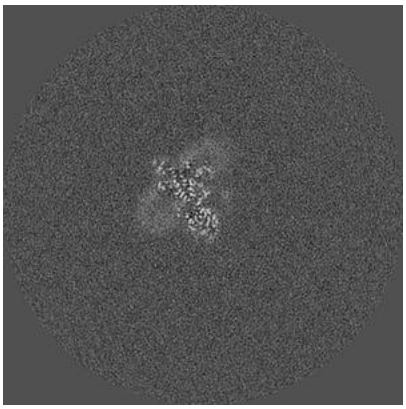
6.2.1 Primary map



X Index: 225

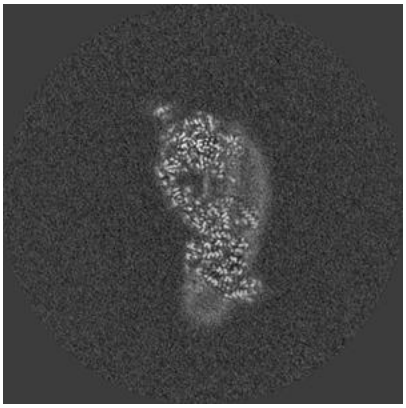


Y Index: 225

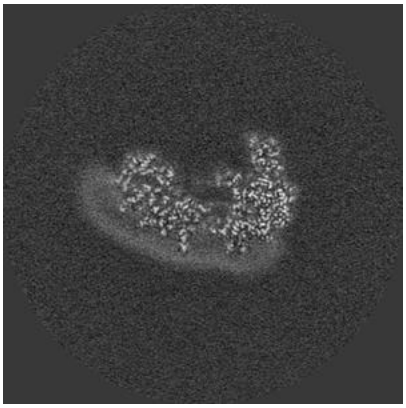


Z Index: 225

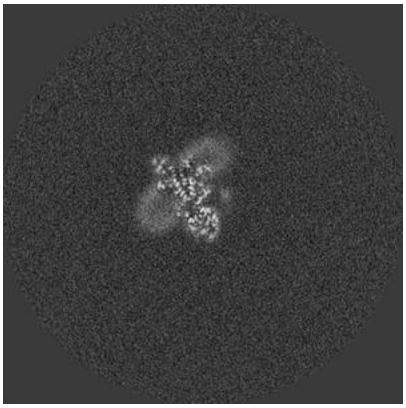
6.2.2 Raw map



X Index: 225



Y Index: 225

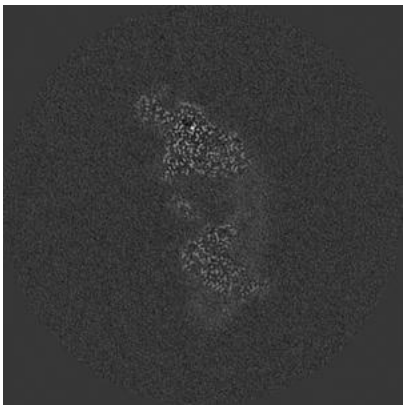


Z Index: 225

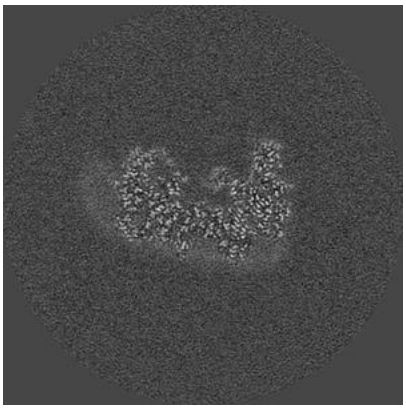
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

