Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 12:12 am GMT

PDB ID	:	6ZTQ
EMDB ID	:	EMD-11424
Title	:	Cryo-EM structure of respiratory complex I from Mus musculus inhibited by piericidin A at 3.0 A
Authors	:	Bridges, H.R.; Blaza, J.N.; Agip, A.N.A.; Hirst, J.
Deposited on	:	2020-07-20
Resolution	:	3.00 Å(reported)

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

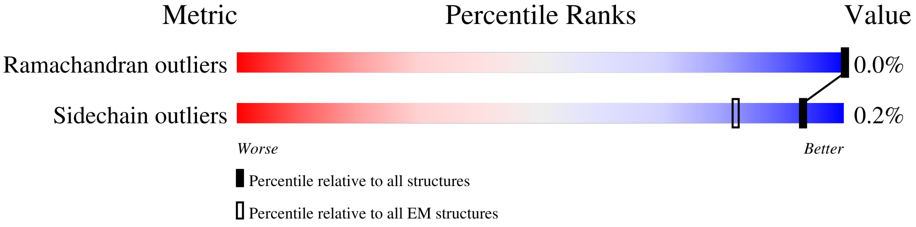
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance ⓘ

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

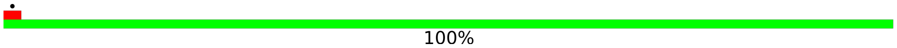
The reported resolution of this entry is 3.00 Å.

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	
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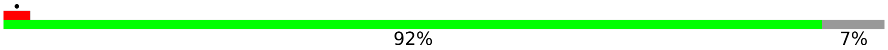
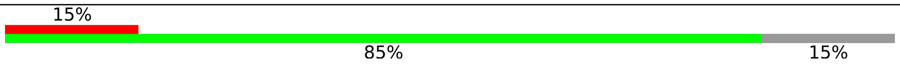
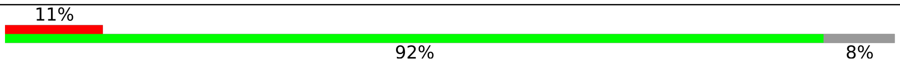
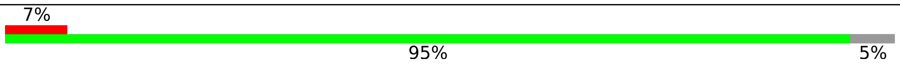
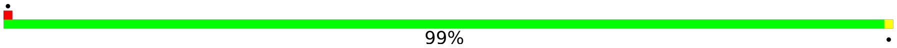
3	C	263	
4	D	463	
5	E	248	
6	F	464	
7	G	727	
8	H	318	
9	I	212	

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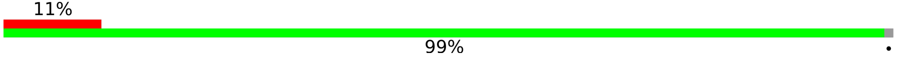
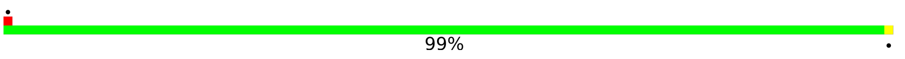
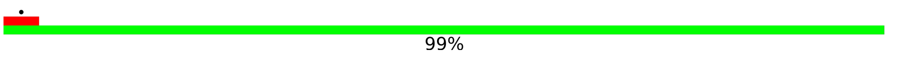
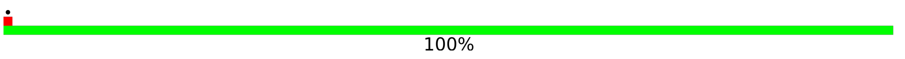
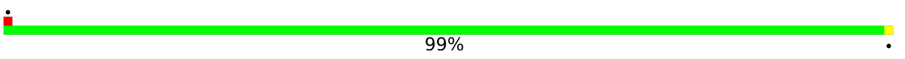
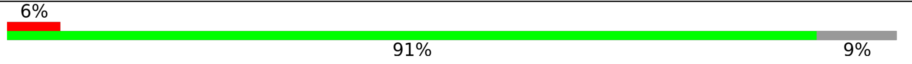
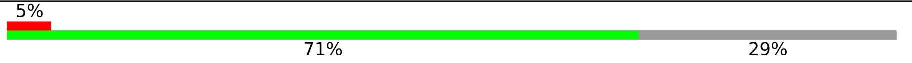
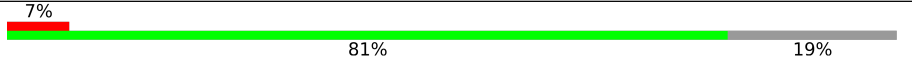
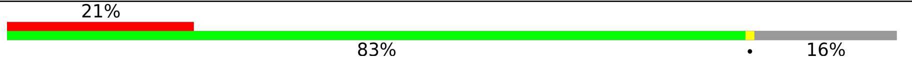
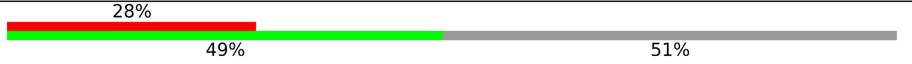
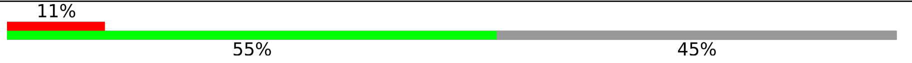
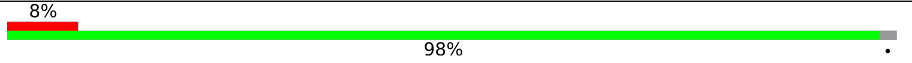
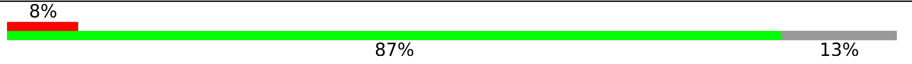
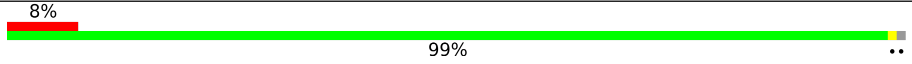
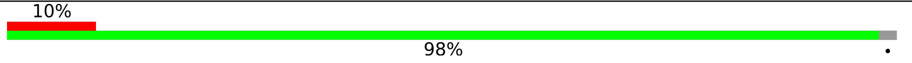
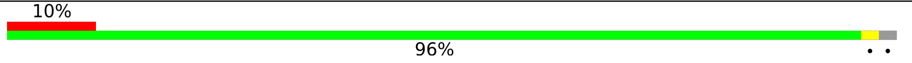
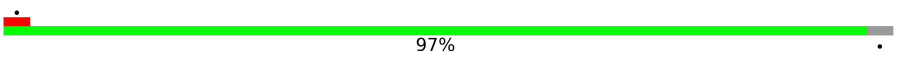
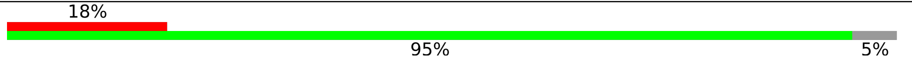
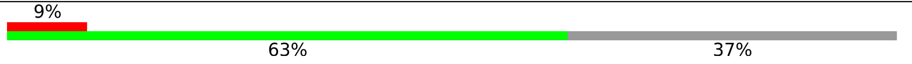
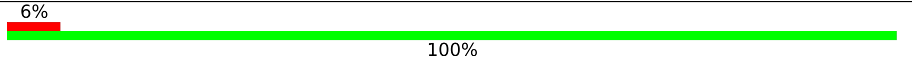
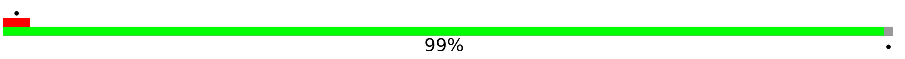
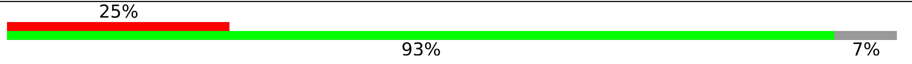
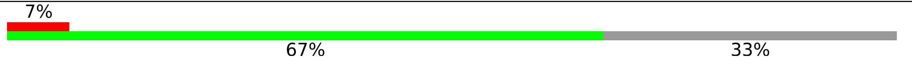
Mol	Chain	Length	Quality of chain
10	J	172	
11	K	98	
12	L	607	
13	M	459	
14	N	345	
15	O	355	
16	P	377	
17	Q	175	
18	R	116	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	131	
23	X	172	
24	Y	143	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	
29	d	120	
30	e	106	
31	f	57	
32	g	151	
33	h	189	

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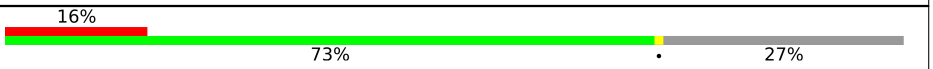
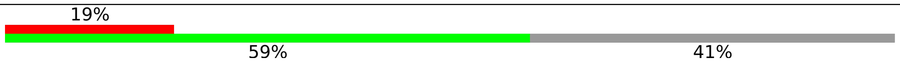
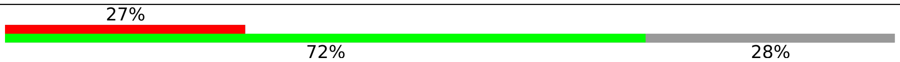
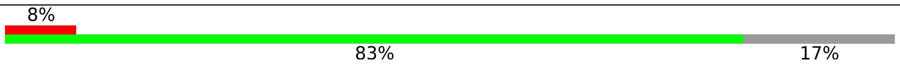
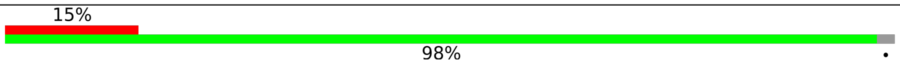
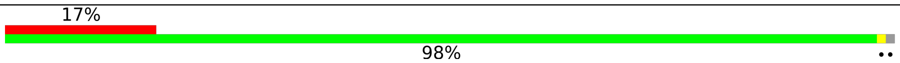
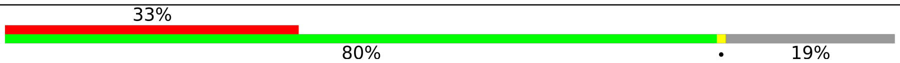
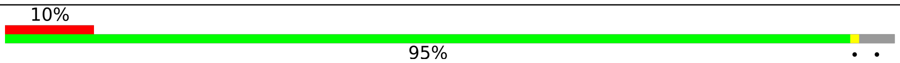
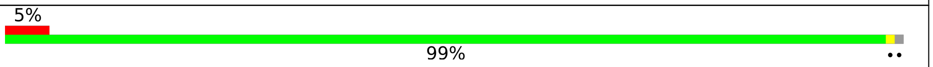
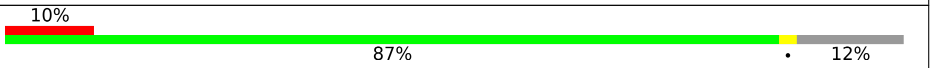
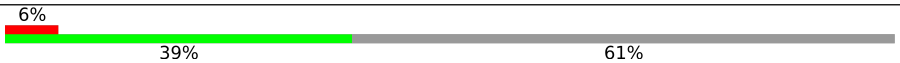
Mol	Chain	Length	Quality of chain
34	i	128	
35	j	105	
36	k	104	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	104	

2 Entry composition ⓘ

There are 55 unique types of molecules in this entry. The entry contains 67072 atoms, of which 0 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	N	O	S		
1	A	115	933	633	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	N	O	S		
2	B	156	1247	796	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	N	O	S		
3	C	207	1721	1111	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	N	O	S		
4	D	430	3464	2215	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	N	O	S		
5	E	212	1648	1048	277	312	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	428	3300	2080	589	609	22	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	688	5296	3321	919	1015	41	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	318	2540	1706	384	428	22	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	178	1431	898	245	276	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	171	1300	874	185	226	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	98	737	477	112	137	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	606	4800	3182	746	827	45	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	459	3632	2408	567	617	40	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	344	2696	1791	416	452	37	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	320	2607	1674	431	492	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	342	2748	1777	483	481	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	125	1015	642	179	190	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	94	738	458	135	142	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	83	667	419	126	119	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	76	611	392	90	124	5	0	0
20	U	86	692	446	102	139	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	V	114	927	604	154	166	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	W	114	970	619	180	165	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	X	171	1396	889	250	247	10	0	0

- Molecule 24 is a protein called MCG5603.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Y	140	1037	662	175	192	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Z	141	1167	750	207	202	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	68	Total 556	C 360	N 99	O 93	S 4	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	48	Total 398	C 261	N 69	O 67	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	120	Total 996	C 651	N 171	O 165	S 9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	105	Total 877	C 555	N 162	O 152	S 8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	53	Total 456	C 295	N 82	O 77	S 2	0	0

- 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 850	C 549	N 136	O 161	S 4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	h	138	1162	762	194	203	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	i	94	787	515	134	135	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	j	62	537	355	88	93	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	k	75	609	404	103	100	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	l	154	1294	834	215	234	11	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	m	126	1050	676	189	185	0	0

- 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	N	O	S	0	0
			1534	981	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	N	O	S	0	0
			957	605	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	N	O	S	0	0
			1433	901	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	N	O	S	0	0
			1203	773	213	212	5		

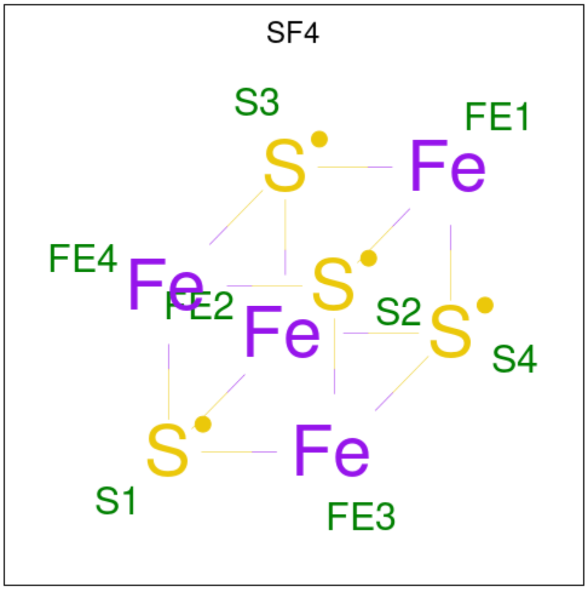
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	100	Total	C	N	O	S	0	0
			802	507	149	143	3		

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

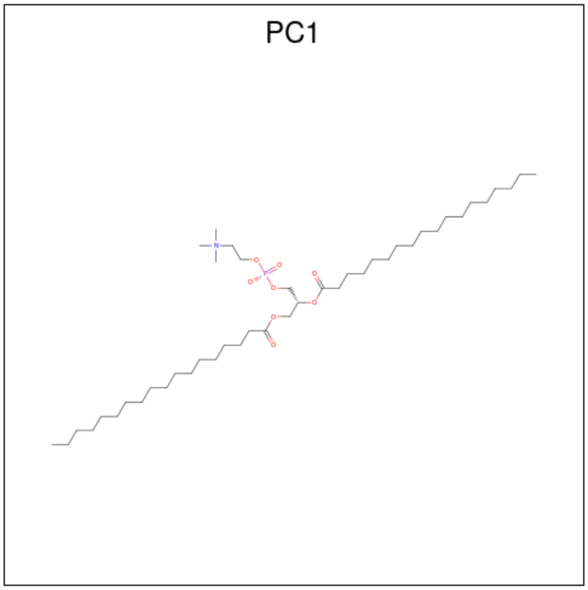
Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	41	Total	C	N	O	0	0
			344	215	61	68		

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



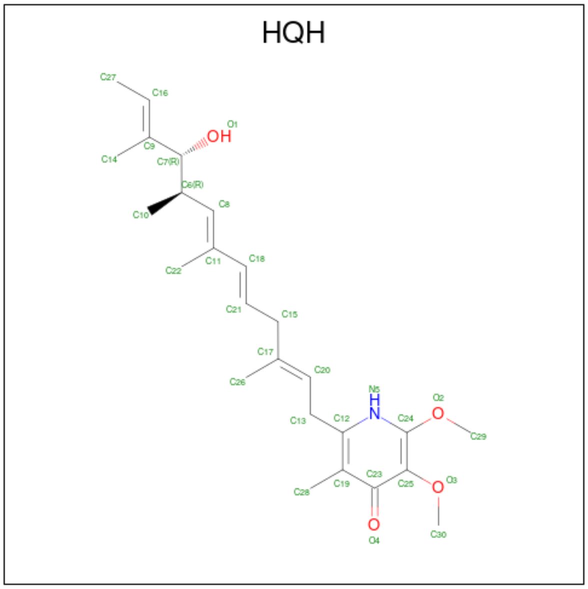
Mol	Chain	Residues	Atoms	AltConf
45	B	1	Total Fe S 8 4 4	0
45	F	1	Total Fe S 8 4 4	0
45	G	1	Total Fe S 16 8 8	0
45	G	1	Total Fe S 16 8 8	0
45	I	1	Total Fe S 16 8 8	0
45	I	1	Total Fe S 16 8 8	0

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



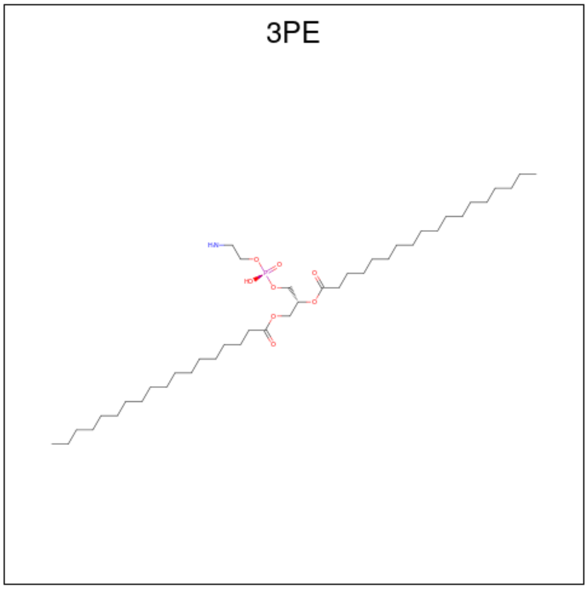
Mol	Chain	Residues	Atoms	AltConf
46	B	1	Total C N O P 78 58 2 16 2	0
46	B	1	Total C N O P 78 58 2 16 2	0
46	J	1	Total C N O P 42 32 1 8 1	0
46	Z	1	Total C N O P 45 35 1 8 1	0

- Molecule 47 is Piericidin A (three-letter code: HQH) (formula: $C_{25}H_{37}NO_4$) (labeled as "Ligand of Interest" by depositor).