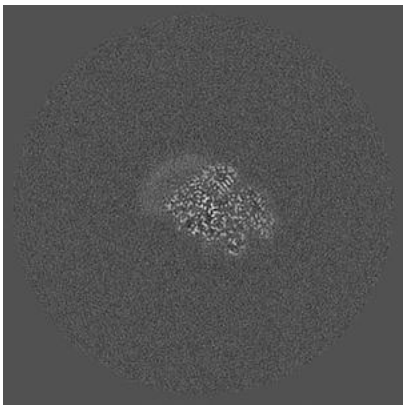
6.3.1 Primary map



X Index: 240

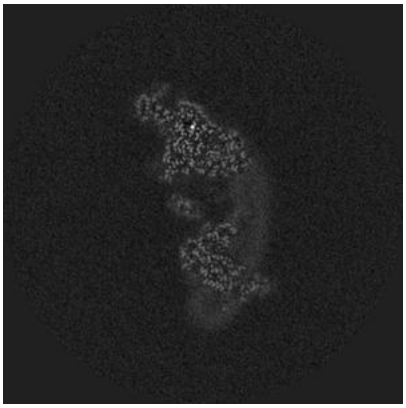


Y Index: 235

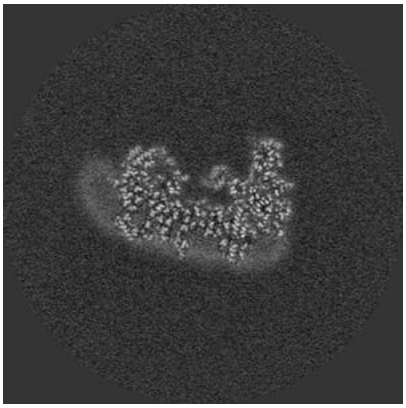


Z Index: 297

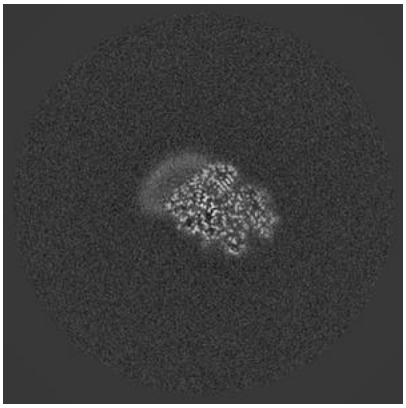
6.3.2 Raw map



X Index: 240



Y Index: 235



Z Index: 297

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

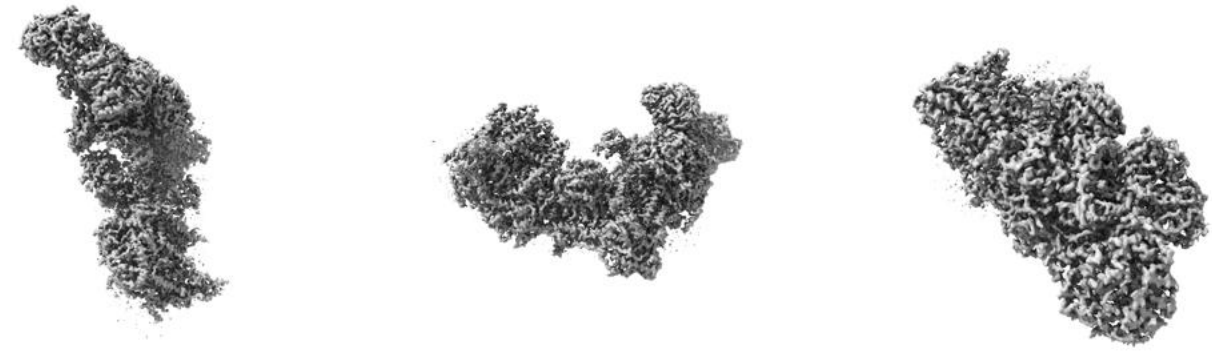
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

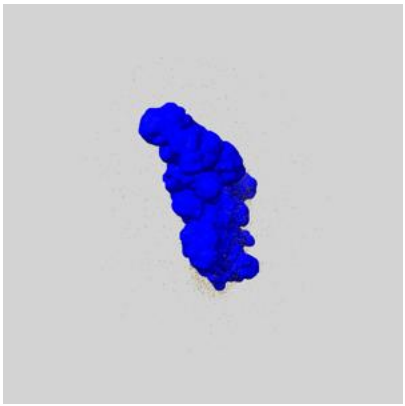
6.5 Mask visualisation (i)

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

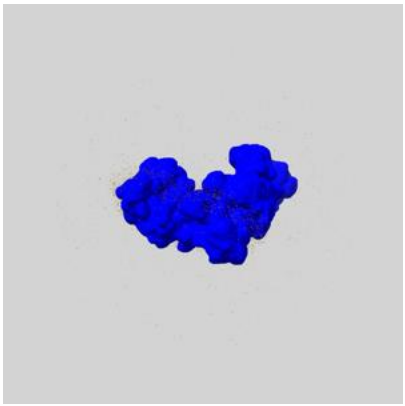
A mask typically either:

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

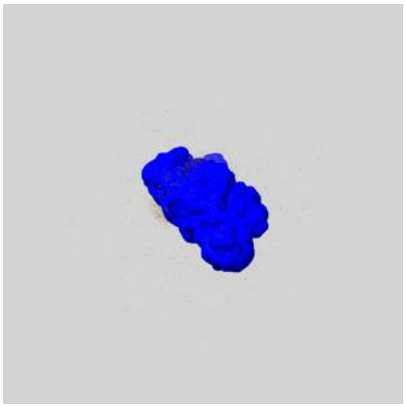
6.5.1 emd_13611_msk_1.map (i)