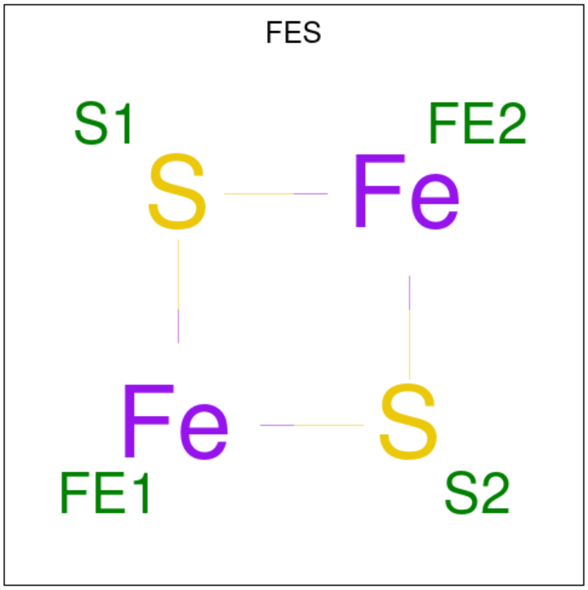
Mol	Chain	Residues	Atoms				AltConf
47	D	1	Total 30	C 25	N 1	O 4	0

- Molecule 48 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



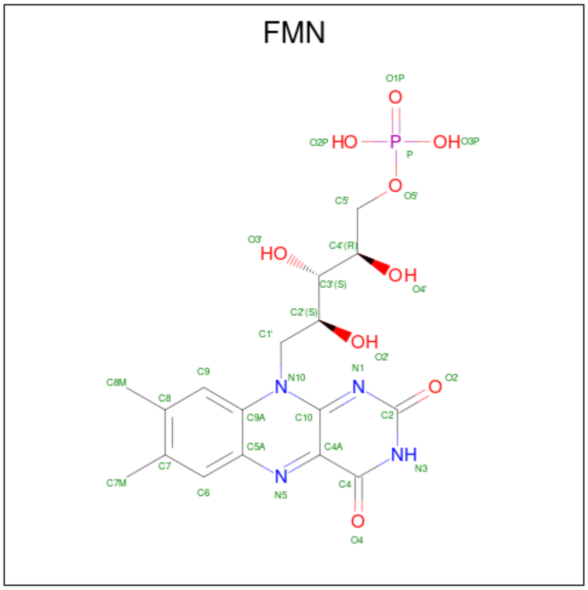
Mol	Chain	Residues	Atoms					AltConf
48	D	1	Total 51	C 41	N 1	O 8	P 1	0
48	H	1	Total 44	C 34	N 1	O 8	P 1	0
48	K	1	Total 33	C 23	N 1	O 8	P 1	0
48	L	1	Total 49	C 39	N 1	O 8	P 1	0
48	M	1	Total 42	C 32	N 1	O 8	P 1	0
48	Y	1	Total 41	C 31	N 1	O 8	P 1	0
48	h	1	Total 37	C 27	N 1	O 8	P 1	0
48	i	1	Total 42	C 32	N 1	O 8	P 1	0
48	l	1	Total 49	C 39	N 1	O 8	P 1	0

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



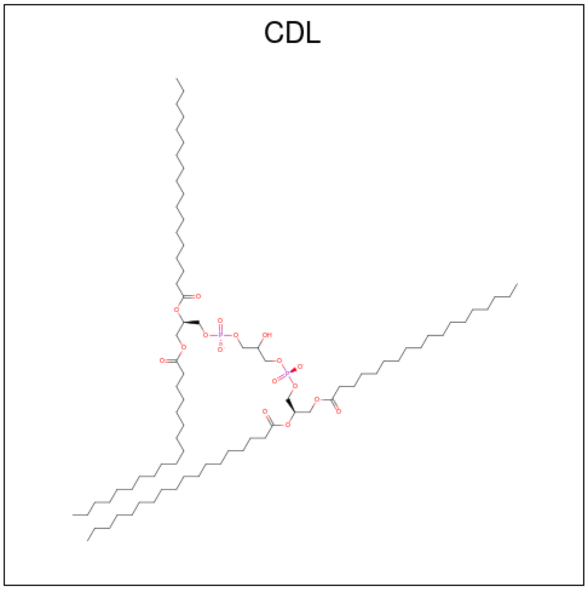
Mol	Chain	Residues	Atoms			AltConf
49	E	1	Total 4	Fe 2	S 2	0
49	G	1	Total 4	Fe 2	S 2	0

- Molecule 50 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



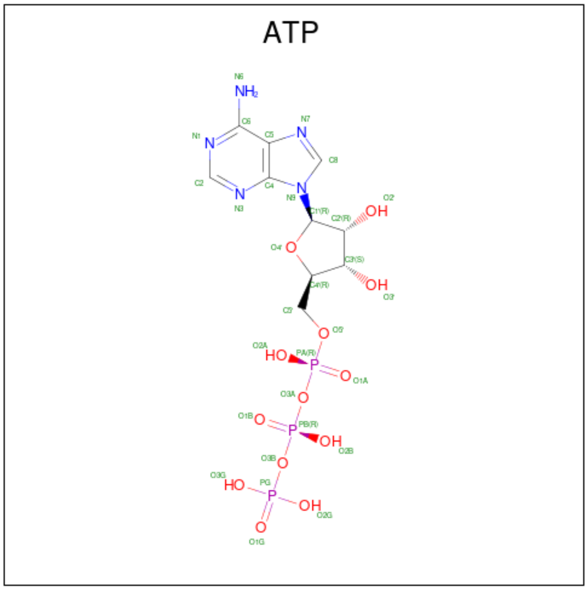
Mol	Chain	Residues	Atoms					AltConf
50	F	1	Total 31	C 17	N 4	O 9	P 1	0

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



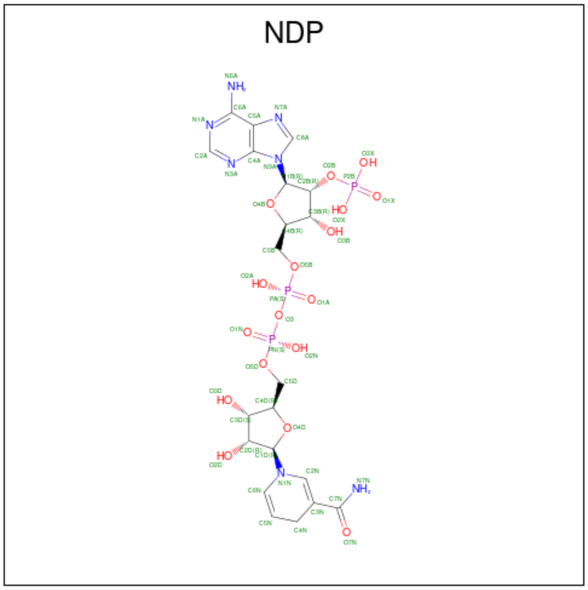
Mol	Chain	Residues	Atoms	AltConf
51	L	1	Total C O P 74 55 17 2	0
51	N	1	Total C O P 124 87 33 4	0
51	N	1	Total C O P 124 87 33 4	0
51	d	1	Total C O P 130 92 34 4	0
51	d	1	Total C O P 130 92 34 4	0
51	h	1	Total C O P 70 51 17 2	0
51	q	1	Total C O P 57 38 17 2	0

- 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
			Total	C	N	O	P	
52	O	1	31	10	5	13	3	0

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

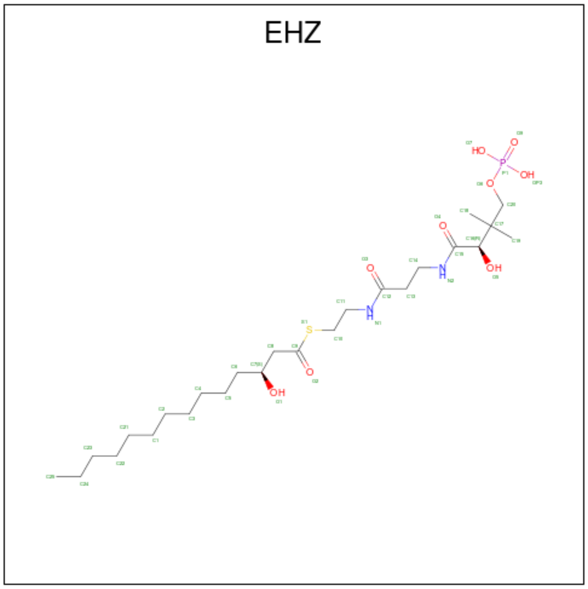


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
53	P	1	48	21	7	17	3	0

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

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

- 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: $C_{25}H_{49}N_2O_9PS$).



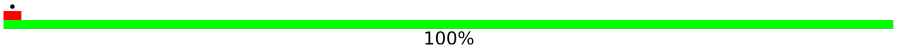
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
55	T	1	37	25	2	8	1	1	0
55	U	1	37	25	2	8	1	1	0

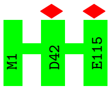
3 Residue-property plots

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

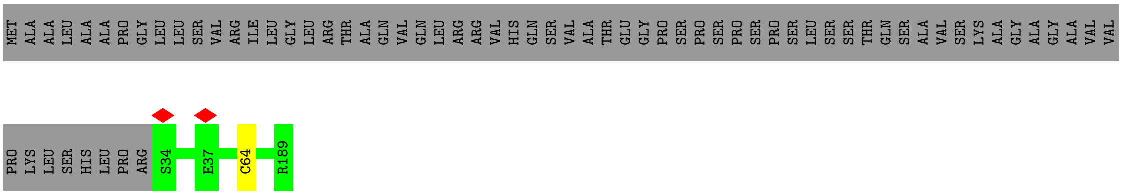
Chain A:





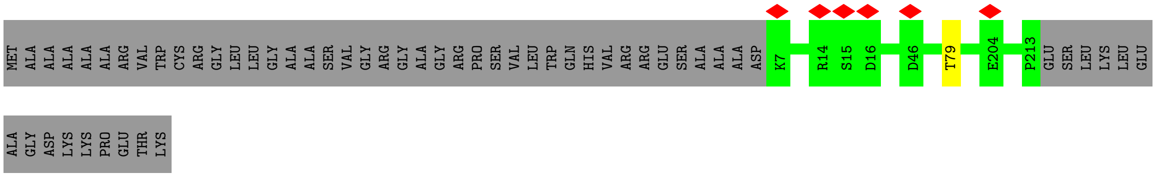
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B:



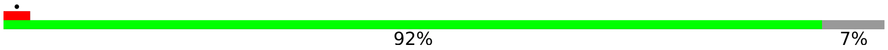
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

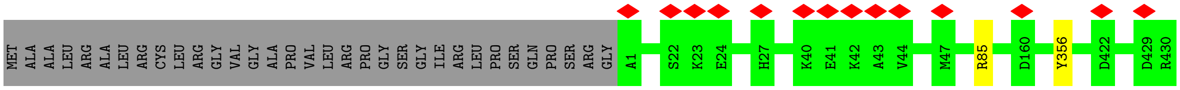
Chain C:



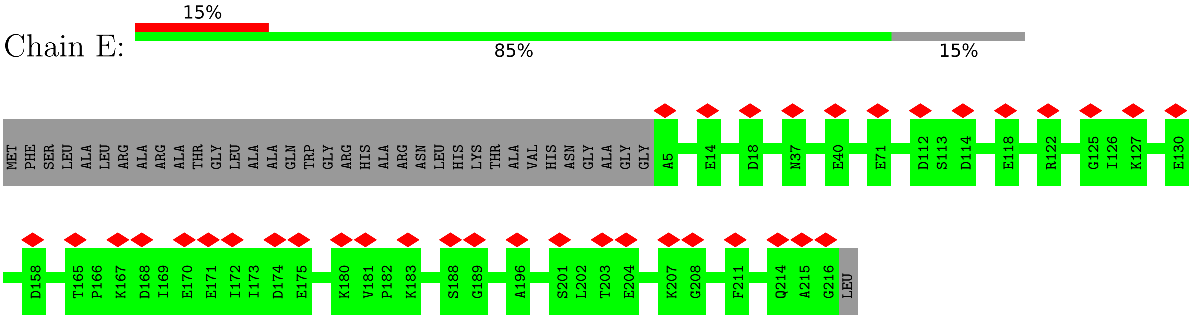
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D:

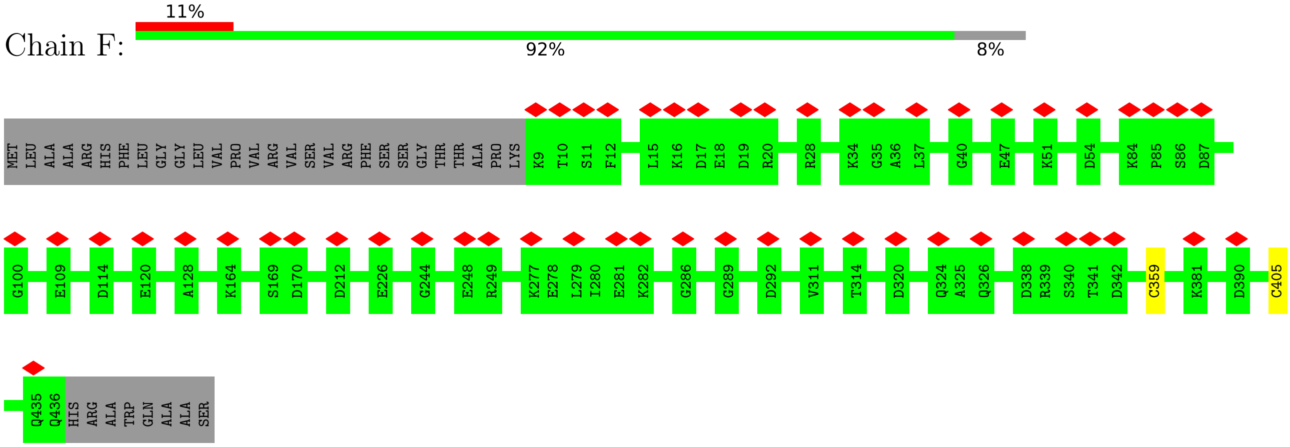




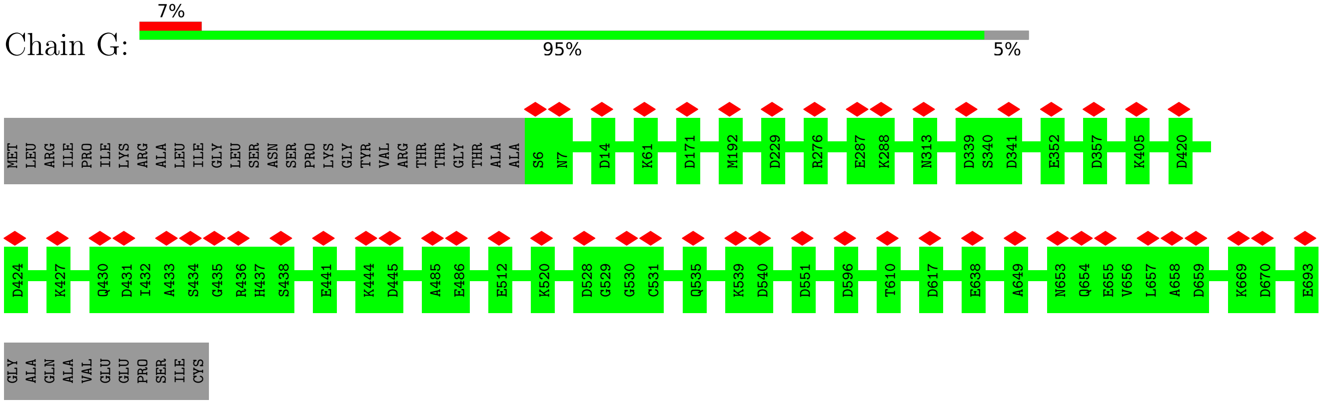
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



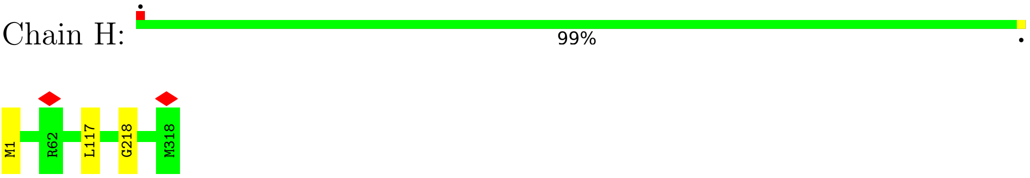
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



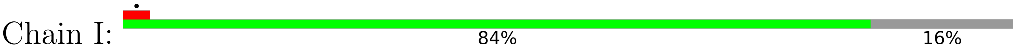
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

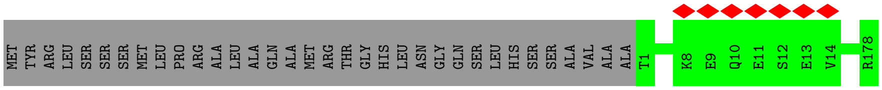


- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



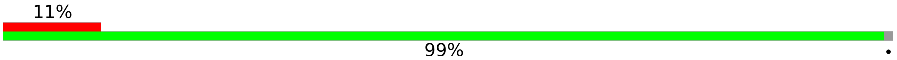
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

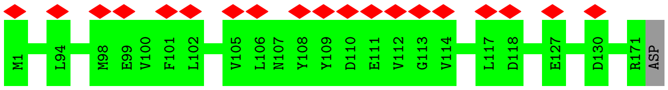




- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

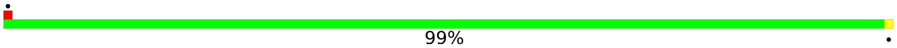
Chain J:

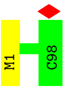




- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

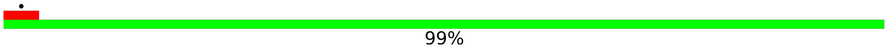
Chain K:

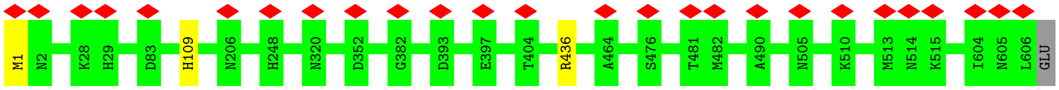




- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

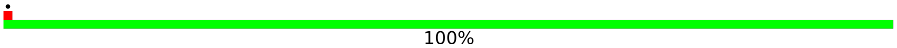
Chain L:

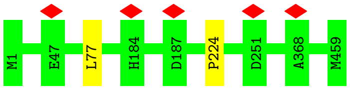




- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

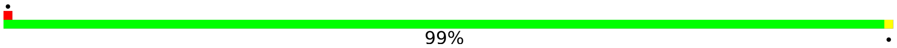
Chain M:

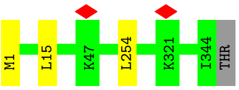




- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

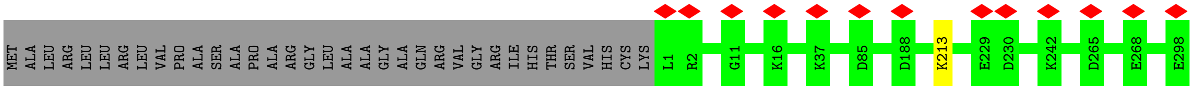
Chain N:

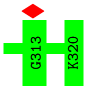




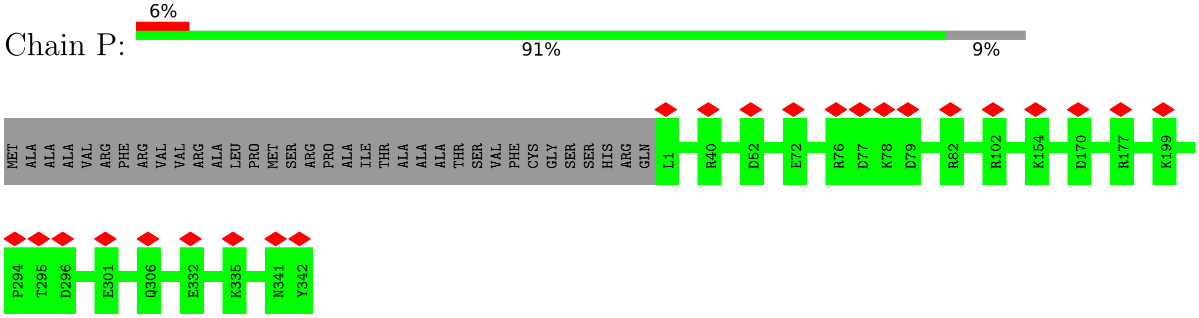
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:

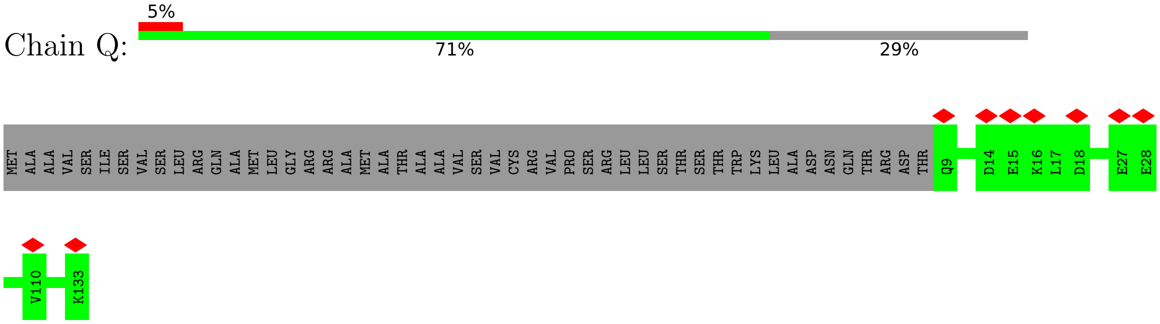




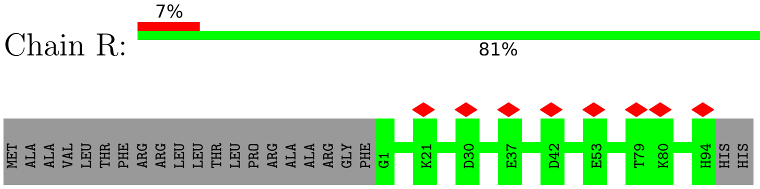
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



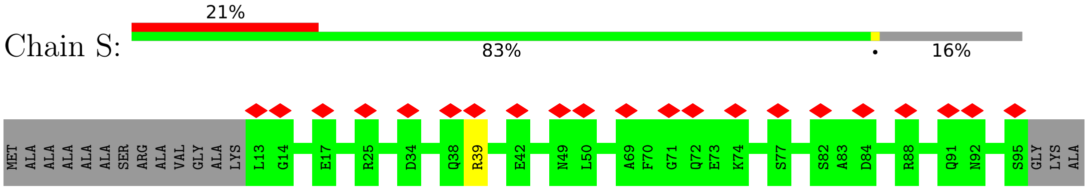
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



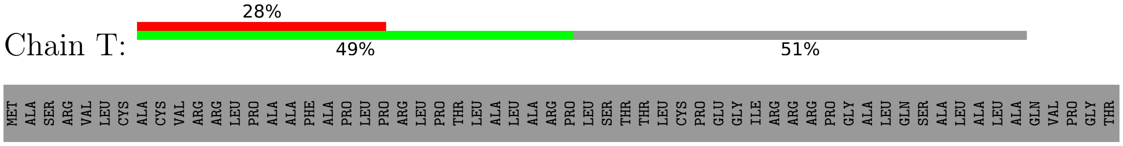
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