X



Y

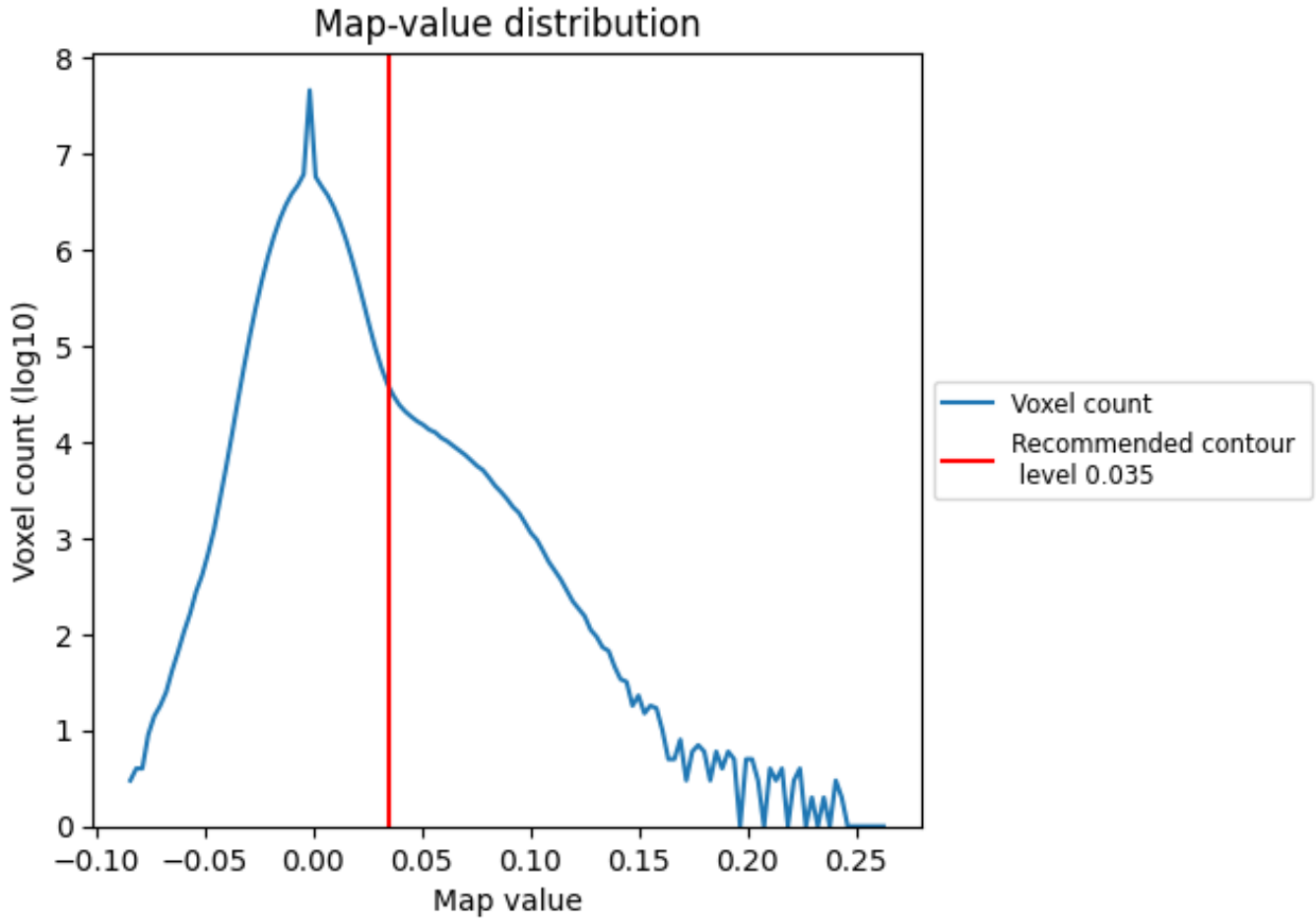


Z

7 Map analysis