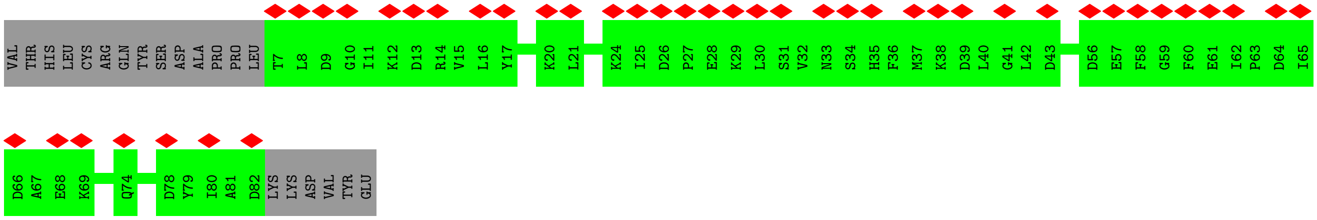


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

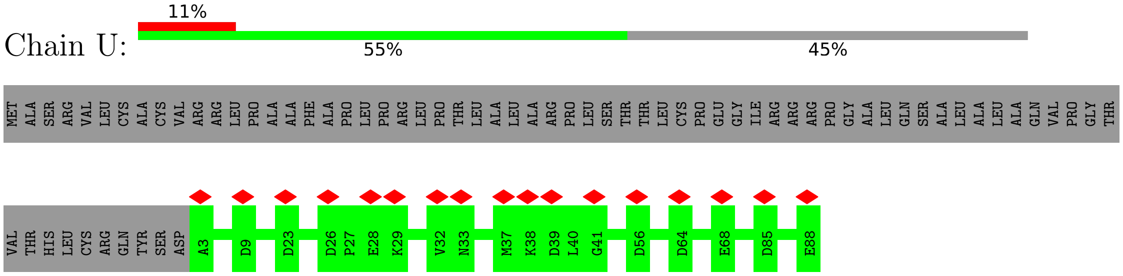


- Molecule 20: Acyl carrier protein, mitochondrial

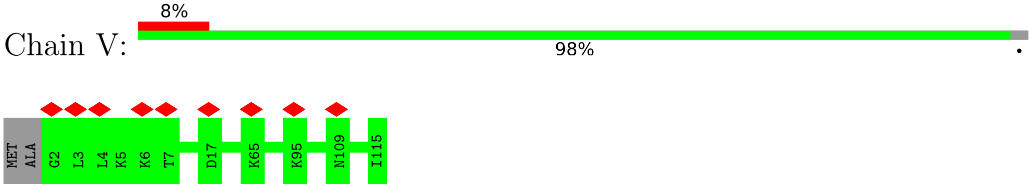




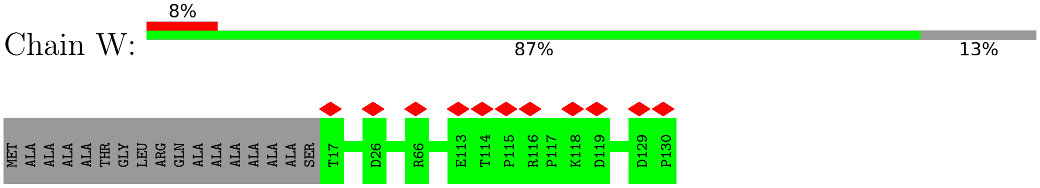
- Molecule 20: Acyl carrier protein, mitochondrial



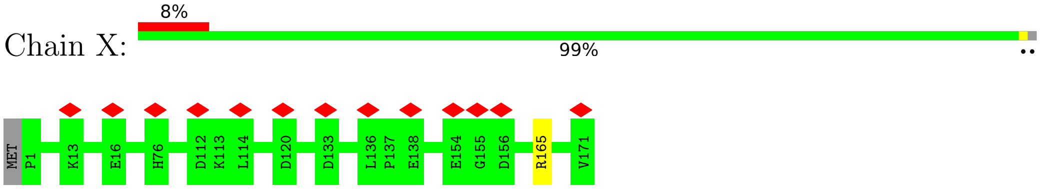
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



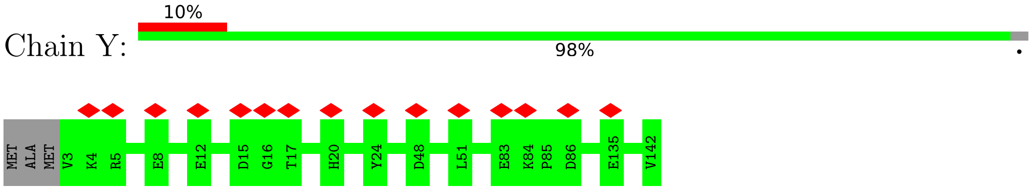
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



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

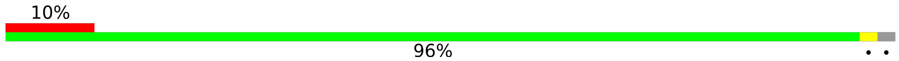


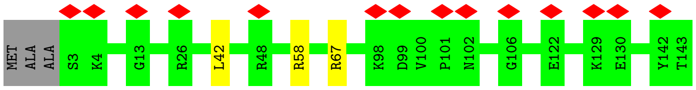
- Molecule 24: MCG5603



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

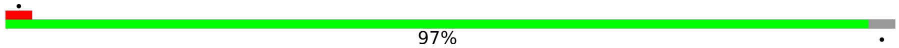
Chain Z:

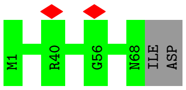




- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

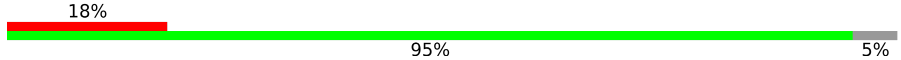
Chain a:

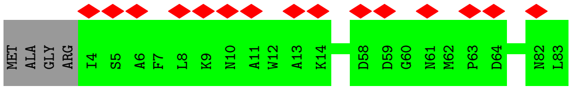




- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

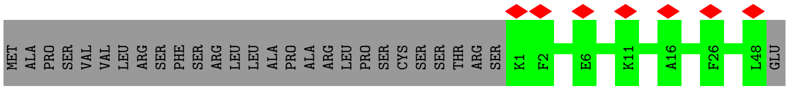
Chain b:





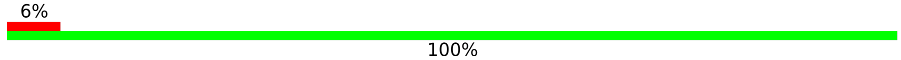
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

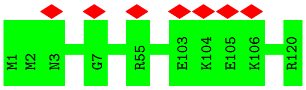
Chain c:



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

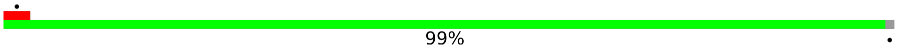
Chain d:

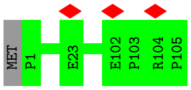




- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

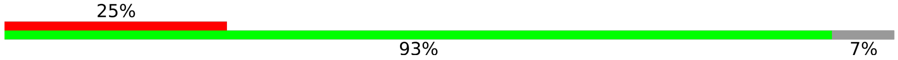
Chain e:

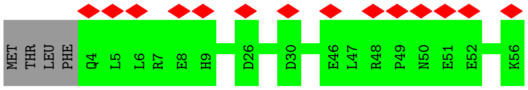




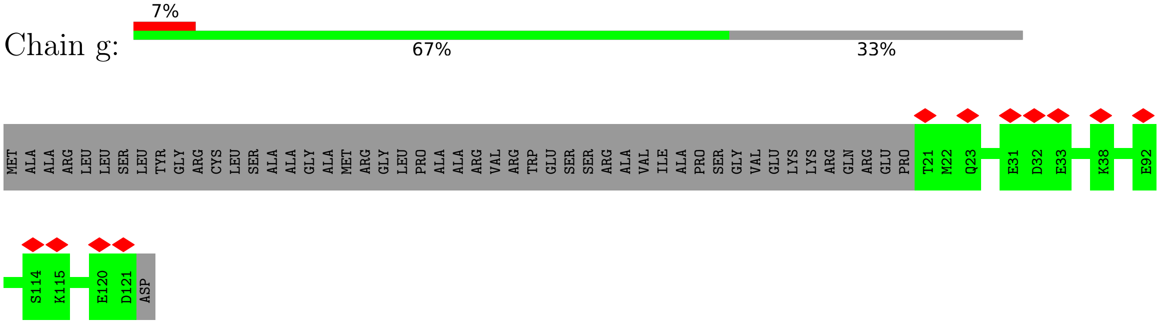
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:

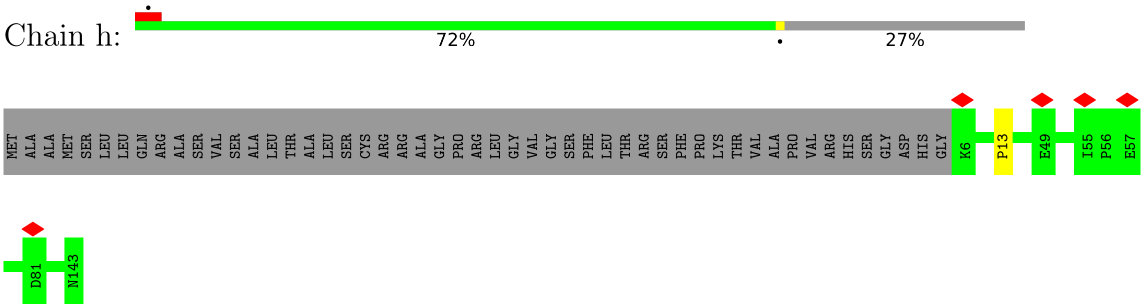




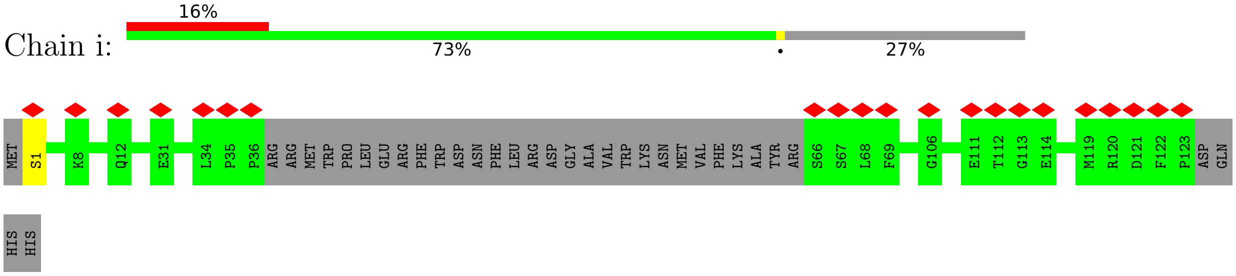
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



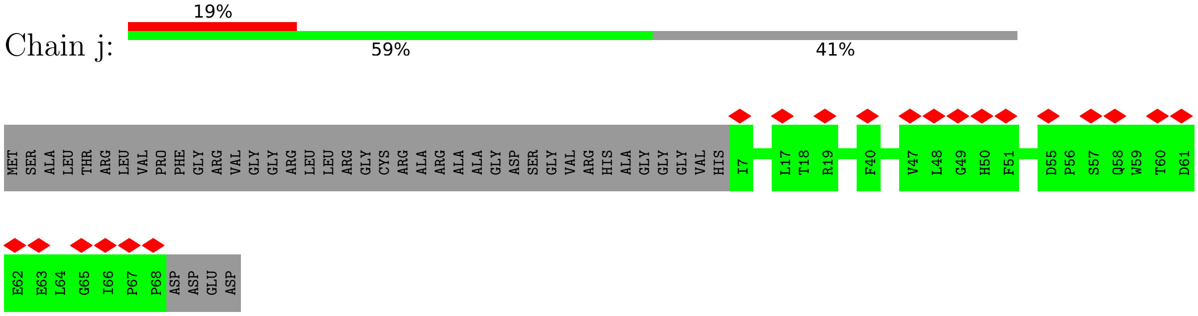
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



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

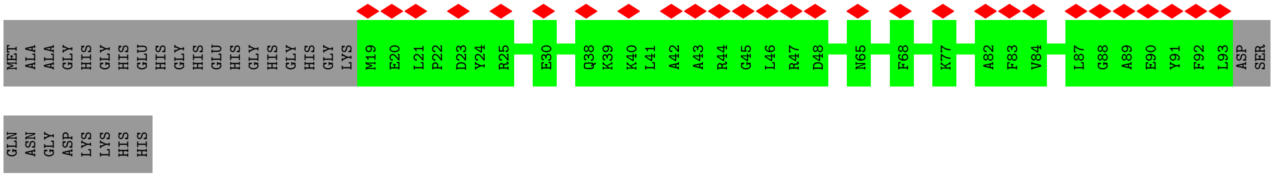


- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



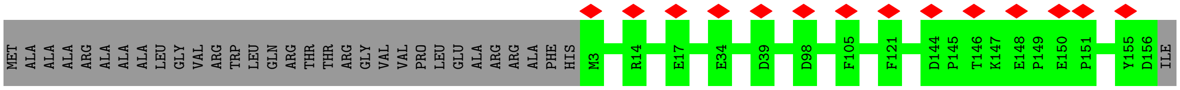
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



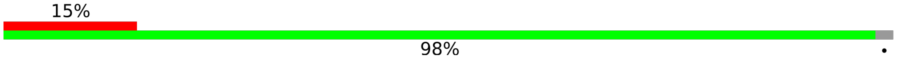
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

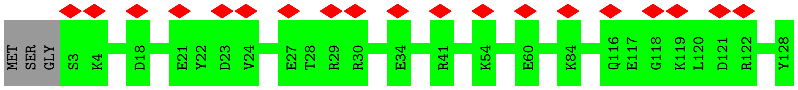
Chain l:



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

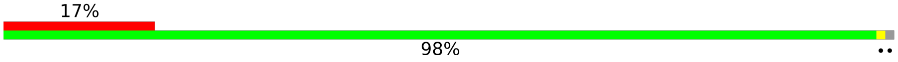
Chain m:

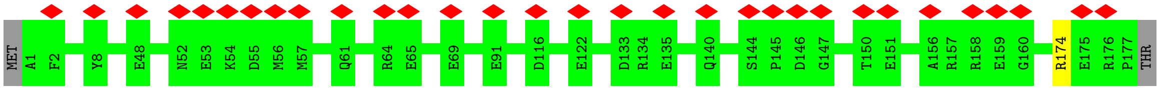




- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

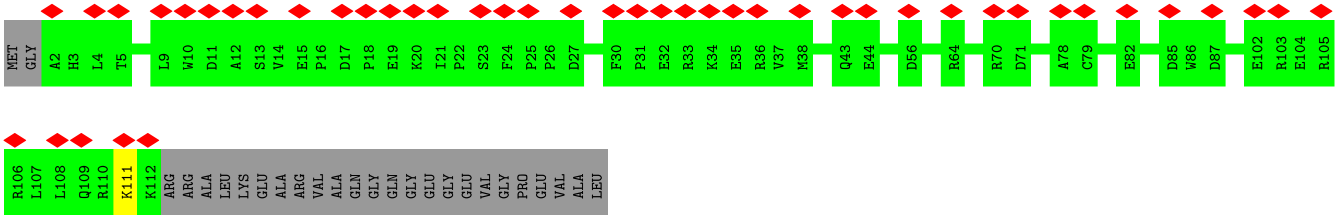
Chain n:





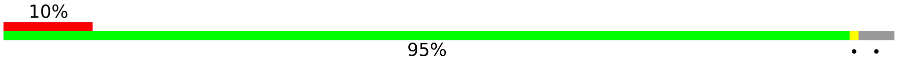
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

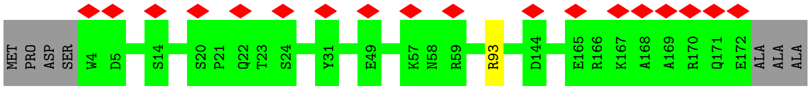
Chain o:



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

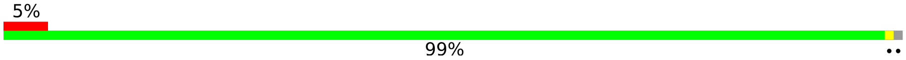
Chain p:

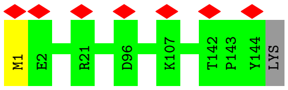




- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

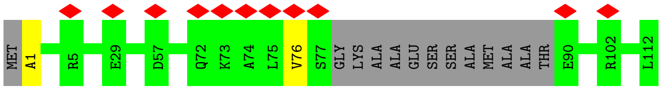
Chain q:





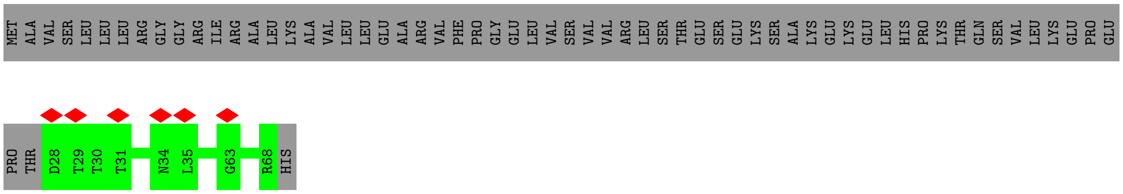
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:



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

Chain s:



4 Experimental information

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27193	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 $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	2200	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	47600	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.137	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0241	Depositor
Map size (Å)	472.49997, 472.49997, 472.49997	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.44	0/949	0.61	0/1297
2	B	0.59	0/1278	0.66	0/1730
3	C	0.54	0/1771	0.66	0/2412
4	D	0.54	0/3540	0.62	0/4795
5	E	0.40	0/1688	0.59	0/2300
6	F	0.41	0/3374	0.61	0/4557
7	G	0.45	0/5383	0.62	0/7293
8	H	0.50	0/2607	0.62	1/3564 (0.0%)
9	I	0.57	0/1461	0.65	0/1974
10	J	0.46	0/1322	0.58	0/1799
11	K	0.45	0/738	0.56	0/1002
12	L	0.42	0/4913	0.58	0/6686
13	M	0.44	0/3709	0.59	1/5052 (0.0%)
14	N	0.45	0/2748	0.61	3/3741 (0.1%)
15	O	0.47	0/2674	0.57	0/3626
16	P	0.45	0/2823	0.63	0/3828
17	Q	0.46	0/1038	0.60	0/1401
18	R	0.47	0/751	0.60	0/1011
19	S	0.38	0/678	0.67	0/915
20	T	0.35	0/620	0.53	0/836
20	U	0.38	0/704	0.51	0/951
21	V	0.42	0/949	0.57	0/1286
22	W	0.43	0/993	0.61	0/1335
23	X	0.42	0/1434	0.59	0/1937
24	Y	0.38	0/1061	0.56	0/1439
25	Z	0.44	0/1198	0.62	1/1616 (0.1%)
26	a	0.49	0/569	0.59	0/766
27	b	0.42	0/651	0.49	0/895
28	c	0.40	0/409	0.54	0/555
29	d	0.46	0/1028	0.59	0/1387
30	e	0.39	0/900	0.63	0/1199
31	f	0.38	0/468	0.59	0/630

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	g	0.45	0/878	0.56	0/1196
33	h	0.45	0/1197	0.60	0/1621
34	i	0.40	0/804	0.61	0/1094
35	j	0.36	0/561	0.54	0/768
36	k	0.36	0/629	0.52	0/851
37	l	0.44	0/1348	0.55	0/1840
38	m	0.42	0/1079	0.61	0/1463
39	n	0.40	0/1589	0.60	1/2152 (0.0%)
40	o	0.35	0/982	0.57	0/1320
41	p	0.42	0/1466	0.60	1/1981 (0.1%)
42	q	0.49	0/1234	0.59	0/1681
43	r	0.44	0/812	0.68	1/1098 (0.1%)
44	s	0.37	0/353	0.56	0/479
All	All	0.45	0/67361	0.60	9/91359 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	r	76	VAL	CG1-CB-CG2	6.99	122.09	110.90
14	N	254	LEU	CB-CG-CD2	6.74	122.47	111.00
14	N	15	LEU	CB-CG-CD2	6.13	121.42	111.00
25	Z	58	ARG	NE-CZ-NH1	5.60	123.10	120.30
13	M	77	LEU	CA-CB-CG	5.55	128.07	115.30
8	H	117	LEU	CA-CB-CG	5.39	127.69	115.30
14	N	15	LEU	CB-CG-CD1	5.08	119.64	111.00
41	p	93	ARG	NE-CZ-NH1	5.04	122.82	120.30
39	n	174	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	105 (93%)	8 (7%)	0	100	100
2	B	154/224 (69%)	141 (92%)	13 (8%)	0	100	100
3	C	205/263 (78%)	191 (93%)	14 (7%)	0	100	100
4	D	427/463 (92%)	399 (93%)	28 (7%)	0	100	100
5	E	210/248 (85%)	194 (92%)	16 (8%)	0	100	100
6	F	426/464 (92%)	383 (90%)	43 (10%)	0	100	100
7	G	686/727 (94%)	633 (92%)	53 (8%)	0	100	100
8	H	316/318 (99%)	291 (92%)	24 (8%)	1 (0%)	41	76
9	I	176/212 (83%)	166 (94%)	10 (6%)	0	100	100
10	J	169/172 (98%)	153 (90%)	16 (10%)	0	100	100
11	K	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
12	L	604/607 (100%)	555 (92%)	49 (8%)	0	100	100
13	M	457/459 (100%)	434 (95%)	22 (5%)	1 (0%)	47	82
14	N	342/345 (99%)	320 (94%)	22 (6%)	0	100	100
15	O	318/355 (90%)	283 (89%)	35 (11%)	0	100	100
16	P	340/377 (90%)	303 (89%)	37 (11%)	0	100	100
17	Q	123/175 (70%)	114 (93%)	9 (7%)	0	100	100
18	R	92/116 (79%)	86 (94%)	6 (6%)	0	100	100
19	S	81/99 (82%)	73 (90%)	8 (10%)	0	100	100
20	T	74/156 (47%)	63 (85%)	11 (15%)	0	100	100
20	U	84/156 (54%)	79 (94%)	5 (6%)	0	100	100
21	V	112/116 (97%)	106 (95%)	6 (5%)	0	100	100
22	W	112/131 (86%)	106 (95%)	6 (5%)	0	100	100
23	X	169/172 (98%)	156 (92%)	13 (8%)	0	100	100
24	Y	138/143 (96%)	132 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Z	139/144 (96%)	129 (93%)	10 (7%)	0	100	100
26	a	66/70 (94%)	61 (92%)	5 (8%)	0	100	100
27	b	78/84 (93%)	70 (90%)	8 (10%)	0	100	100
28	c	46/76 (60%)	45 (98%)	1 (2%)	0	100	100
29	d	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
30	e	103/106 (97%)	93 (90%)	10 (10%)	0	100	100
31	f	51/57 (90%)	45 (88%)	6 (12%)	0	100	100
32	g	99/151 (66%)	89 (90%)	10 (10%)	0	100	100
33	h	136/189 (72%)	123 (90%)	12 (9%)	1 (1%)	22	60
34	i	90/128 (70%)	85 (94%)	5 (6%)	0	100	100
35	j	60/105 (57%)	54 (90%)	6 (10%)	0	100	100
36	k	73/104 (70%)	69 (94%)	4 (6%)	0	100	100
37	l	152/186 (82%)	135 (89%)	17 (11%)	0	100	100
38	m	124/129 (96%)	115 (93%)	9 (7%)	0	100	100
39	n	175/179 (98%)	162 (93%)	13 (7%)	0	100	100
40	o	109/137 (80%)	101 (93%)	8 (7%)	0	100	100
41	p	167/176 (95%)	155 (93%)	12 (7%)	0	100	100
42	q	142/145 (98%)	128 (90%)	14 (10%)	0	100	100
43	r	96/113 (85%)	82 (85%)	14 (15%)	0	100	100
44	s	39/104 (38%)	35 (90%)	4 (10%)	0	100	100
All	All	8087/9214 (88%)	7445 (92%)	639 (8%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	h	13	PRO
13	M	224	PRO
8	H	218	GLY

5.3.2 Protein sidechains ⓘ

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%)	131 (99%)	1 (1%)	81	93
3	C	189/227 (83%)	188 (100%)	1 (0%)	88	96
4	D	370/394 (94%)	369 (100%)	1 (0%)	92	97
5	E	183/206 (89%)	183 (100%)	0	100	100
6	F	343/370 (93%)	341 (99%)	2 (1%)	86	95
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%)	546 (100%)	2 (0%)	91	97
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	97
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%)	73 (99%)	1 (1%)	67	88
20	T	70/135 (52%)	70 (100%)	0	100	100
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%)	152 (99%)	1 (1%)	84	94
24	Y	105/107 (98%)	105 (100%)	0	100	100
25	Z	122/123 (99%)	120 (98%)	2 (2%)	62	86
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	92 (100%)	0	100	100
33	h	123/162 (76%)	123 (100%)	0	100	100
34	i	88/119 (74%)	88 (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%)	162 (100%)	0	100	100
40	o	104/121 (86%)	103 (99%)	1 (1%)	76	91
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%)	89 (100%)	0	100	100
44	s	40/95 (42%)	40 (100%)	0	100	100
All	All	7176/7947 (90%)	7163 (100%)	13 (0%)	93	98

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	64	CYS
3	C	79	THR
4	D	356	TYR
6	F	359	CYS
6	F	405	CYS
12	L	109	HIS
12	L	436	ARG
15	O	213	LYS
19	S	39	ARG
23	X	165	ARG
25	Z	42	LEU
25	Z	67	ARG
40	o	111	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	116	GLN
4	D	237	ASN
4	D	252	ASN
6	F	165	ASN
6	F	283	HIS
6	F	293	ASN
8	H	169	GLN
9	I	67	HIS
12	L	269	ASN
12	L	452	ASN
13	M	26	ASN
14	N	223	ASN
15	O	251	GLN
20	T	35	HIS
28	c	46	ASN
30	e	96	HIS
41	p	99	GLN
41	p	139	GLN
43	r	24	GLN
44	s	34	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

11 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	$\#\|Z\| > 2$
4	2MR	D	85	4	10,12,13	2.43	3 (30%)	5,13,15	2.90	2 (40%)
43	AYA	r	1	43	6,7,8	1.80	1 (16%)	5,8,10	1.07	0
8	FME	H	1	8	8,9,10	0.90	0	7,9,11	1.80	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
34	SAC	i	1	34	7,8,9	0.59	0	8,9,11	1.12	1 (12%)
1	FME	A	1	1	8,9,10	0.98	0	7,9,11	0.87	0
14	FME	N	1	14	8,9,10	0.91	0	7,9,11	1.47	1 (14%)
42	AME	q	1	42	9,10,11	1.46	1 (11%)	9,11,13	1.44	2 (22%)
12	FME	L	1	12	8,9,10	1.04	0	7,9,11	0.94	1 (14%)
11	FME	K	1	11	8,9,10	1.02	0	7,9,11	1.57	1 (14%)
13	FME	M	1	13	8,9,10	0.96	0	7,9,11	1.07	0
10	FME	J	1	10	8,9,10	0.95	0	7,9,11	0.95	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	2MR	D	85	4	-	2/10/13/15	-
43	AYA	r	1	43	-	0/4/6/8	-
8	FME	H	1	8	-	5/7/9/11	-
34	SAC	i	1	34	-	3/7/8/10	-
1	FME	A	1	1	-	3/7/9/11	-
14	FME	N	1	14	-	2/7/9/11	-
42	AME	q	1	42	-	0/9/10/12	-
12	FME	L	1	12	-	2/7/9/11	-
11	FME	K	1	11	-	3/7/9/11	-
13	FME	M	1	13	-	1/7/9/11	-
10	FME	J	1	10	-	1/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NE	5.00	1.45	1.34
4	D	85	2MR	CZ-NH2	4.42	1.43	1.33
42	q	1	AME	CT1-N	3.24	1.45	1.34
43	r	1	AYA	CT-N	3.01	1.44	1.34
4	D	85	2MR	CQ1-NH1	-2.68	1.41	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	85	2MR	NE-CZ-NH2	-4.43	115.42	119.48
4	D	85	2MR	CD-NE-CZ	4.42	131.69	123.41
8	H	1	FME	CA-N-CN	3.93	128.87	122.82
11	K	1	FME	C-CA-N	3.48	116.01	109.73
14	N	1	FME	C-CA-N	3.42	115.91	109.73
34	i	1	SAC	O-C-CA	-2.96	117.02	124.78
42	q	1	AME	CE-SD-CG	2.62	109.42	100.40
8	H	1	FME	C-CA-N	2.40	114.06	109.73
12	L	1	FME	CG-CB-CA	2.18	119.01	112.95
42	q	1	AME	O-C-CA	-2.12	119.22	124.78

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
8	H	1	FME	CB-CA-N-CN
8	H	1	FME	C-CA-CB-CG
11	K	1	FME	CB-CA-N-CN
11	K	1	FME	N-CA-CB-CG
14	N	1	FME	CB-CA-N-CN
34	i	1	SAC	CB-CA-N-C1A
10	J	1	FME	CA-CB-CG-SD
11	K	1	FME	CA-CB-CG-SD
4	D	85	2MR	NE-CD-CG-CB
8	H	1	FME	CB-CG-SD-CE
12	L	1	FME	CB-CG-SD-CE
14	N	1	FME	CB-CG-SD-CE
8	H	1	FME	N-CA-CB-CG
13	M	1	FME	CB-CG-SD-CE
4	D	85	2MR	CA-CB-CG-CD
8	H	1	FME	CA-CB-CG-SD
34	i	1	SAC	C2A-C1A-N-CA
34	i	1	SAC	OAC-C1A-N-CA
1	A	1	FME	C-CA-CB-CG
12	L	1	FME	N-CA-CB-CG
1	A	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
49	FES	G	803	7	0,4,4	-	-	-		
48	3PE	Y	401	-	40,40,50	0.97	4 (10%)	43,45,55	1.06	2 (4%)
48	3PE	l	701	-	48,48,50	0.89	3 (6%)	51,53,55	1.14	3 (5%)
48	3PE	h	202	-	36,36,50	1.01	3 (8%)	39,41,55	1.00	2 (5%)
45	SF4	B	201	2	0,12,12	-	-	-		
51	CDL	q	201	-	56,56,99	1.14	8 (14%)	62,68,111	1.08	4 (6%)
46	PC1	J	201	-	41,41,53	1.05	4 (9%)	47,49,61	1.01	2 (4%)
45	SF4	I	202	9	0,12,12	-	-	-		
45	SF4	G	802	7	0,12,12	-	-	-		
50	FMN	F	501	-	33,33,33	1.13	2 (6%)	48,50,50	1.44	9 (18%)
53	NDP	P	501	-	45,52,52	2.22	5 (11%)	53,80,80	1.67	9 (16%)
46	PC1	Z	201	-	44,44,53	1.04	4 (9%)	50,52,61	1.06	2 (4%)
51	CDL	N	401	-	58,58,99	1.02	6 (10%)	63,69,111	0.99	3 (4%)
45	SF4	F	502	6	0,12,12	-	-	-		
51	CDL	d	201	-	66,66,99	1.06	8 (12%)	72,78,111	1.10	4 (5%)
48	3PE	i	201	-	41,41,50	0.96	4 (9%)	44,46,55	1.07	2 (4%)
49	FES	E	301	5	0,4,4	-	-	-		
51	CDL	h	201	-	69,69,99	1.02	8 (11%)	75,81,111	1.06	4 (5%)
51	CDL	d	202	-	62,62,99	1.09	8 (12%)	68,74,111	1.12	5 (7%)
51	CDL	N	402	-	64,64,99	1.08	8 (12%)	70,76,111	1.06	4 (5%)
46	PC1	B	202	-	34,34,53	1.17	4 (11%)	40,42,61	1.04	2 (5%)
51	CDL	L	701	-	73,73,99	1.01	7 (9%)	79,85,111	1.11	4 (5%)
48	3PE	K	201	-	32,32,50	1.06	4 (12%)	35,37,55	1.11	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	3PE	D	502	-	50,50,50	0.88	4 (8%)	53,55,55	1.15	3 (5%)
55	EHZ	U	201	20	29,36,37	1.73	4 (13%)	35,44,47	2.36	12 (34%)
48	3PE	H	401	-	43,43,50	0.92	4 (9%)	46,48,55	1.16	2 (4%)
52	ATP	O	401	-	26,33,33	0.91	1 (3%)	31,52,52	1.67	4 (12%)
48	3PE	M	501	-	41,41,50	0.94	3 (7%)	44,46,55	1.07	2 (4%)
45	SF4	G	801	7	0,12,12	-	-	-		
46	PC1	B	203	-	42,42,53	1.07	4 (9%)	48,50,61	0.95	2 (4%)
45	SF4	I	201	9	0,12,12	-	-	-		
48	3PE	L	702	-	48,48,50	0.86	4 (8%)	51,53,55	1.05	2 (3%)
55	EHZ	T	201	20	29,36,37	1.72	6 (20%)	35,44,47	1.56	5 (14%)
47	HQH	D	501	-	29,30,30	0.89	1 (3%)	28,40,40	1.38	4 (14%)

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
49	FES	G	803	7	-	-	0/1/1/1
48	3PE	Y	401	-	-	23/44/44/54	-
48	3PE	l	701	-	-	19/52/52/54	-
48	3PE	h	202	-	-	17/40/40/54	-
45	SF4	B	201	2	-	-	0/6/5/5
51	CDL	q	201	-	-	27/67/67/110	-
46	PC1	J	201	-	-	20/45/45/57	-
45	SF4	I	202	9	-	-	0/6/5/5
45	SF4	G	802	7	-	-	0/6/5/5
50	FMN	F	501	-	-	5/18/18/18	0/3/3/3
53	NDP	P	501	-	-	6/30/77/77	0/5/5/5
46	PC1	Z	201	-	-	19/48/48/57	-
51	CDL	N	401	-	-	32/67/67/110	-
45	SF4	F	502	6	-	-	0/6/5/5
51	CDL	d	201	-	-	33/77/77/110	-
48	3PE	i	201	-	-	18/45/45/54	-
49	FES	E	301	5	-	-	0/1/1/1
51	CDL	h	201	-	-	29/80/80/110	-
51	CDL	d	202	-	-	31/73/73/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	CDL	N	402	-	-	36/75/75/110	-
46	PC1	B	202	-	-	11/38/38/57	-
51	CDL	L	701	-	-	34/84/84/110	-
48	3PE	K	201	-	-	19/36/36/54	-
48	3PE	D	502	-	-	22/54/54/54	-
55	EHZ	U	201	20	-	13/42/44/45	-
48	3PE	H	401	-	-	19/47/47/54	-
52	ATP	O	401	-	-	5/18/38/38	0/3/3/3
48	3PE	M	501	-	-	19/45/45/54	-
45	SF4	G	801	7	-	-	0/6/5/5
46	PC1	B	203	-	-	18/46/46/57	-
45	SF4	I	201	9	-	-	0/6/5/5
48	3PE	L	702	-	-	23/52/52/54	-
55	EHZ	T	201	20	-	16/42/44/45	-
47	HQH	D	501	-	-	10/27/29/29	0/1/1/1

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	P	501	NDP	P2B-O2B	12.11	1.82	1.59
55	U	201	EHZ	C15-N2	5.91	1.46	1.33
55	T	201	EHZ	C15-N2	5.66	1.46	1.33
55	T	201	EHZ	C12-N1	5.17	1.45	1.33
55	U	201	EHZ	C12-N1	4.99	1.44	1.33
53	P	501	NDP	PN-O5D	4.04	1.75	1.59
53	P	501	NDP	O2B-C2B	-3.21	1.32	1.44
50	F	501	FMN	C4A-N5	3.18	1.36	1.30
47	D	501	HQH	C12-C19	3.08	1.41	1.37
48	l	701	3PE	O21-C2	-2.72	1.39	1.46
48	D	502	3PE	O31-C3	-2.70	1.39	1.45
51	L	701	CDL	OB6-CB4	-2.69	1.39	1.46
48	M	501	3PE	O21-C2	-2.69	1.39	1.46
46	B	203	PC1	O21-C2	-2.67	1.39	1.46
48	h	202	3PE	O21-C2	-2.64	1.40	1.46
48	L	702	3PE	O21-C2	-2.63	1.40	1.46
51	N	402	CDL	OA6-CA4	-2.63	1.40	1.46
55	U	201	EHZ	O4-C15	-2.59	1.18	1.23
48	i	201	3PE	O21-C2	-2.55	1.40	1.46
48	i	201	3PE	O31-C31	2.55	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	M	501	3PE	O31-C3	-2.54	1.39	1.45
51	N	401	CDL	OB8-CB7	2.53	1.40	1.33
48	H	401	3PE	O31-C3	-2.51	1.39	1.45
55	U	201	EHZ	O3-C12	-2.51	1.18	1.23
46	Z	201	PC1	O21-C21	2.51	1.41	1.34
51	h	201	CDL	OB6-CB4	-2.49	1.40	1.46
46	B	202	PC1	O21-C2	-2.48	1.40	1.46
51	N	402	CDL	OB6-CB4	-2.48	1.40	1.46
51	h	201	CDL	OA6-CA4	-2.48	1.40	1.46
51	d	201	CDL	OB8-CB7	2.47	1.40	1.33
51	q	201	CDL	OB6-CB4	-2.47	1.40	1.46
48	D	502	3PE	O21-C2	-2.47	1.40	1.46
51	q	201	CDL	OB8-CB7	2.46	1.40	1.33
48	K	201	3PE	O21-C2	-2.46	1.40	1.46
48	h	202	3PE	O31-C31	2.46	1.40	1.33
51	L	701	CDL	OA8-CA7	2.45	1.40	1.33
46	B	203	PC1	O31-C31	2.45	1.40	1.33
48	K	201	3PE	O31-C3	-2.45	1.39	1.45
51	N	401	CDL	OA8-CA7	2.44	1.40	1.33
51	N	402	CDL	OB8-CB7	2.44	1.40	1.33
51	q	201	CDL	OA8-CA6	-2.43	1.39	1.45
46	Z	201	PC1	O31-C31	2.42	1.40	1.33
51	N	402	CDL	OA8-CA7	2.42	1.40	1.33
48	l	701	3PE	O31-C3	-2.42	1.39	1.45
51	d	202	CDL	OB8-CB7	2.40	1.40	1.33
51	d	201	CDL	OA6-CA4	-2.40	1.40	1.46
51	d	202	CDL	OA8-CA7	2.39	1.40	1.33
48	Y	401	3PE	O31-C31	2.39	1.40	1.33
55	T	201	EHZ	C9-S1	2.39	1.81	1.76
46	J	201	PC1	O31-C31	2.39	1.40	1.33
51	h	201	CDL	OB8-CB7	2.38	1.40	1.33
55	T	201	EHZ	O4-C15	-2.38	1.18	1.23
51	d	202	CDL	OB6-CB4	-2.38	1.40	1.46
53	P	501	NDP	O4B-C4B	-2.37	1.39	1.45
46	B	202	PC1	O31-C31	2.37	1.40	1.33
48	H	401	3PE	O31-C31	2.37	1.40	1.33
51	L	701	CDL	OB8-CB7	2.36	1.40	1.33
51	d	202	CDL	OA6-CA4	-2.35	1.40	1.46
51	h	201	CDL	OA8-CA7	2.35	1.40	1.33
48	Y	401	3PE	O21-C2	-2.35	1.40	1.46
51	d	201	CDL	OA8-CA7	2.34	1.40	1.33
48	D	502	3PE	O21-C21	2.34	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	J	201	PC1	O21-C2	-2.32	1.40	1.46
51	d	201	CDL	OB6-CB4	-2.31	1.40	1.46
46	J	201	PC1	O21-C21	2.30	1.40	1.34
51	q	201	CDL	OA8-CA7	2.29	1.40	1.33
51	d	202	CDL	OB6-CB5	2.28	1.40	1.34
48	Y	401	3PE	O31-C3	-2.28	1.39	1.45
51	L	701	CDL	OA6-CA4	-2.28	1.40	1.46
48	K	201	3PE	O31-C31	2.28	1.40	1.33
48	Y	401	3PE	O21-C21	2.28	1.40	1.34
51	q	201	CDL	OA6-CA4	-2.27	1.40	1.46
48	H	401	3PE	O21-C21	2.27	1.40	1.34
48	L	702	3PE	O31-C31	2.27	1.40	1.33
51	d	201	CDL	OA8-CA6	-2.26	1.40	1.45
51	N	401	CDL	OB6-CB4	-2.26	1.40	1.46
51	N	402	CDL	OB6-CB5	2.25	1.40	1.34
51	L	701	CDL	OB8-CB6	-2.24	1.40	1.45
51	q	201	CDL	OB6-CB5	2.23	1.40	1.34
55	T	201	EHZ	O3-C12	-2.22	1.18	1.23
51	h	201	CDL	OB8-CB6	-2.21	1.40	1.45
46	B	202	PC1	O21-C21	2.21	1.40	1.34
46	Z	201	PC1	O31-C3	-2.21	1.40	1.45
51	q	201	CDL	OA6-CA5	2.20	1.40	1.34
48	i	201	3PE	O21-C21	2.20	1.40	1.34
46	J	201	PC1	O31-C3	-2.19	1.40	1.45
51	N	401	CDL	OB6-CB5	2.19	1.40	1.34
50	F	501	FMN	C10-N1	2.19	1.37	1.33
51	L	701	CDL	OA8-CA6	-2.19	1.40	1.45
51	d	202	CDL	OA8-CA6	-2.18	1.40	1.45
51	N	402	CDL	OA8-CA6	-2.18	1.40	1.45
51	q	201	CDL	OB8-CB6	-2.18	1.40	1.45
51	d	202	CDL	OA6-CA5	2.18	1.40	1.34
51	d	202	CDL	OB8-CB6	-2.18	1.40	1.45
48	K	201	3PE	O21-C21	2.18	1.40	1.34
48	l	701	3PE	O31-C31	2.17	1.39	1.33
48	L	702	3PE	O31-C3	-2.17	1.40	1.45
51	d	201	CDL	OB8-CB6	-2.16	1.40	1.45
51	h	201	CDL	OB6-CB5	2.16	1.40	1.34
48	h	202	3PE	O31-C3	-2.15	1.40	1.45
51	N	401	CDL	OA8-CA6	-2.15	1.40	1.45
51	h	201	CDL	OA6-CA5	2.14	1.40	1.34
46	B	202	PC1	O31-C3	-2.14	1.40	1.45
52	O	401	ATP	C5-C4	2.13	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	d	201	CDL	OA6-CA5	2.12	1.40	1.34
51	N	402	CDL	OB8-CB6	-2.12	1.40	1.45
51	N	401	CDL	OB8-CB6	-2.11	1.40	1.45
51	d	201	CDL	OB6-CB5	2.11	1.40	1.34
46	Z	201	PC1	O21-C2	-2.10	1.41	1.46
46	B	203	PC1	O21-C21	2.09	1.40	1.34
48	H	401	3PE	O21-C2	-2.09	1.41	1.46
48	M	501	3PE	O31-C31	2.09	1.39	1.33
51	L	701	CDL	OA6-CA5	2.08	1.40	1.34
55	T	201	EHZ	O6-C20	-2.08	1.39	1.44
51	N	402	CDL	OA6-CA5	2.08	1.40	1.34
51	h	201	CDL	OA8-CA6	-2.08	1.40	1.45
48	i	201	3PE	O31-C3	-2.06	1.40	1.45
53	P	501	NDP	O5D-C5D	-2.03	1.37	1.44
46	B	203	PC1	O31-C3	-2.02	1.40	1.45
48	L	702	3PE	O21-C21	2.02	1.40	1.34
48	D	502	3PE	O31-C31	2.01	1.39	1.33