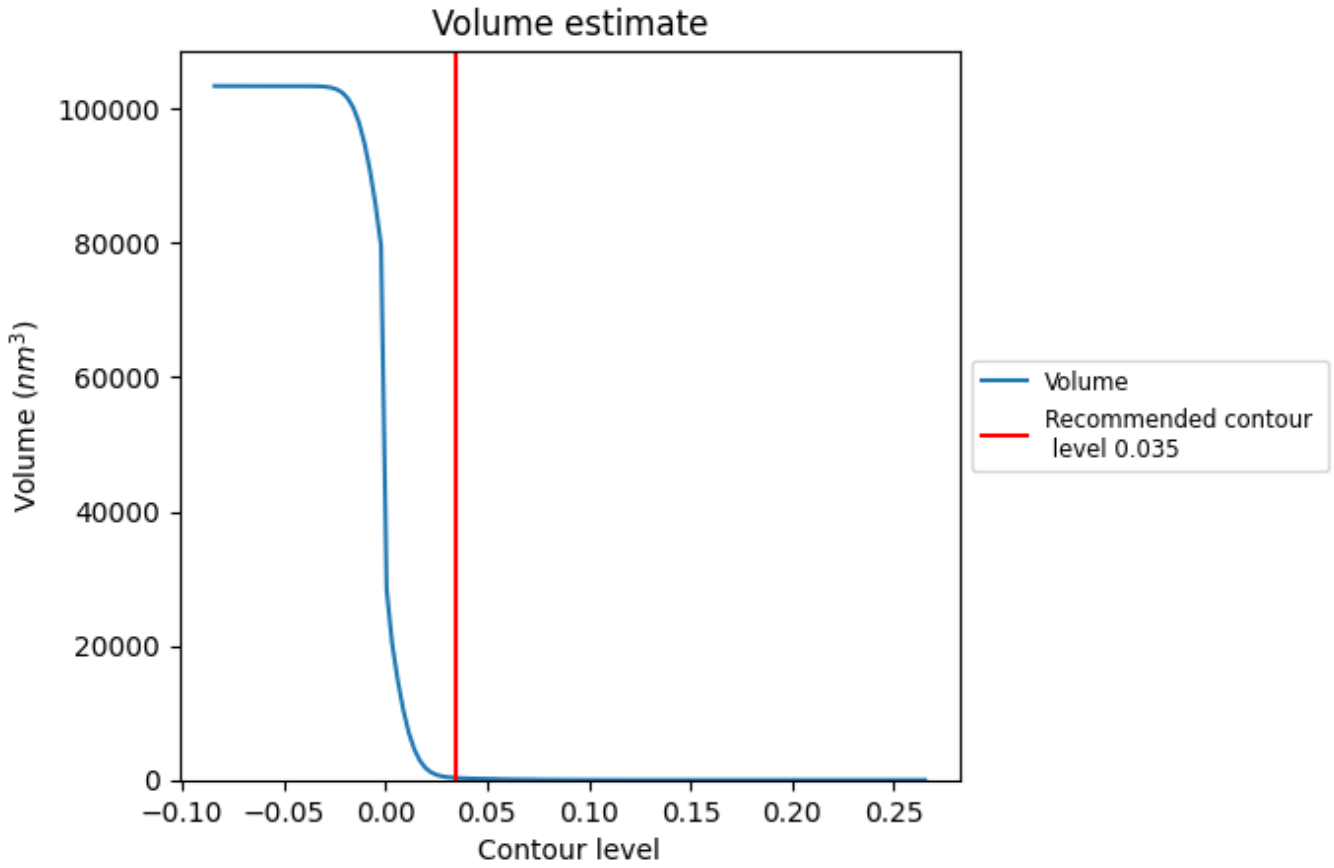
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