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	-7.11	108.41	132.83
55	U	201	EHZ	C16-C15-N2	6.03	128.58	116.58
55	T	201	EHZ	C8-C9-S1	5.86	120.88	113.63
48	l	701	3PE	O21-C21-C22	5.01	122.30	111.50
55	U	201	EHZ	O4-C15-N2	-4.69	112.93	122.99
48	i	201	3PE	O21-C21-C22	4.51	121.22	111.50
46	Z	201	PC1	O21-C21-C22	4.39	120.95	111.50
52	O	401	ATP	PA-O3A-PB	-4.31	118.03	132.83
48	H	401	3PE	O21-C21-C22	4.17	120.49	111.50
55	U	201	EHZ	C13-C12-N1	4.16	123.43	116.42
51	d	201	CDL	OB6-CB5-C51	4.13	120.39	111.50
51	N	402	CDL	OA6-CA5-C11	4.12	120.37	111.50
46	B	202	PC1	O21-C21-C22	4.11	120.37	111.50
48	D	502	3PE	O21-C21-C22	4.08	120.28	111.50
48	Y	401	3PE	O21-C21-C22	4.06	120.26	111.50
46	J	201	PC1	O21-C21-C22	4.01	120.14	111.50
55	U	201	EHZ	C11-N1-C12	-3.98	115.44	122.84
50	F	501	FMN	C4-N3-C2	-3.96	118.32	125.64
48	K	201	3PE	O21-C21-C22	3.93	119.97	111.50
52	O	401	ATP	PB-O3B-PG	-3.93	119.34	132.83
51	h	201	CDL	OA6-CA5-C11	3.90	119.92	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	U	201	EHZ	C14-N2-C15	3.88	129.50	122.59
51	h	201	CDL	OB6-CB5-C51	3.84	119.77	111.50
51	d	201	CDL	OA6-CA5-C11	3.83	119.75	111.50
52	O	401	ATP	N3-C2-N1	-3.79	122.75	128.68
51	N	401	CDL	OB6-CB5-C51	3.75	119.58	111.50
55	U	201	EHZ	C14-C13-C12	-3.74	106.12	112.36
51	L	701	CDL	OB6-CB5-C51	3.73	119.53	111.50
51	d	202	CDL	OB6-CB5-C51	3.69	119.44	111.50
51	d	202	CDL	OA6-CA5-C11	3.67	119.41	111.50
55	U	201	EHZ	C8-C9-S1	3.65	118.15	113.63
48	h	202	3PE	O21-C21-C22	3.65	119.37	111.50
51	L	701	CDL	OA6-CA5-C11	3.64	119.35	111.50
48	M	501	3PE	O21-C21-C22	3.63	119.31	111.50
48	L	702	3PE	O21-C21-C22	3.54	119.12	111.50
51	q	201	CDL	OA6-CA5-C11	3.51	119.06	111.50
55	U	201	EHZ	C10-S1-C9	3.44	112.58	101.87
46	B	203	PC1	O21-C21-C22	3.42	118.87	111.50
51	q	201	CDL	OB6-CB5-C51	3.38	118.78	111.50
50	F	501	FMN	C4A-C10-N10	3.35	121.38	116.48
47	D	501	HQH	O2-C24-N5	3.31	123.44	113.49
53	P	501	NDP	O2B-P2B-O1X	-3.31	96.62	109.39
55	U	201	EHZ	C19-C17-C16	3.26	114.48	108.82
51	N	402	CDL	OB6-CB5-C51	3.19	118.39	111.50
47	D	501	HQH	O3-C25-C23	3.13	127.13	116.56
48	H	401	3PE	O31-C31-C32	3.10	121.64	111.91
50	F	501	FMN	C4A-C4-N3	3.09	121.04	113.19
50	F	501	FMN	O4-C4-C4A	-2.93	118.84	126.60
50	F	501	FMN	C4A-C10-N1	-2.86	118.09	124.73
51	L	701	CDL	OB8-CB7-C71	2.83	120.80	111.91
51	d	202	CDL	OA8-CA7-C31	2.81	120.73	111.91
53	P	501	NDP	PA-O5B-C5B	-2.79	105.30	121.68
51	N	401	CDL	OB8-CB7-C71	2.77	120.59	111.91
46	J	201	PC1	O31-C31-C32	2.73	120.47	111.91
51	q	201	CDL	OA8-CA7-C31	2.73	120.47	111.91
51	d	201	CDL	OA8-CA7-C31	2.72	120.45	111.91
51	L	701	CDL	OA8-CA7-C31	2.72	120.45	111.91
48	h	202	3PE	O31-C31-C32	2.72	120.44	111.91
51	N	402	CDL	OA8-CA7-C31	2.68	120.33	111.91
53	P	501	NDP	O4B-C4B-C3B	2.65	110.37	105.11
51	d	201	CDL	OB8-CB7-C71	2.65	120.22	111.91
47	D	501	HQH	C21-C18-C11	2.65	129.90	125.89
51	h	201	CDL	OB8-CB7-C71	2.63	120.17	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	Z	201	PC1	O31-C31-C32	2.63	120.16	111.91
53	P	501	NDP	C2A-N1A-C6A	-2.58	114.34	118.75
48	Y	401	3PE	O31-C31-C32	2.57	119.98	111.91
51	N	401	CDL	OA8-CA7-C31	2.56	119.95	111.91
53	P	501	NDP	O3X-P2B-O2X	2.53	117.30	107.64
51	d	202	CDL	OB8-CB7-C71	2.52	119.83	111.91
46	B	202	PC1	O31-C31-C32	2.52	119.82	111.91
55	U	201	EHZ	O3-C12-N1	-2.51	118.27	123.01
48	l	701	3PE	O31-C31-C32	2.51	119.79	111.91
51	d	202	CDL	CA6-CA4-CA3	-2.50	105.88	111.79
48	M	501	3PE	O31-C31-C32	2.48	119.71	111.91
48	L	702	3PE	O31-C31-C32	2.48	119.69	111.91
53	P	501	NDP	PN-O5D-C5D	-2.45	107.32	121.68
50	F	501	FMN	C1'-N10-C9A	2.44	124.59	120.51
48	l	701	3PE	O21-C21-O22	-2.44	117.81	123.70
55	T	201	EHZ	O2-C9-S1	-2.43	119.45	122.61
46	B	203	PC1	O31-C31-C32	2.43	119.52	111.91
51	q	201	CDL	OB8-CB7-C71	2.41	119.48	111.91
51	N	402	CDL	OB8-CB7-C71	2.41	119.47	111.91
48	K	201	3PE	O31-C31-C32	2.41	119.47	111.91
48	D	502	3PE	O31-C31-C32	2.40	119.43	111.91
52	O	401	ATP	C3'-C2'-C1'	2.37	104.55	100.98
51	h	201	CDL	OA8-CA7-C31	2.30	119.14	111.91
53	P	501	NDP	O2N-PN-O1N	2.24	123.31	112.24
48	D	502	3PE	C3-C2-C1	-2.22	106.53	111.79
53	P	501	NDP	O5D-PN-O1N	-2.20	100.45	109.07
50	F	501	FMN	C10-N1-C2	2.16	121.21	116.90
55	T	201	EHZ	C10-S1-C9	2.14	108.54	101.87
50	F	501	FMN	C4-C4A-C10	2.13	120.38	116.79
47	D	501	HQH	C15-C21-C18	2.10	127.45	124.18
48	i	201	3PE	O31-C31-C32	2.09	118.48	111.91
55	T	201	EHZ	C13-C12-N1	2.06	119.89	116.42
50	F	501	FMN	C10-C4A-N5	-2.04	120.53	124.86
55	U	201	EHZ	O3-C12-C13	-2.03	118.30	122.02
55	T	201	EHZ	C11-N1-C12	-2.01	119.10	122.84
55	U	201	EHZ	C7-C8-C9	-2.00	109.32	113.89

There are no chirality outliers.

All (524) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	B	202	PC1	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
46	B	202	PC1	C11-O13-P-O14
46	B	202	PC1	C11-O13-P-O11
46	B	202	PC1	C1-O11-P-O13
46	B	203	PC1	C11-O13-P-O14
46	B	203	PC1	C1-O11-P-O14
46	B	203	PC1	O13-C11-C12-N
46	J	201	PC1	O13-C11-C12-N
46	Z	201	PC1	C1-O11-P-O13
46	Z	201	PC1	O13-C11-C12-N
47	D	501	HQH	C22-C11-C18-C21
47	D	501	HQH	C8-C11-C18-C21
47	D	501	HQH	C19-C12-C13-C20
47	D	501	HQH	C6-C7-C9-C14
47	D	501	HQH	C6-C7-C9-C16
47	D	501	HQH	O1-C7-C9-C16
48	H	401	3PE	C1-O11-P-O14
48	H	401	3PE	C11-O13-P-O14
48	K	201	3PE	C1-O11-P-O14
48	K	201	3PE	C11-O13-P-O11
48	K	201	3PE	C11-O13-P-O12
48	K	201	3PE	C11-O13-P-O14
48	K	201	3PE	O13-C11-C12-N
48	L	702	3PE	C1-O11-P-O12
48	L	702	3PE	C1-O11-P-O14
48	L	702	3PE	C11-O13-P-O14
48	L	702	3PE	O13-C11-C12-N
48	M	501	3PE	C11-O13-P-O14
48	M	501	3PE	O13-C11-C12-N
48	Y	401	3PE	C1-O11-P-O14
48	Y	401	3PE	C11-O13-P-O11
48	Y	401	3PE	C11-O13-P-O12
48	Y	401	3PE	C11-O13-P-O14
48	Y	401	3PE	O13-C11-C12-N
48	h	202	3PE	C1-O11-P-O12
48	h	202	3PE	C1-O11-P-O14
48	h	202	3PE	C11-O13-P-O11
48	h	202	3PE	C11-O13-P-O12
48	h	202	3PE	C11-O13-P-O14
48	h	202	3PE	O13-C11-C12-N
48	h	202	3PE	O22-C21-O21-C2
48	i	201	3PE	O13-C11-C12-N
48	i	201	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
48	l	701	3PE	C1-O11-P-O14
48	l	701	3PE	O13-C11-C12-N
48	l	701	3PE	C22-C21-O21-C2
50	F	501	FMN	N10-C1'-C2'-O2'
50	F	501	FMN	N10-C1'-C2'-C3'
50	F	501	FMN	C5'-O5'-P-O1P
50	F	501	FMN	C5'-O5'-P-O2P
50	F	501	FMN	C5'-O5'-P-O3P
51	L	701	CDL	OB7-CB5-OB6-CB4
51	L	701	CDL	C51-CB5-OB6-CB4
51	N	401	CDL	CB2-C1-CA2-OA2
51	N	401	CDL	CB2-OB2-PB2-OB3
51	N	401	CDL	CB2-OB2-PB2-OB4
51	N	401	CDL	C51-CB5-OB6-CB4
51	N	402	CDL	C1-CA2-OA2-PA1
51	N	402	CDL	C11-CA5-OA6-CA4
51	N	402	CDL	CB2-OB2-PB2-OB4
51	N	402	CDL	CB2-OB2-PB2-OB5
51	d	201	CDL	CA2-C1-CB2-OB2
51	d	201	CDL	CA3-OA5-PA1-OA3
51	d	201	CDL	C51-CB5-OB6-CB4
51	d	202	CDL	CB2-OB2-PB2-OB3
51	h	201	CDL	O1-C1-CB2-OB2
51	h	201	CDL	CA2-C1-CB2-OB2
51	h	201	CDL	CA2-OA2-PA1-OA4
51	h	201	CDL	CA3-OA5-PA1-OA2
51	h	201	CDL	CA3-OA5-PA1-OA3
51	h	201	CDL	CA3-OA5-PA1-OA4
51	h	201	CDL	CB2-OB2-PB2-OB3
51	q	201	CDL	OB6-CB4-CB6-OB8
52	O	401	ATP	C5'-O5'-PA-O3A
53	P	501	NDP	O4D-C4D-C5D-O5D
53	P	501	NDP	O4D-C1D-N1N-C6N
55	T	201	EHZ	C6-C7-C8-C9
55	T	201	EHZ	C7-C8-C9-O2
55	T	201	EHZ	C16-C17-C20-O6
55	U	201	EHZ	O1-C7-C8-C9
55	U	201	EHZ	C6-C7-C8-C9
55	U	201	EHZ	C11-C10-S1-C9
55	U	201	EHZ	C16-C15-N2-C14
46	J	201	PC1	O32-C31-O31-C3
48	D	502	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
48	H	401	3PE	O32-C31-O31-C3
51	N	402	CDL	OA9-CA7-OA8-CA6
46	J	201	PC1	C32-C31-O31-C3
48	H	401	3PE	C32-C31-O31-C3
51	d	201	CDL	C71-CB7-OB8-CB6
51	q	201	CDL	C31-CA7-OA8-CA6
48	L	702	3PE	O32-C31-O31-C3
48	h	202	3PE	O32-C31-O31-C3
51	d	201	CDL	OA9-CA7-OA8-CA6
51	d	201	CDL	OB9-CB7-OB8-CB6
51	d	202	CDL	OA9-CA7-OA8-CA6
51	d	202	CDL	OB9-CB7-OB8-CB6
51	h	201	CDL	OB9-CB7-OB8-CB6
51	q	201	CDL	OA9-CA7-OA8-CA6
48	M	501	3PE	O22-C21-O21-C2
48	i	201	3PE	O22-C21-O21-C2
48	l	701	3PE	O22-C21-O21-C2
51	N	401	CDL	OB7-CB5-OB6-CB4
51	N	402	CDL	OA7-CA5-OA6-CA4
51	d	201	CDL	OB7-CB5-OB6-CB4
48	D	502	3PE	C32-C31-O31-C3
48	L	702	3PE	C32-C31-O31-C3
51	N	402	CDL	C31-CA7-OA8-CA6
51	d	202	CDL	C31-CA7-OA8-CA6
51	d	202	CDL	C71-CB7-OB8-CB6
51	h	201	CDL	C71-CB7-OB8-CB6
48	M	501	3PE	C22-C21-O21-C2
48	h	202	3PE	C22-C21-O21-C2
48	K	201	3PE	C32-C31-O31-C3
48	h	202	3PE	C32-C31-O31-C3
51	d	201	CDL	C31-CA7-OA8-CA6
51	N	401	CDL	O1-C1-CA2-OA2
51	d	201	CDL	O1-C1-CB2-OB2
51	q	201	CDL	O1-C1-CB2-OB2
48	Y	401	3PE	C32-C31-O31-C3
48	l	701	3PE	C32-C31-O31-C3
51	N	402	CDL	C71-CB7-OB8-CB6
48	K	201	3PE	O32-C31-O31-C3
48	l	701	3PE	O32-C31-O31-C3
55	U	201	EHZ	O4-C15-N2-C14
46	B	202	PC1	C22-C21-O21-C2
48	L	702	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
51	h	201	CDL	C11-CA5-OA6-CA4
48	h	202	3PE	C37-C38-C39-C3A
51	L	701	CDL	C71-CB7-OB8-CB6
51	N	402	CDL	OB9-CB7-OB8-CB6
48	Y	401	3PE	O32-C31-O31-C3
51	L	701	CDL	OB9-CB7-OB8-CB6
51	d	202	CDL	CB2-C1-CA2-OA2
51	h	201	CDL	OA7-CA5-OA6-CA4
46	B	203	PC1	C32-C31-O31-C3
51	N	401	CDL	C31-CA7-OA8-CA6
51	q	201	CDL	C71-CB7-OB8-CB6
51	L	701	CDL	O1-C1-CA2-OA2
46	B	203	PC1	O32-C31-O31-C3
48	H	401	3PE	C22-C21-O21-C2
51	d	201	CDL	CA5-C11-C12-C13
51	N	402	CDL	CA7-C31-C32-C33
47	D	501	HQH	C24-C25-O3-C30
46	J	201	PC1	C21-C22-C23-C24
48	i	201	3PE	C21-C22-C23-C24
48	l	701	3PE	C21-C22-C23-C24
51	d	201	CDL	CB5-C51-C52-C53
53	P	501	NDP	C3D-C4D-C5D-O5D
55	T	201	EHZ	C5-C6-C7-O1
46	B	202	PC1	O22-C21-O21-C2
48	L	702	3PE	O22-C21-O21-C2
51	d	202	CDL	CA7-C31-C32-C33
51	N	401	CDL	OA9-CA7-OA8-CA6
51	q	201	CDL	OB9-CB7-OB8-CB6
51	N	401	CDL	OA5-CA3-CA4-OA6
51	h	201	CDL	CB7-C71-C72-C73
48	h	202	3PE	C34-C35-C36-C37
46	B	203	PC1	C11-O13-P-O11
48	H	401	3PE	C11-O13-P-O11
48	L	702	3PE	C1-O11-P-O13
48	L	702	3PE	C11-O13-P-O11
48	M	501	3PE	C1-O11-P-O13
48	h	202	3PE	C1-O11-P-O13
51	N	401	CDL	CB2-OB2-PB2-OB5
51	N	401	CDL	CB3-OB5-PB2-OB2
51	d	201	CDL	CA3-OA5-PA1-OA2
51	d	201	CDL	CB2-OB2-PB2-OB5
51	h	201	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
51	h	201	CDL	CB2-OB2-PB2-OB5
51	N	401	CDL	C71-CB7-OB8-CB6
51	L	701	CDL	CB2-C1-CA2-OA2
51	N	401	CDL	OA5-CA3-CA4-CA6
51	q	201	CDL	CA2-C1-CB2-OB2
48	H	401	3PE	O22-C21-O21-C2
48	M	501	3PE	C32-C31-O31-C3
48	M	501	3PE	C36-C37-C38-C39
51	N	401	CDL	C31-C32-C33-C34
48	D	502	3PE	C28-C29-C2A-C2B
48	h	202	3PE	C25-C26-C27-C28
46	J	201	PC1	C27-C28-C29-C2A
48	i	201	3PE	C22-C23-C24-C25
51	q	201	CDL	C31-C32-C33-C34
48	H	401	3PE	C34-C35-C36-C37
48	Y	401	3PE	C33-C34-C35-C36
51	d	201	CDL	C31-C32-C33-C34
51	h	201	CDL	C18-C19-C20-C21
46	B	202	PC1	C2-C1-O11-P
51	N	402	CDL	C79-C80-C81-C82
51	d	202	CDL	O1-C1-CA2-OA2
51	q	201	CDL	C15-C16-C17-C18
46	B	203	PC1	C22-C23-C24-C25
48	l	701	3PE	C22-C23-C24-C25
51	h	201	CDL	C51-C52-C53-C54
48	M	501	3PE	C22-C23-C24-C25
51	L	701	CDL	C52-C53-C54-C55
46	B	203	PC1	C3B-C3C-C3D-C3E
46	Z	201	PC1	C2C-C2D-C2E-C2F
51	L	701	CDL	OA7-CA5-OA6-CA4
51	L	701	CDL	C11-CA5-OA6-CA4
51	N	402	CDL	C83-C84-C85-C86
46	B	202	PC1	C21-C22-C23-C24
48	D	502	3PE	C21-C22-C23-C24
48	K	201	3PE	C31-C32-C33-C34
48	l	701	3PE	C39-C3A-C3B-C3C
48	l	701	3PE	C3B-C3C-C3D-C3E
51	d	202	CDL	CA5-C11-C12-C13
51	N	401	CDL	OB9-CB7-OB8-CB6
46	Z	201	PC1	C29-C2A-C2B-C2C
48	Y	401	3PE	C37-C38-C39-C3A
48	l	701	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
51	N	401	CDL	C54-C55-C56-C57
48	H	401	3PE	C39-C3A-C3B-C3C
48	L	702	3PE	C38-C39-C3A-C3B
48	M	501	3PE	C3D-C3E-C3F-C3G
51	N	402	CDL	C52-C53-C54-C55
51	L	701	CDL	CB3-CB4-CB6-OB8
46	B	203	PC1	C22-C21-O21-C2
51	d	201	CDL	C56-C57-C58-C59
51	d	201	CDL	C59-C60-C61-C62
48	M	501	3PE	O32-C31-O31-C3
51	h	201	CDL	CA5-C11-C12-C13
51	N	402	CDL	O1-C1-CA2-OA2
48	L	702	3PE	C32-C33-C34-C35
48	K	201	3PE	C23-C24-C25-C26
46	Z	201	PC1	C27-C28-C29-C2A
46	B	203	PC1	C35-C36-C37-C38
51	L	701	CDL	C74-C75-C76-C77
51	d	202	CDL	C11-CA5-OA6-CA4
46	J	201	PC1	C24-C25-C26-C27
46	B	203	PC1	O22-C21-O21-C2
48	D	502	3PE	O22-C21-O21-C2
55	U	201	EHZ	C2-C3-C4-C5
51	h	201	CDL	CB5-C51-C52-C53
51	L	701	CDL	C78-C79-C80-C81
51	L	701	CDL	C36-C37-C38-C39
55	U	201	EHZ	C3-C4-C5-C6
48	D	502	3PE	C22-C21-O21-C2
48	Y	401	3PE	C22-C21-O21-C2
51	q	201	CDL	C51-CB5-OB6-CB4
48	D	502	3PE	O11-C1-C2-O21
51	L	701	CDL	OA5-CA3-CA4-OA6
48	Y	401	3PE	O22-C21-O21-C2
46	J	201	PC1	O21-C2-C3-O31
48	Y	401	3PE	O21-C2-C3-O31
51	L	701	CDL	OB6-CB4-CB6-OB8
48	L	702	3PE	C34-C35-C36-C37
51	d	202	CDL	OA7-CA5-OA6-CA4
51	q	201	CDL	OB7-CB5-OB6-CB4
51	d	201	CDL	C11-CA5-OA6-CA4
51	d	202	CDL	C76-C77-C78-C79
48	M	501	3PE	C11-O13-P-O11
48	Y	401	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
51	h	201	CDL	C1-CA2-OA2-PA1
55	T	201	EHZ	C21-C1-C2-C3
47	D	501	HQH	C11-C18-C21-C15
48	K	201	3PE	O11-C1-C2-C3
51	L	701	CDL	OA5-CA3-CA4-CA6
48	i	201	3PE	C24-C25-C26-C27
51	L	701	CDL	C76-C77-C78-C79
51	N	402	CDL	CA2-C1-CB2-OB2
48	D	502	3PE	C37-C38-C39-C3A
48	l	701	3PE	C2E-C2F-C2G-C2H
48	D	502	3PE	C2B-C2C-C2D-C2E
48	l	701	3PE	C27-C28-C29-C2A
51	N	402	CDL	C76-C77-C78-C79
46	B	203	PC1	C1-C2-C3-O31
46	Z	201	PC1	C1-C2-C3-O31
48	M	501	3PE	C1-C2-C3-O31
48	h	202	3PE	C1-C2-C3-O31
51	d	201	CDL	CB3-CB4-CB6-OB8
51	d	202	CDL	CB3-CB4-CB6-OB8
51	h	201	CDL	CA3-CA4-CA6-OA8
46	J	201	PC1	C39-C3A-C3B-C3C
48	D	502	3PE	C3C-C3D-C3E-C3F
51	d	202	CDL	C33-C34-C35-C36
51	N	402	CDL	CB5-C51-C52-C53
46	J	201	PC1	C34-C35-C36-C37
51	d	201	CDL	C34-C35-C36-C37
46	B	203	PC1	C3F-C3G-C3H-C3I
51	L	701	CDL	CA6-CA4-OA6-CA5
51	N	401	CDL	CB4-CB3-OB5-PB2
48	D	502	3PE	C32-C33-C34-C35
48	M	501	3PE	C3A-C3B-C3C-C3D
48	Y	401	3PE	C23-C24-C25-C26
51	L	701	CDL	CA7-C31-C32-C33
46	Z	201	PC1	C25-C26-C27-C28
48	K	201	3PE	C33-C34-C35-C36
48	L	702	3PE	C3F-C3G-C3H-C3I
51	N	402	CDL	O1-C1-CB2-OB2
46	Z	201	PC1	O21-C2-C3-O31
46	J	201	PC1	C32-C33-C34-C35
53	P	501	NDP	PN-O3-PA-O1A
51	L	701	CDL	C57-C58-C59-C60
48	L	702	3PE	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
51	L	701	CDL	C33-C34-C35-C36
51	N	402	CDL	C54-C55-C56-C57
47	D	501	HQH	O1-C7-C9-C14
48	H	401	3PE	C36-C37-C38-C39
51	N	401	CDL	C71-C72-C73-C74
48	D	502	3PE	O11-C1-C2-C3
51	N	402	CDL	OA5-CA3-CA4-CA6
48	D	502	3PE	O13-C11-C12-N
48	h	202	3PE	C31-C32-C33-C34
48	i	201	3PE	C31-C32-C33-C34
51	d	201	CDL	OA7-CA5-OA6-CA4
51	d	202	CDL	C73-C74-C75-C76
48	Y	401	3PE	C35-C36-C37-C38
46	J	201	PC1	C1-C2-C3-O31
48	Y	401	3PE	C1-C2-C3-O31
48	i	201	3PE	C1-C2-C3-O31
51	N	402	CDL	CB3-CB4-CB6-OB8
48	D	502	3PE	C1-O11-P-O13
48	H	401	3PE	C1-O11-P-O13
48	K	201	3PE	C1-O11-P-O13
48	l	701	3PE	C1-O11-P-O13
51	d	202	CDL	CB2-OB2-PB2-OB5
51	q	201	CDL	CB3-OB5-PB2-OB2
46	B	203	PC1	O21-C2-C3-O31
51	h	201	CDL	C74-C75-C76-C77
51	L	701	CDL	C1-CA2-OA2-PA1
55	T	201	EHZ	O2-C9-S1-C10
51	N	402	CDL	C81-C82-C83-C84
51	q	201	CDL	C71-C72-C73-C74
48	l	701	3PE	O11-C1-C2-C3
51	q	201	CDL	OA5-CA3-CA4-CA6
51	L	701	CDL	C14-C15-C16-C17
51	d	202	CDL	C79-C80-C81-C82
55	T	201	EHZ	C5-C6-C7-C8
48	H	401	3PE	C3-C2-O21-C21
51	N	401	CDL	CB6-CB4-OB6-CB5
51	d	202	CDL	CA6-CA4-OA6-CA5
55	T	201	EHZ	C8-C9-S1-C10
51	q	201	CDL	C17-C18-C19-C20
51	d	202	CDL	CA4-CA3-OA5-PA1
48	l	701	3PE	O11-C1-C2-O21
51	q	201	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
51	L	701	CDL	C35-C36-C37-C38
51	L	701	CDL	C31-C32-C33-C34
51	d	201	CDL	C13-C14-C15-C16
55	T	201	EHZ	O1-C7-C8-C9
55	U	201	EHZ	C15-C16-C17-C19
46	Z	201	PC1	C37-C38-C39-C3A
48	i	201	3PE	O21-C2-C3-O31
51	d	201	CDL	OB6-CB4-CB6-OB8
51	h	201	CDL	OA6-CA4-CA6-OA8
51	L	701	CDL	C11-C12-C13-C14
51	N	402	CDL	CA5-C11-C12-C13
48	D	502	3PE	C35-C36-C37-C38
48	H	401	3PE	C26-C27-C28-C29
48	Y	401	3PE	C25-C26-C27-C28
55	U	201	EHZ	C1-C2-C3-C4
55	U	201	EHZ	C4-C5-C6-C7
51	q	201	CDL	CB7-C71-C72-C73
51	N	401	CDL	C56-C57-C58-C59
51	L	701	CDL	CB3-OB5-PB2-OB2
51	N	401	CDL	CA2-OA2-PA1-OA5
51	N	402	CDL	CA3-OA5-PA1-OA2
48	L	702	3PE	C24-C25-C26-C27
51	N	401	CDL	C77-C78-C79-C80
48	D	502	3PE	C1-O11-P-O12
48	H	401	3PE	C11-O13-P-O12
48	K	201	3PE	C1-O11-P-O12
48	L	702	3PE	C11-O13-P-O12
48	M	501	3PE	C1-O11-P-O12
48	M	501	3PE	C1-O11-P-O14
48	M	501	3PE	C11-O13-P-O12
48	Y	401	3PE	C1-O11-P-O12
51	N	401	CDL	CB3-OB5-PB2-OB3
51	N	401	CDL	CB3-OB5-PB2-OB4
51	N	402	CDL	CA3-OA5-PA1-OA3
51	N	402	CDL	CA3-OA5-PA1-OA4
51	N	402	CDL	CB2-OB2-PB2-OB3
51	d	201	CDL	CA3-OA5-PA1-OA4
51	d	201	CDL	CB2-OB2-PB2-OB3
51	q	201	CDL	CA2-OA2-PA1-OA3
51	q	201	CDL	CA2-OA2-PA1-OA4
51	q	201	CDL	CB3-OB5-PB2-OB4
52	O	401	ATP	C5’-O5’-PA-O1A