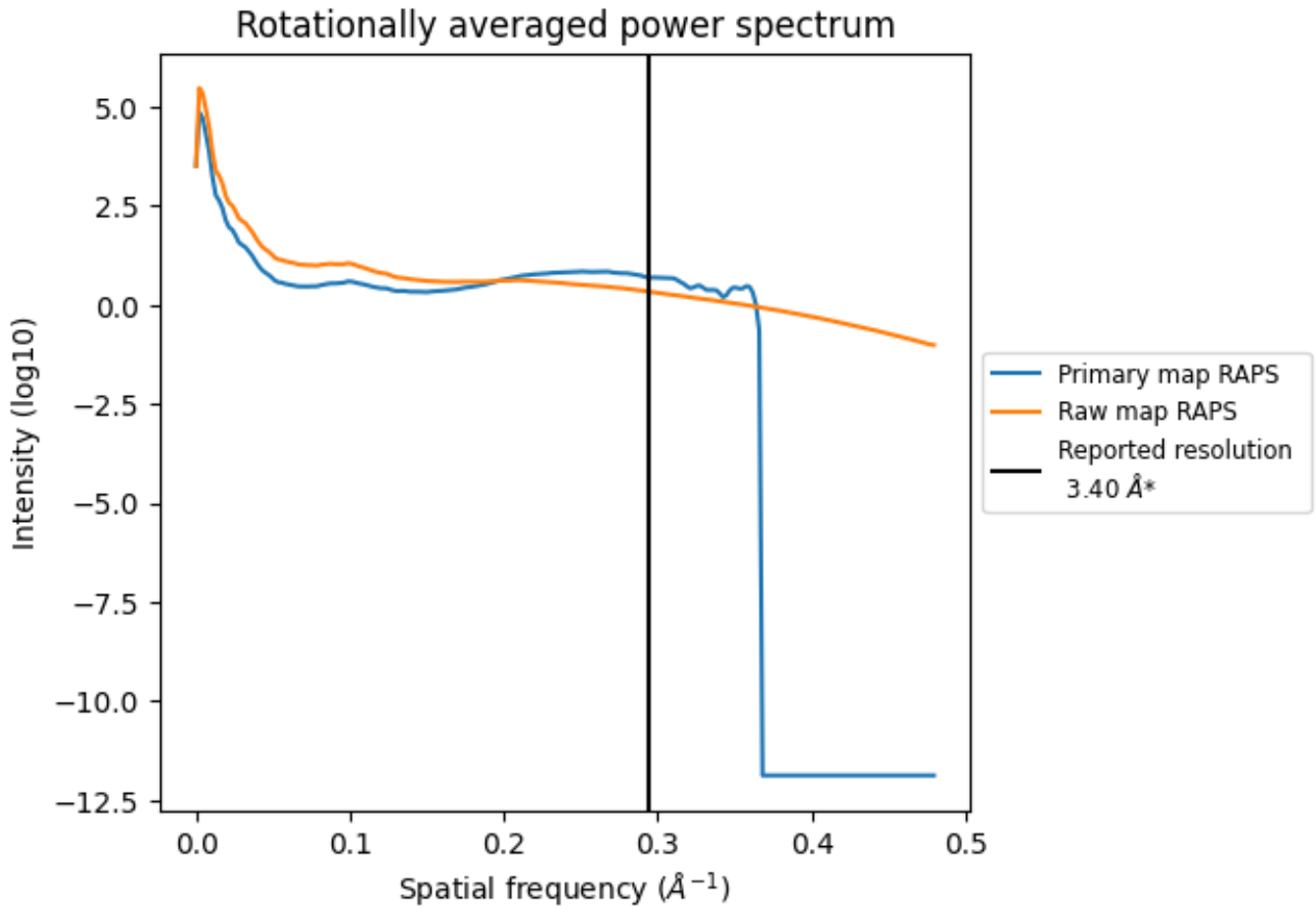
7.2 Volume estimate



The volume at the recommended contour level is 306 nm^3; this corresponds to an approximate mass of 276 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)

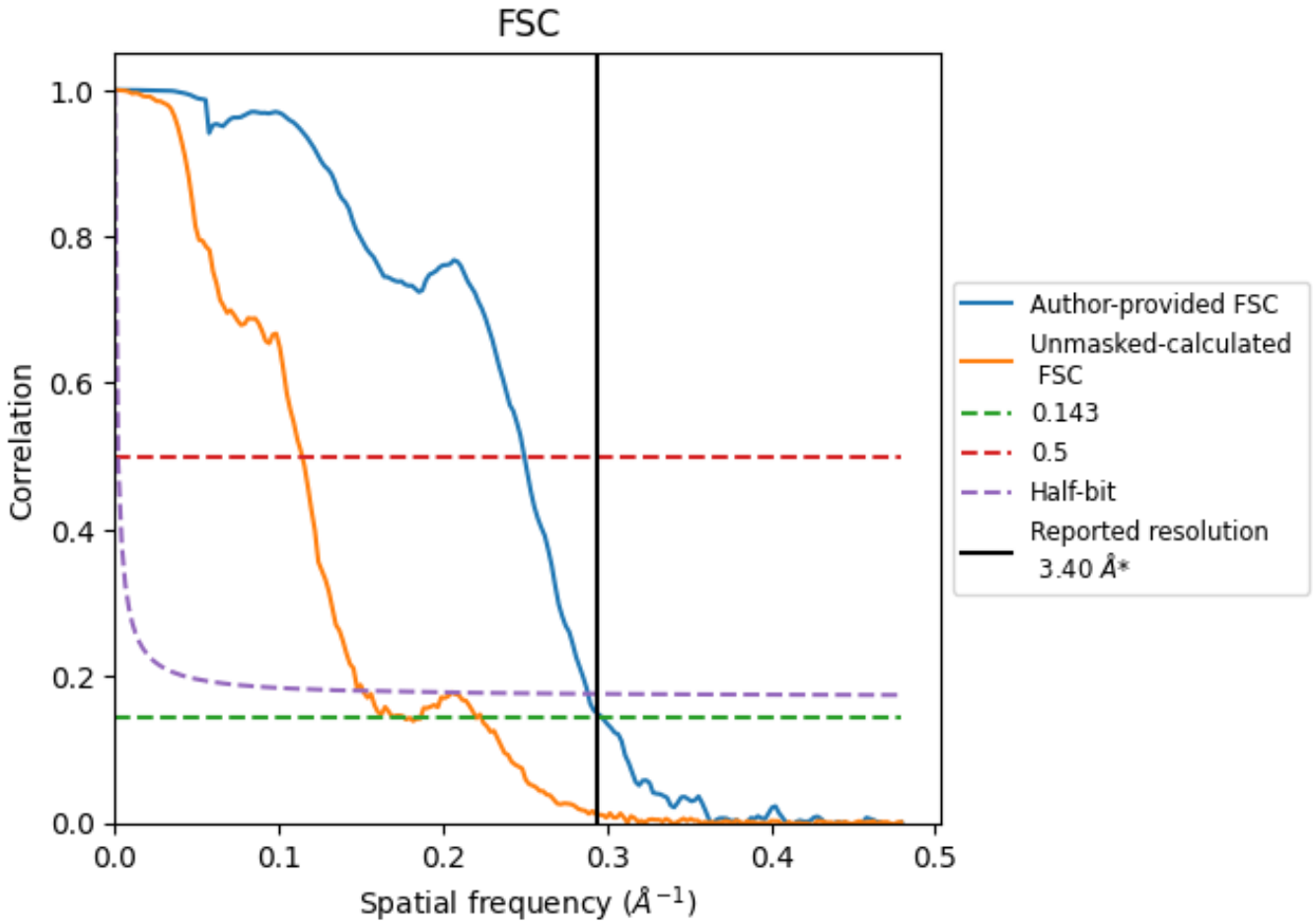


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

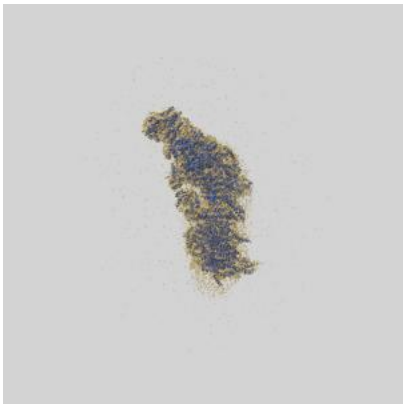
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.37	4.01	3.47
Unmasked-calculated*	5.66	8.76	6.60

*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 5.66 differs from the reported value 3.4 by more than 10 %

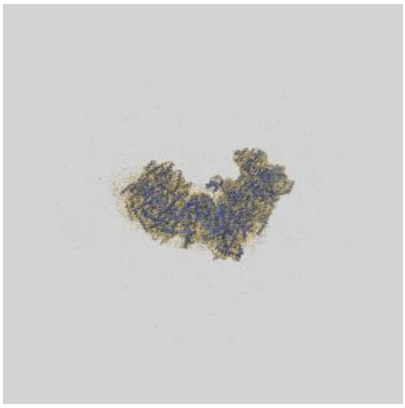
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13611 and PDB model 7PSA. Per-residue inclusion information can be found in section 3 on page 20.