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Mol	Chain	Res	Type	Atoms
48	i	201	3PE	C27-C28-C29-C2A
48	H	401	3PE	O11-C1-C2-C3
48	Y	401	3PE	C39-C3A-C3B-C3C
48	i	201	3PE	C34-C35-C36-C37
51	q	201	CDL	C52-C53-C54-C55
46	B	202	PC1	C12-C11-O13-P
48	K	201	3PE	C12-C11-O13-P
48	L	702	3PE	C12-C11-O13-P
48	H	401	3PE	C24-C25-C26-C27
51	d	202	CDL	CA2-C1-CB2-OB2
48	l	701	3PE	C29-C2A-C2B-C2C
51	N	402	CDL	OA5-CA3-CA4-OA6
55	U	201	EHZ	C15-C16-C17-C20
51	d	201	CDL	C12-C13-C14-C15
46	B	203	PC1	C37-C38-C39-C3A
46	B	202	PC1	O13-C11-C12-N
51	q	201	CDL	CB3-CB4-CB6-OB8
48	h	202	3PE	O21-C2-C3-O31
51	N	402	CDL	OB6-CB4-CB6-OB8
48	i	201	3PE	C2B-C2C-C2D-C2E
48	D	502	3PE	C25-C26-C27-C28
51	d	201	CDL	CA7-C31-C32-C33
46	Z	201	PC1	C22-C23-C24-C25
53	P	501	NDP	O4B-C4B-C5B-O5B
48	M	501	3PE	C33-C34-C35-C36
55	T	201	EHZ	C18-C17-C20-O6
55	T	201	EHZ	C19-C17-C20-O6
51	d	201	CDL	CB3-CB4-OB6-CB5
51	h	201	CDL	CB6-CB4-OB6-CB5
51	q	201	CDL	CA6-CA4-OA6-CA5
46	Z	201	PC1	O11-C1-C2-C3
46	Z	201	PC1	C36-C37-C38-C39
51	N	402	CDL	C74-C75-C76-C77
51	N	401	CDL	C72-C71-CB7-OB8
51	d	201	CDL	C71-C72-C73-C74
51	h	201	CDL	C1-CB2-OB2-PB2
48	L	702	3PE	C25-C26-C27-C28
48	K	201	3PE	O11-C1-C2-O21
48	M	501	3PE	O21-C2-C3-O31
51	d	202	CDL	OB6-CB4-CB6-OB8
48	H	401	3PE	C38-C39-C3A-C3B
51	d	201	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
46	J	201	PC1	C1-O11-P-O13
48	l	701	3PE	C11-O13-P-O11
51	L	701	CDL	CA3-OA5-PA1-OA2
51	L	701	CDL	CB2-OB2-PB2-OB5
51	d	202	CDL	CB3-OB5-PB2-OB2
51	q	201	CDL	CA2-OA2-PA1-OA5
51	q	201	CDL	CB2-OB2-PB2-OB5
48	i	201	3PE	C2A-C2B-C2C-C2D
51	N	401	CDL	C75-C76-C77-C78
48	D	502	3PE	C2D-C2E-C2F-C2G
51	L	701	CDL	C73-C74-C75-C76
51	h	201	CDL	C32-C33-C34-C35
48	Y	401	3PE	C21-C22-C23-C24
52	O	401	ATP	PB-O3A-PA-O2A
48	l	701	3PE	C2A-C2B-C2C-C2D
52	O	401	ATP	O4'-C4'-C5'-O5'
46	J	201	PC1	O11-C1-C2-O21
46	J	201	PC1	C36-C37-C38-C39
51	N	401	CDL	O1-C1-CB2-OB2
48	i	201	3PE	C2-C1-O11-P
51	d	202	CDL	C1-CA2-OA2-PA1
48	i	201	3PE	C36-C37-C38-C39
47	D	501	HQH	C23-C25-O3-C30
51	h	201	CDL	C24-C25-C26-C27
46	J	201	PC1	C37-C38-C39-C3A
51	d	202	CDL	C12-C13-C14-C15
51	d	201	CDL	CA6-CA4-OA6-CA5
46	Z	201	PC1	C11-C12-N-C14
46	J	201	PC1	C38-C39-C3A-C3B
48	i	201	3PE	O11-C1-C2-O21
55	T	201	EHZ	C21-C22-C23-C24
48	L	702	3PE	C21-C22-C23-C24
55	T	201	EHZ	C11-C10-S1-C9
48	Y	401	3PE	C26-C27-C28-C29
46	J	201	PC1	C28-C29-C2A-C2B
51	N	402	CDL	C82-C83-C84-C85
52	O	401	ATP	PG-O3B-PB-O1B
51	d	201	CDL	C11-C12-C13-C14
46	Z	201	PC1	O21-C21-C22-C23
48	L	702	3PE	C36-C37-C38-C39
48	H	401	3PE	O11-C1-C2-O21
46	J	201	PC1	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
48	i	201	3PE	C32-C33-C34-C35
48	K	201	3PE	C25-C26-C27-C28
48	D	502	3PE	C3E-C3F-C3G-C3H
46	B	203	PC1	C1-O11-P-O13
55	U	201	EHZ	C18-C17-C20-O6
48	K	201	3PE	O21-C21-C22-C23
48	D	502	3PE	O31-C31-C32-C33
51	h	201	CDL	CB3-CB4-OB6-CB5
51	N	402	CDL	C32-C31-CA7-OA8
51	d	202	CDL	C12-C11-CA5-OA6
46	B	203	PC1	C32-C33-C34-C35
51	N	401	CDL	C51-C52-C53-C54
55	T	201	EHZ	C1-C2-C3-C4
48	M	501	3PE	C32-C33-C34-C35
55	U	201	EHZ	C15-C16-C17-C18
51	q	201	CDL	C12-C13-C14-C15
46	J	201	PC1	C3A-C3B-C3C-C3D
46	Z	201	PC1	C11-C12-N-C13
48	D	502	3PE	C22-C23-C24-C25
46	J	201	PC1	C23-C24-C25-C26
53	P	501	NDP	PN-O3-PA-O2A
55	T	201	EHZ	C2-C1-C21-C22
55	T	201	EHZ	C4-C5-C6-C7
51	d	202	CDL	C71-C72-C73-C74
51	d	202	CDL	C12-C11-CA5-OA7
51	N	402	CDL	C32-C31-CA7-OA9
48	L	702	3PE	O31-C31-C32-C33
48	D	502	3PE	C24-C25-C26-C27
48	Y	401	3PE	O21-C21-C22-C23
51	h	201	CDL	OB7-CB5-OB6-CB4
51	q	201	CDL	OA7-CA5-OA6-CA4
48	K	201	3PE	O22-C21-C22-C23
51	N	402	CDL	C75-C76-C77-C78
46	Z	201	PC1	C11-O13-P-O14
46	Z	201	PC1	C1-O11-P-O12
46	Z	201	PC1	C11-C12-N-C15
51	N	401	CDL	CA3-OA5-PA1-OA3
51	N	402	CDL	CA2-OA2-PA1-OA3
51	N	402	CDL	CB3-OB5-PB2-OB4
51	d	201	CDL	CB3-OB5-PB2-OB3
51	d	202	CDL	CA3-OA5-PA1-OA4
51	N	401	CDL	C52-C51-CB5-OB6

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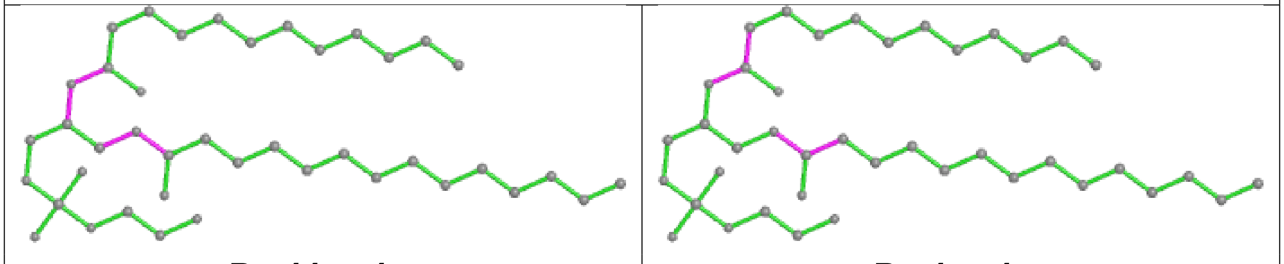
Mol	Chain	Res	Type	Atoms
51	d	202	CDL	C32-C31-CA7-OA8
51	L	701	CDL	C72-C71-CB7-OB8
48	i	201	3PE	C12-C11-O13-P
48	H	401	3PE	O21-C21-C22-C23
46	B	202	PC1	C35-C36-C37-C38
48	K	201	3PE	C27-C28-C29-C2A
51	N	401	CDL	C74-C75-C76-C77
46	B	203	PC1	C23-C24-C25-C26
51	L	701	CDL	C52-C51-CB5-OB6
51	h	201	CDL	C12-C11-CA5-OA6
48	Y	401	3PE	O22-C21-C22-C23
51	d	201	CDL	C64-C65-C66-C67
51	L	701	CDL	C12-C11-CA5-OA6
46	Z	201	PC1	C32-C33-C34-C35
51	L	701	CDL	C53-C54-C55-C56
48	L	702	3PE	O32-C31-C32-C33
51	d	202	CDL	C32-C31-CA7-OA9
51	d	202	CDL	O1-C1-CB2-OB2
51	N	401	CDL	CB7-C71-C72-C73

There are no ring outliers.

No monomer is involved in short contacts.

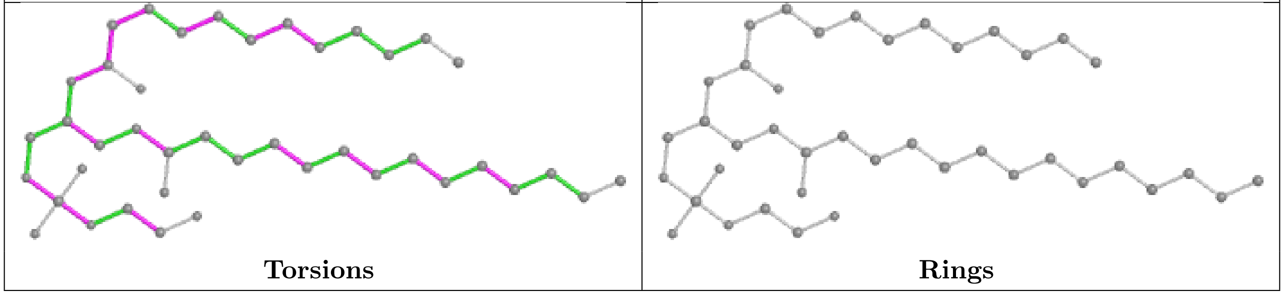
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 3PE Y 401



Bond lengths

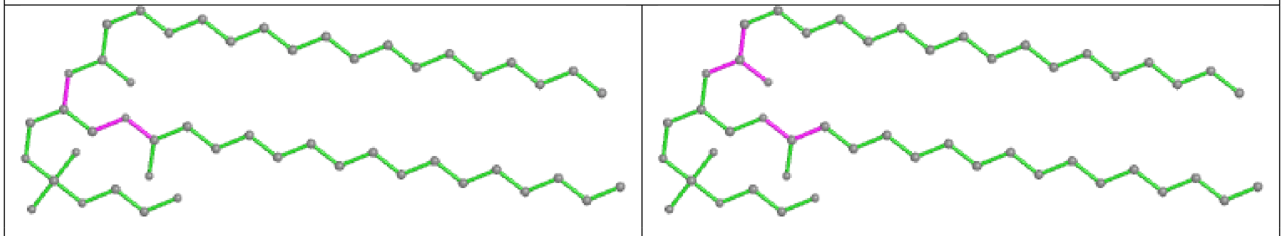
Bond angles



Torsions

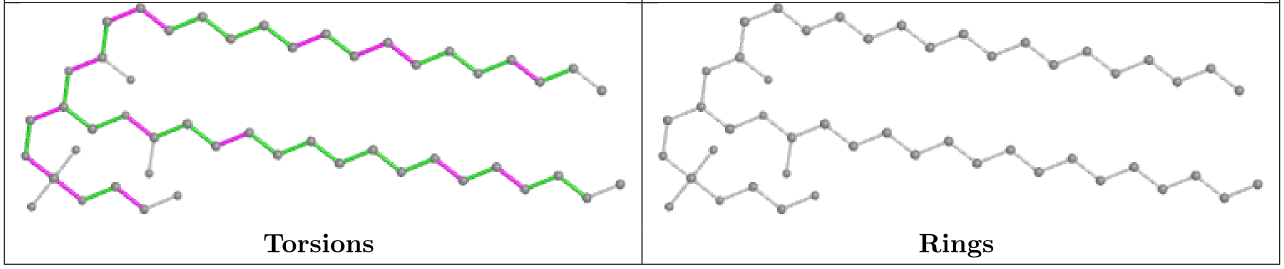
Rings

Ligand 3PE l 701



Bond lengths

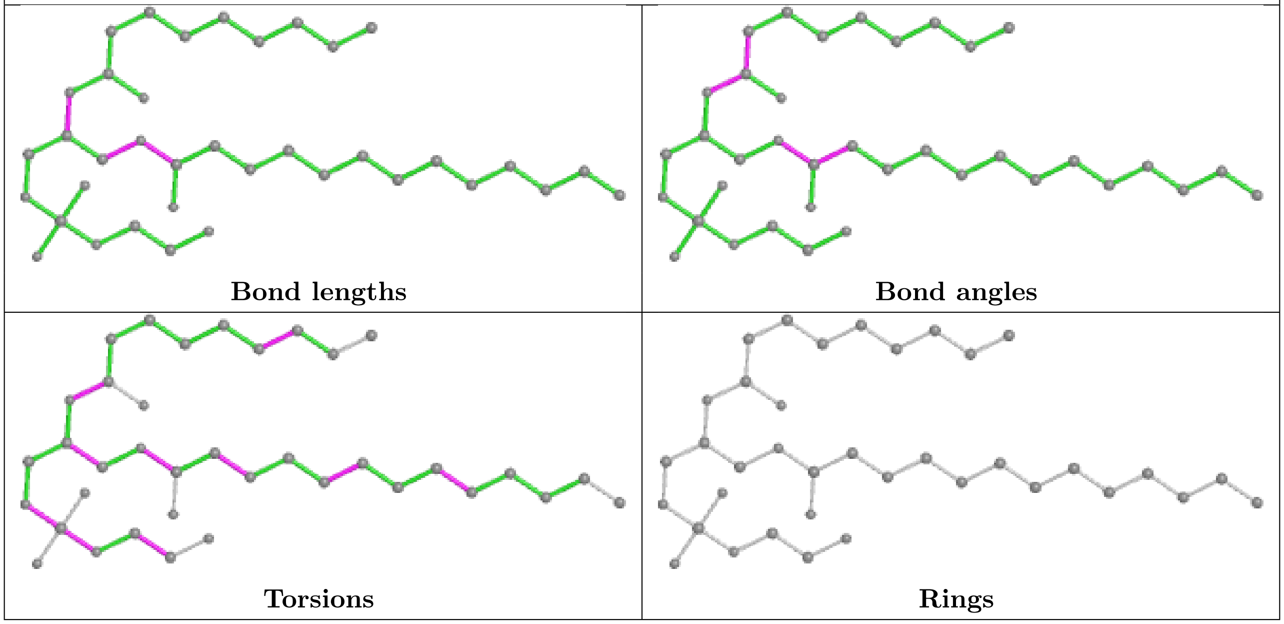
Bond angles



Torsions

Rings

Ligand 3PE h 202



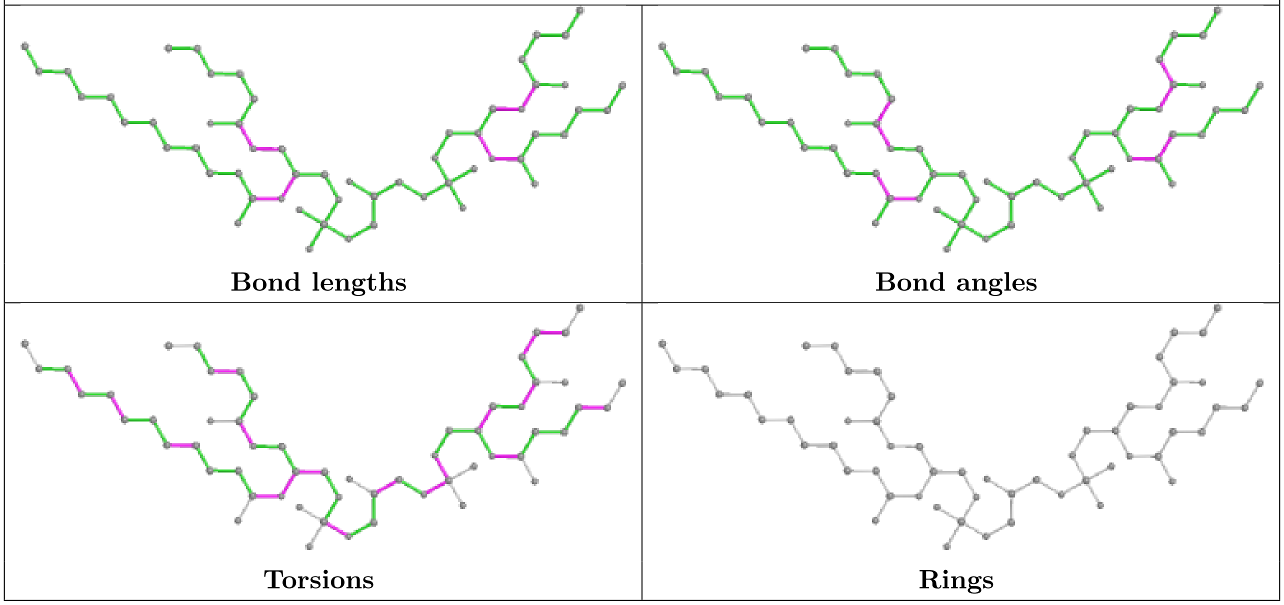
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL q 201