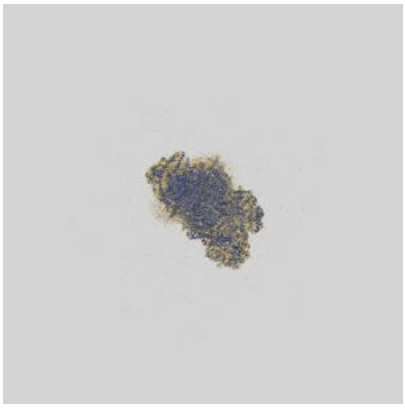
9.1 Map-model overlay



X



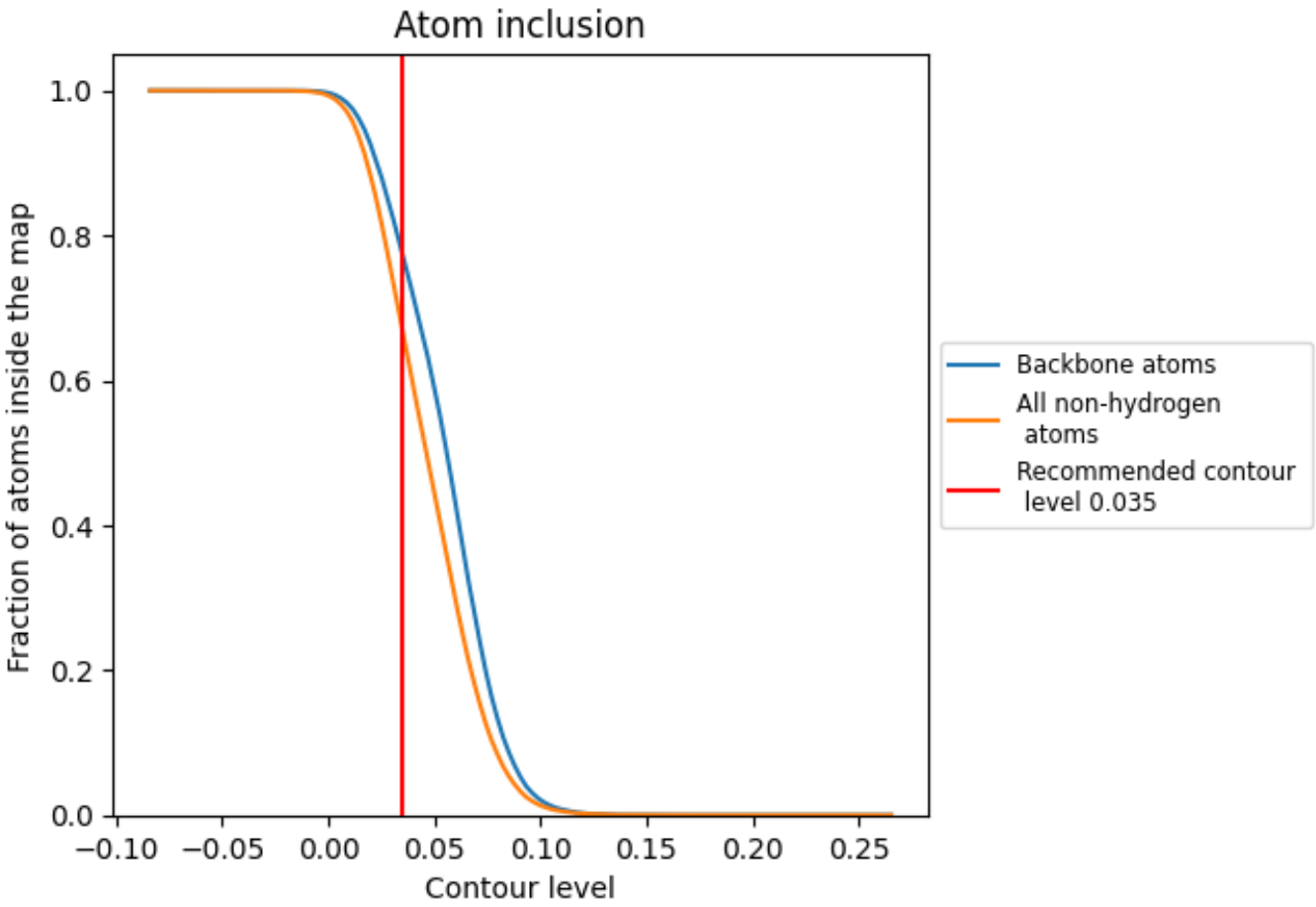
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 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 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.