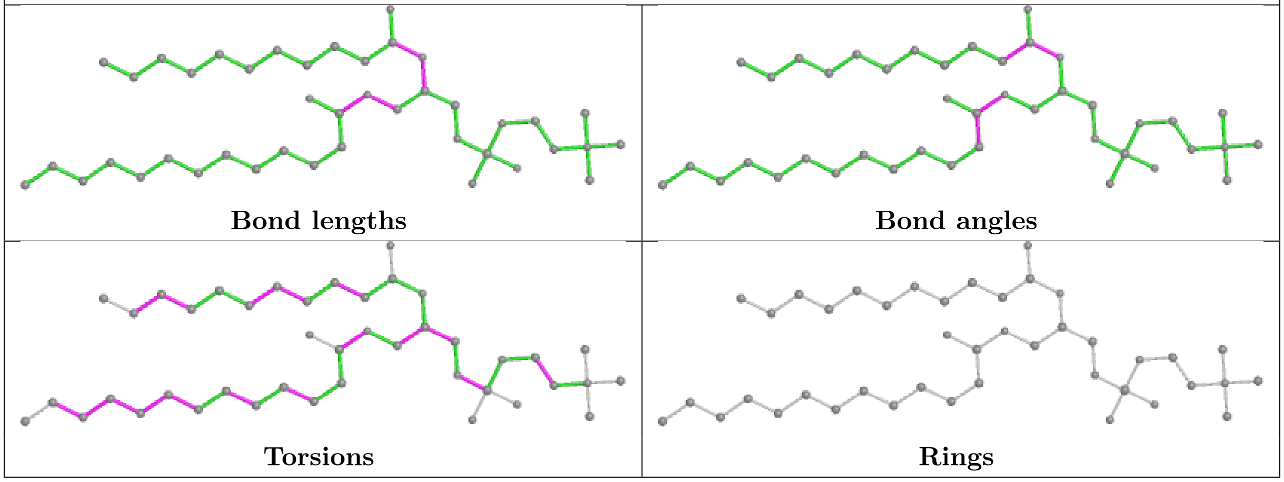
Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 J 201



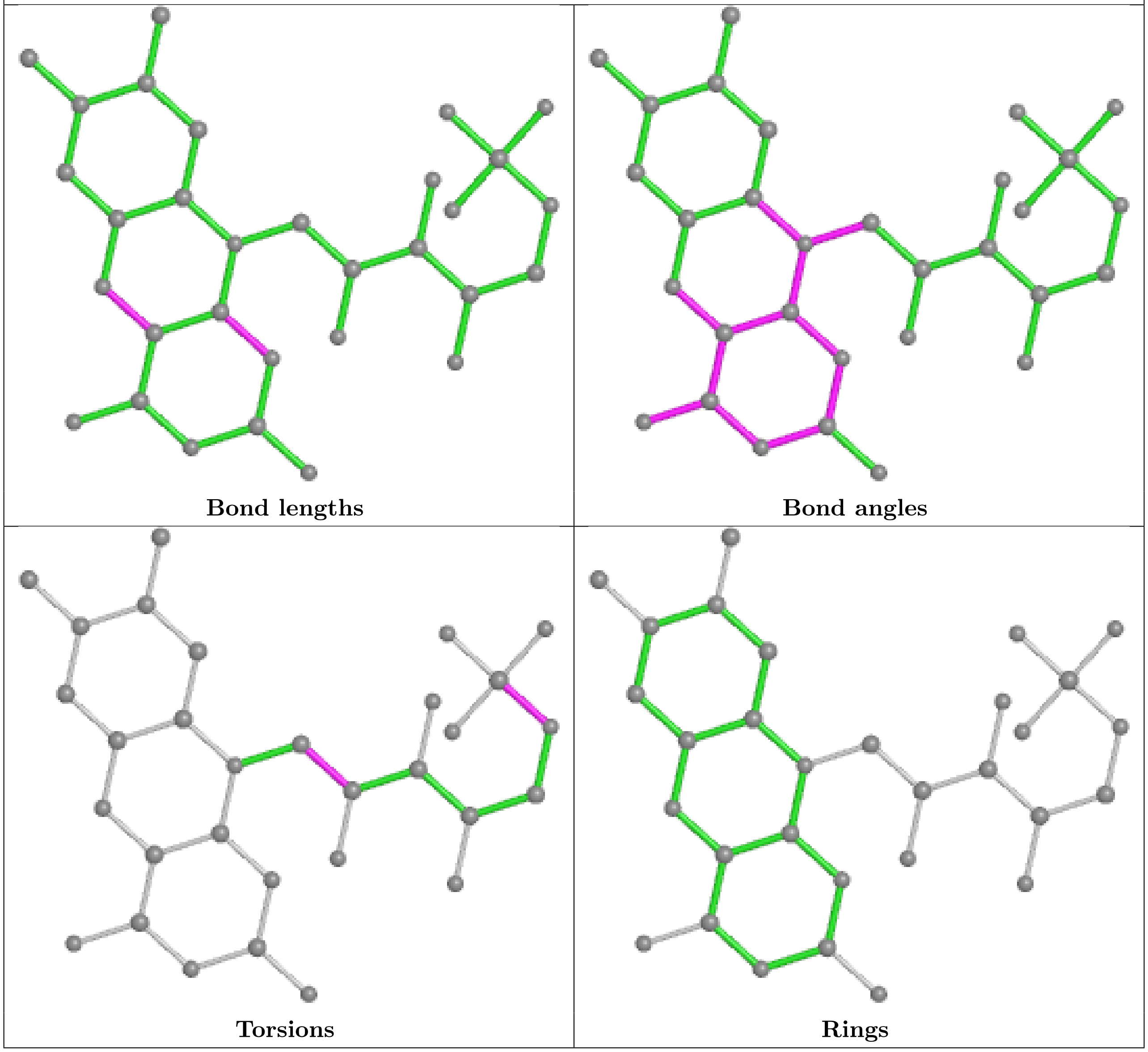
Bond lengths

Bond angles

Torsions

Rings

Ligand FMN F 501



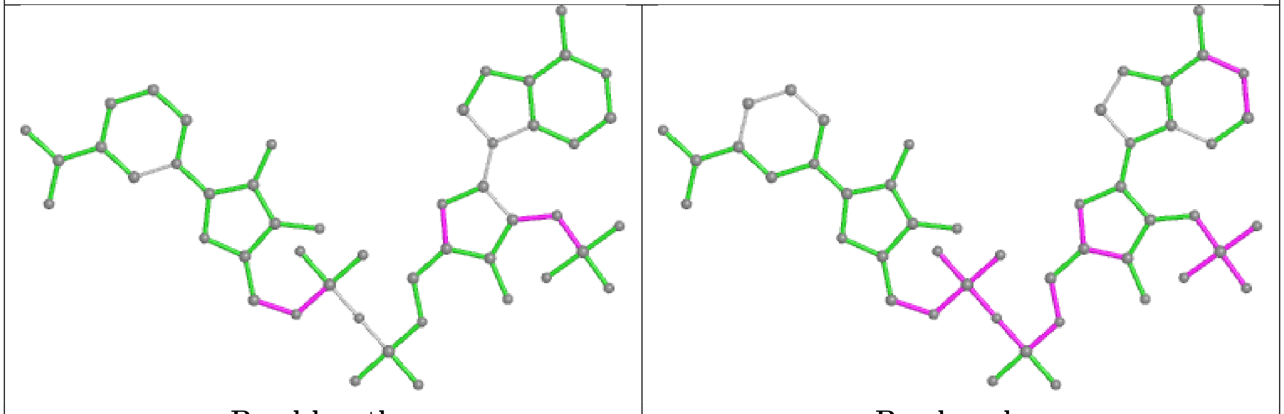
Bond lengths

Bond angles

Torsions

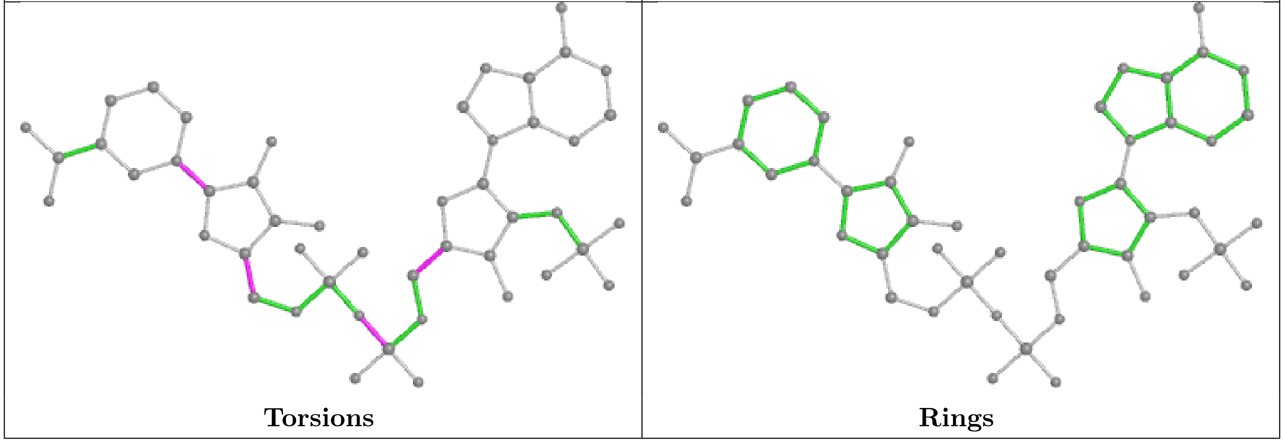
Rings

Ligand NDP P 501



Bond lengths

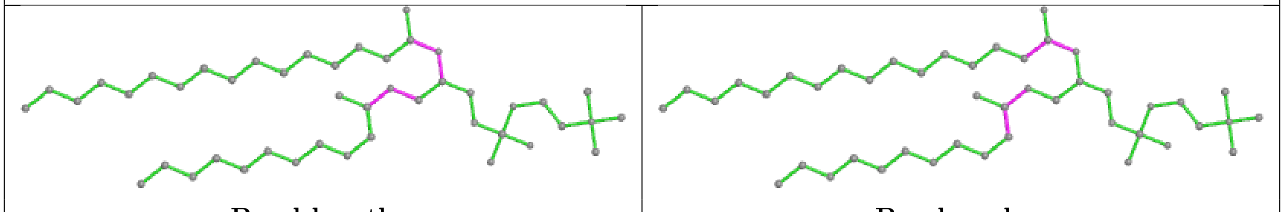
Bond angles



Torsions

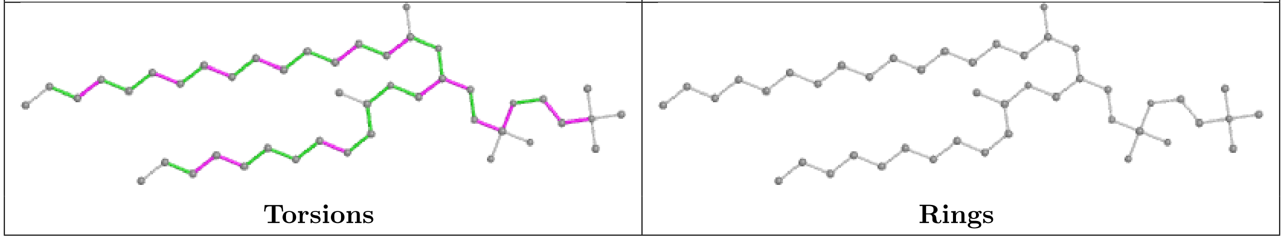
Rings

Ligand PC1 Z 201



Bond lengths

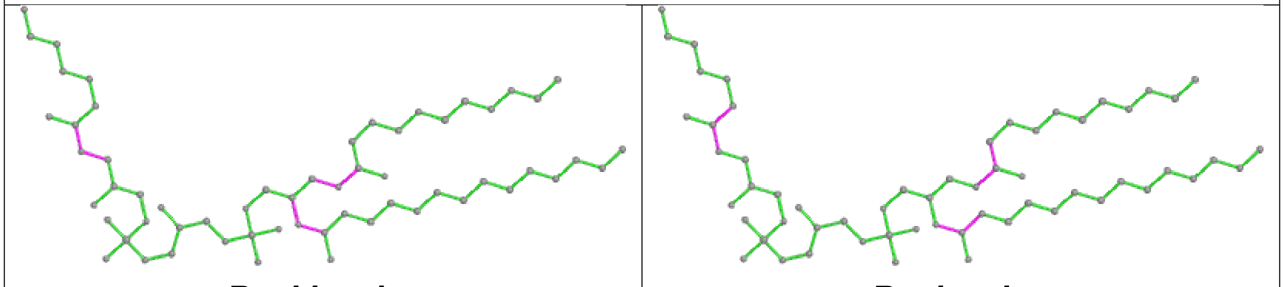
Bond angles



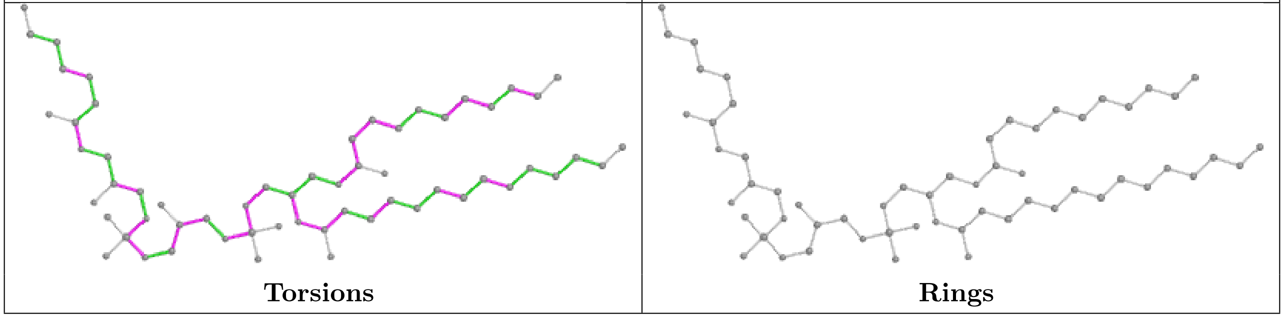
Torsions

Rings

Ligand CDL N 401

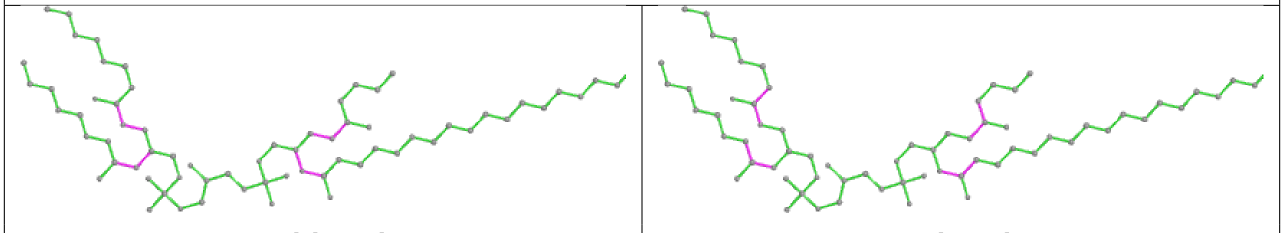


Bond lengths Bond angles

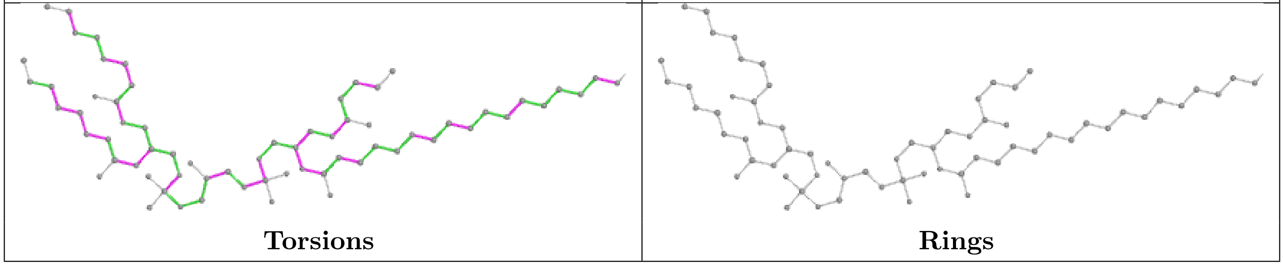


Torsions Rings

Ligand CDL d 201

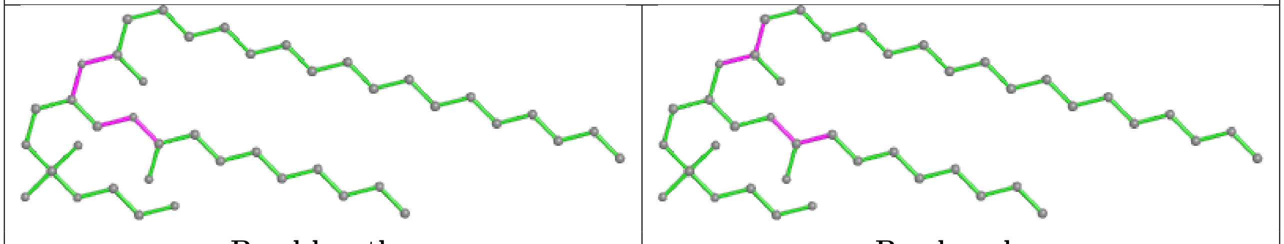


Bond lengths Bond angles



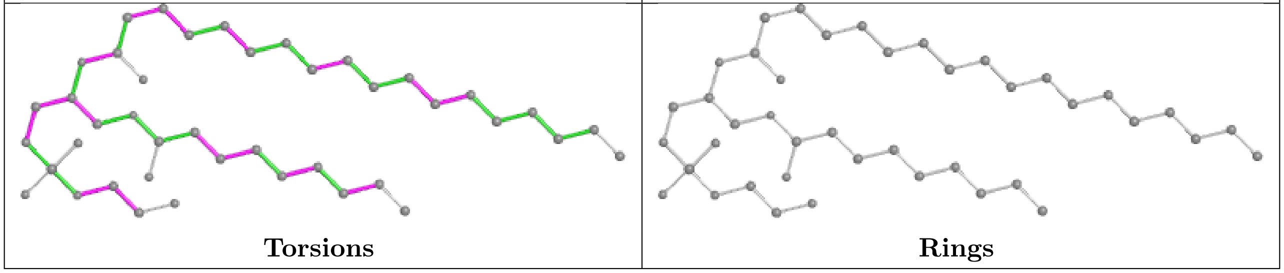
Torsions Rings

Ligand 3PE i 201



Bond lengths

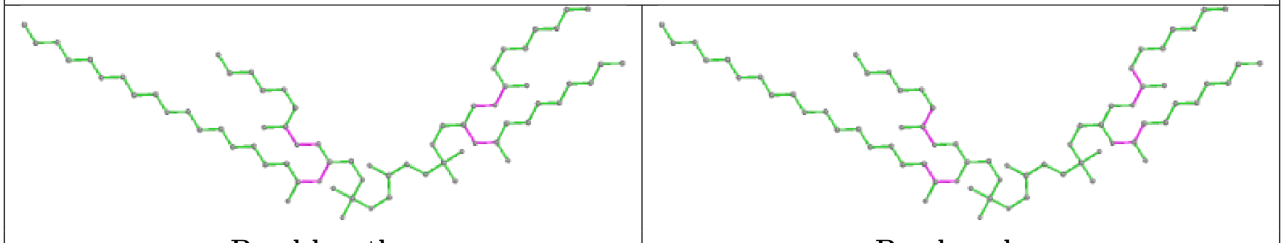
Bond angles



Torsions

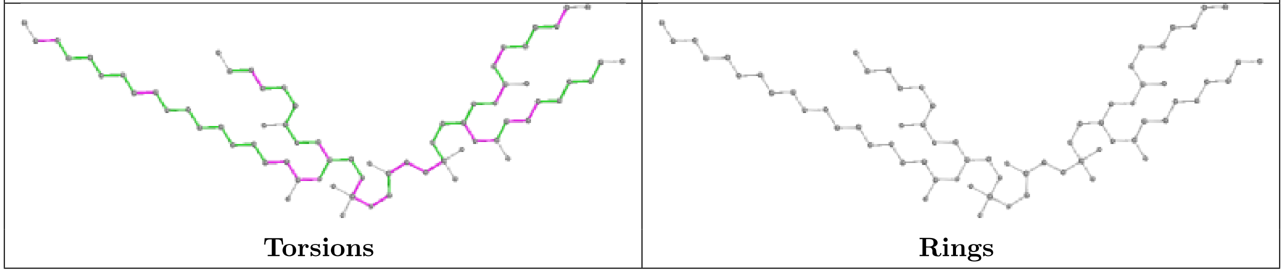
Rings

Ligand CDL h 201



Bond lengths

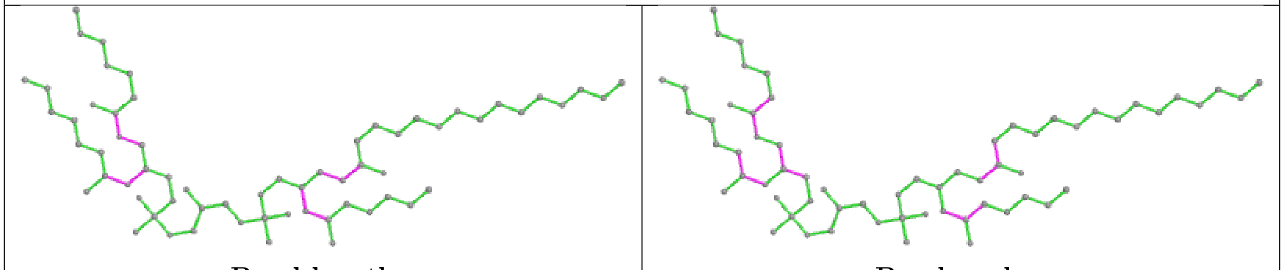
Bond angles



Torsions

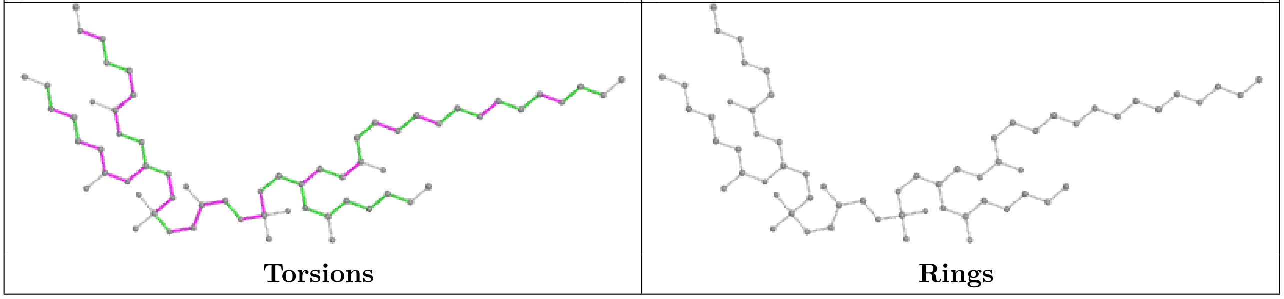
Rings

Ligand CDL d 202



Bond lengths

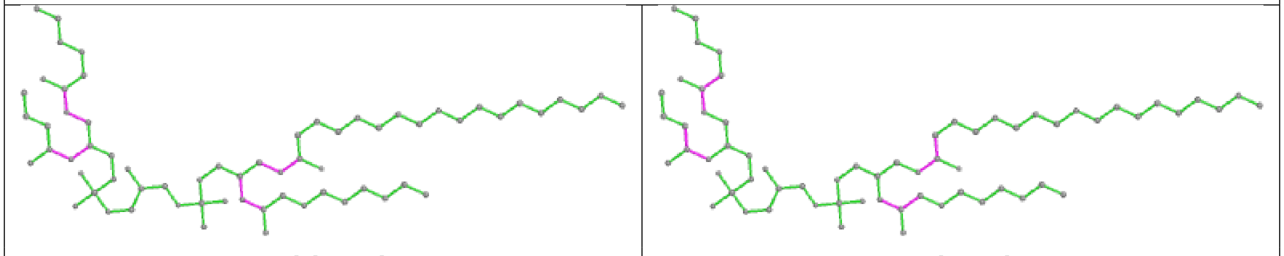
Bond angles



Torsions

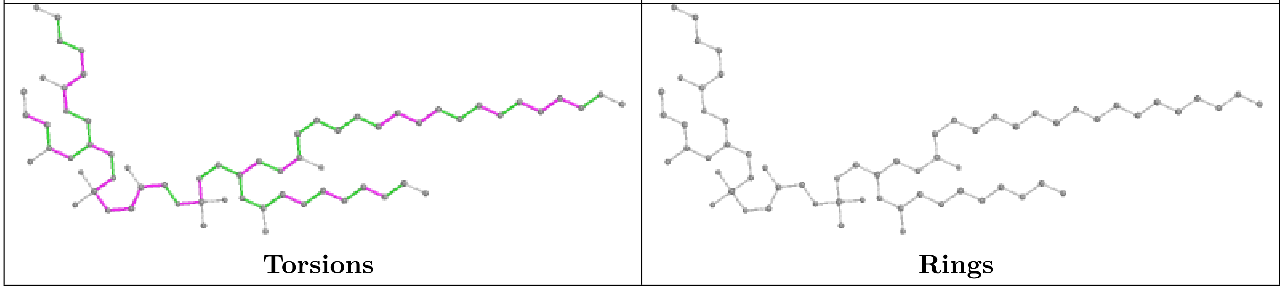
Rings

Ligand CDL N 402



Bond lengths

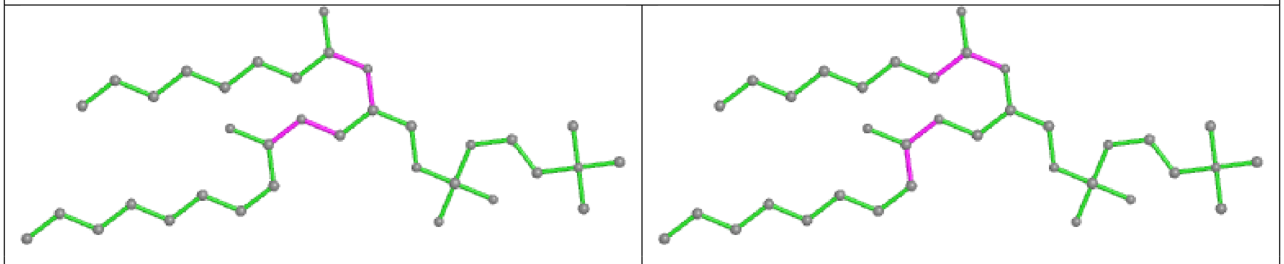
Bond angles



Torsions

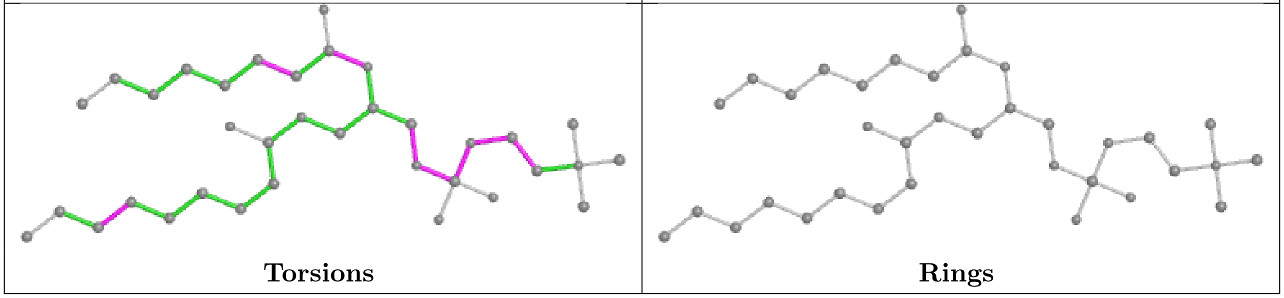
Rings

Ligand PC1 B 202



Bond lengths

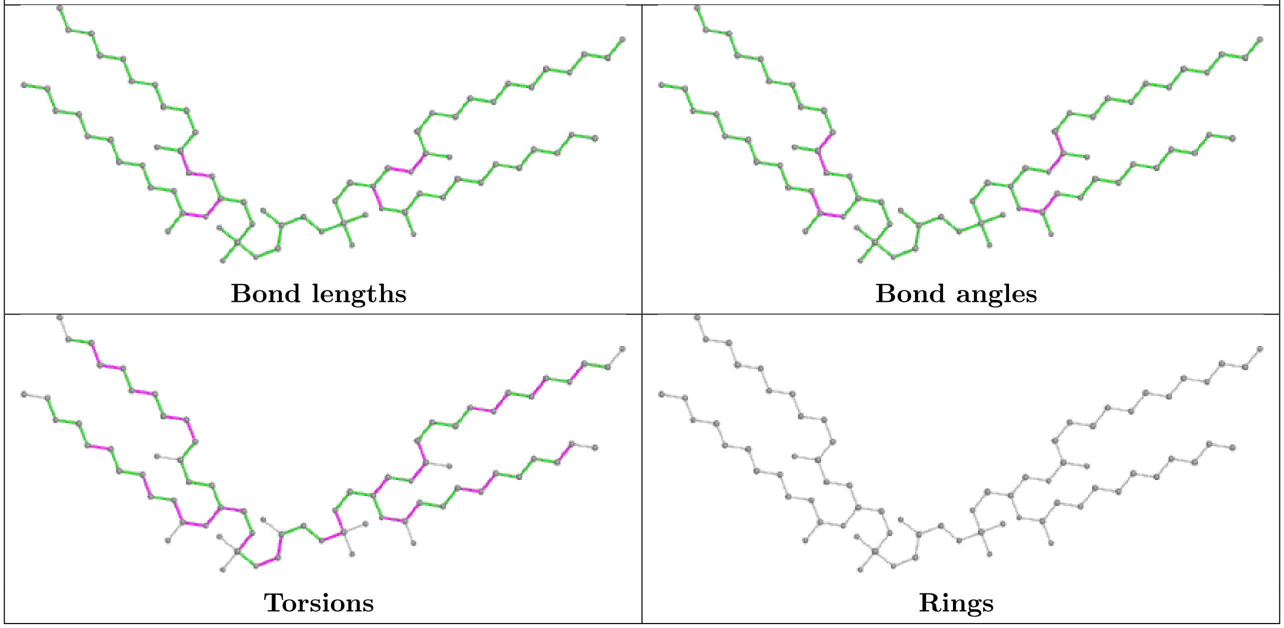
Bond angles



Torsions

Rings

Ligand CDL L 701



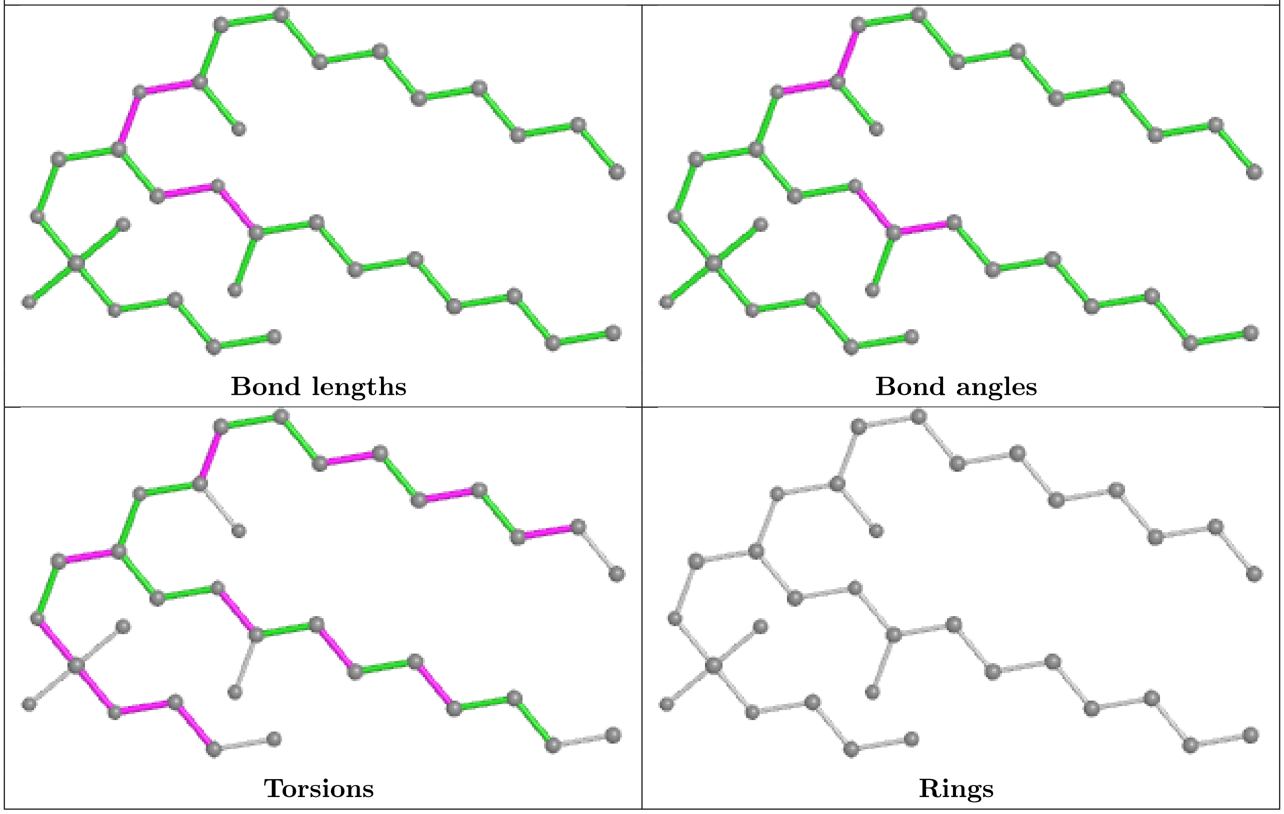
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE K 201



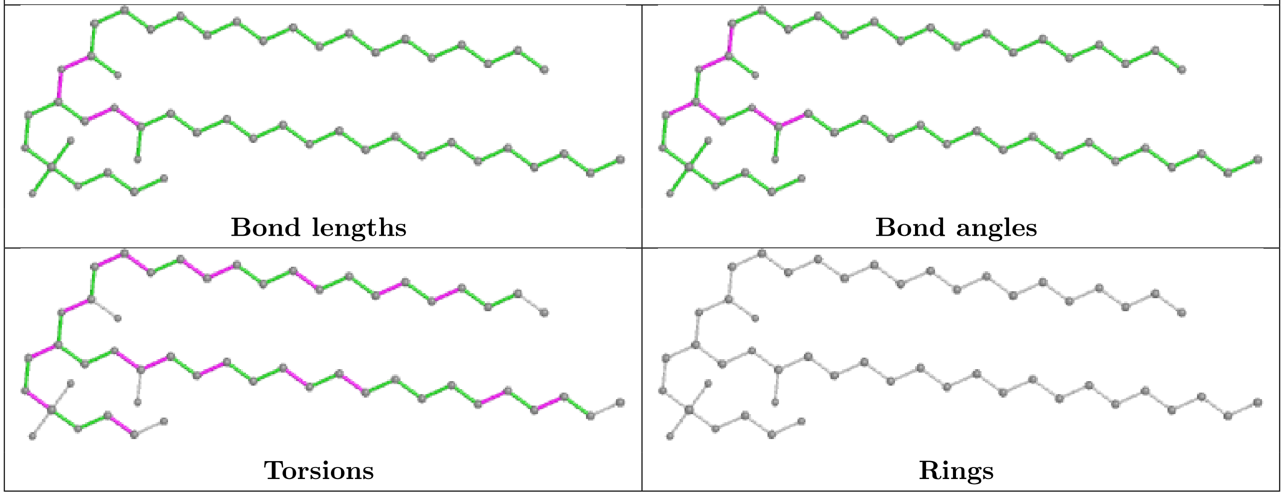
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE D 502



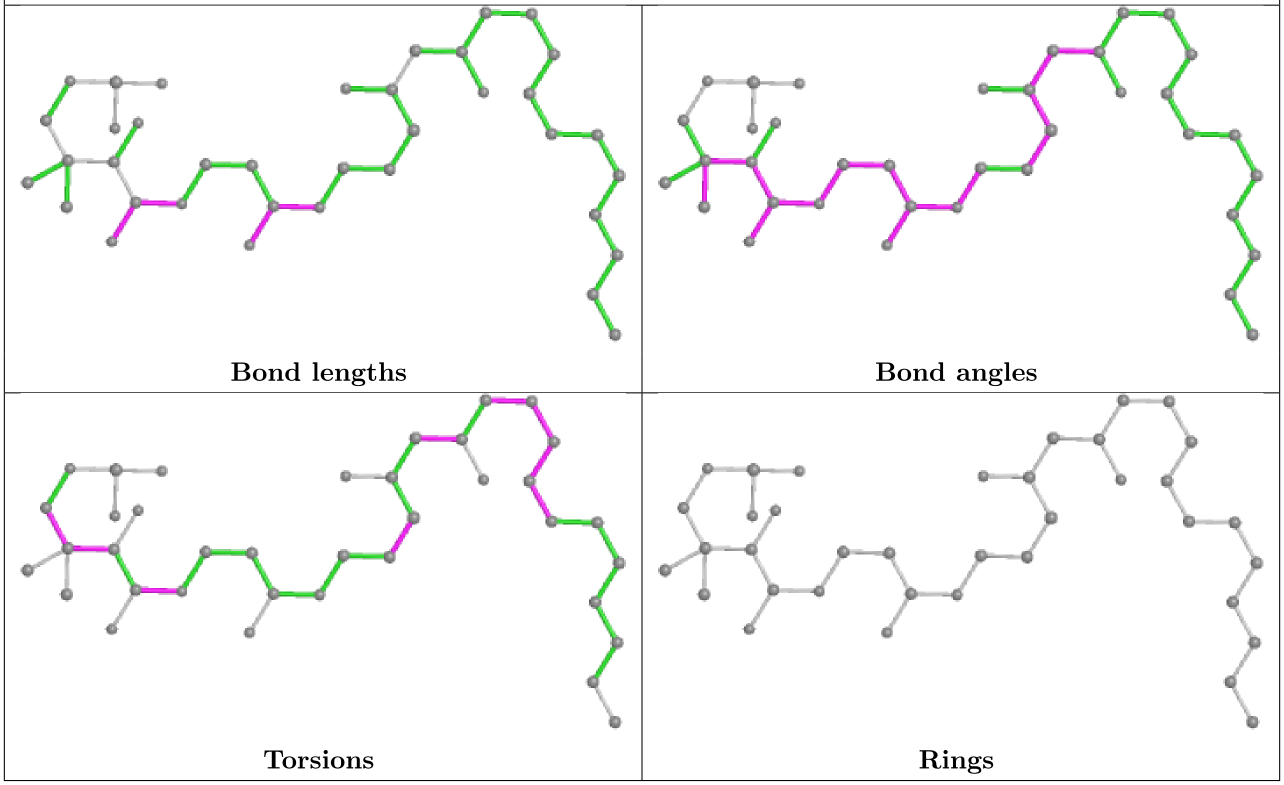
Bond lengths

Bond angles

Torsions

Rings

Ligand EHZ U 201



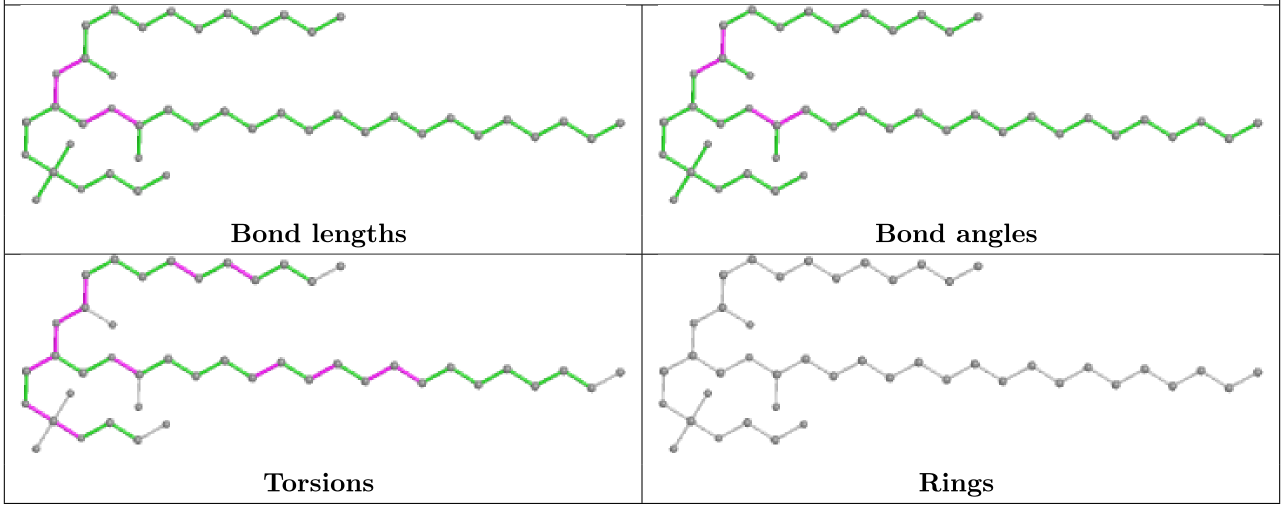
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE H 401



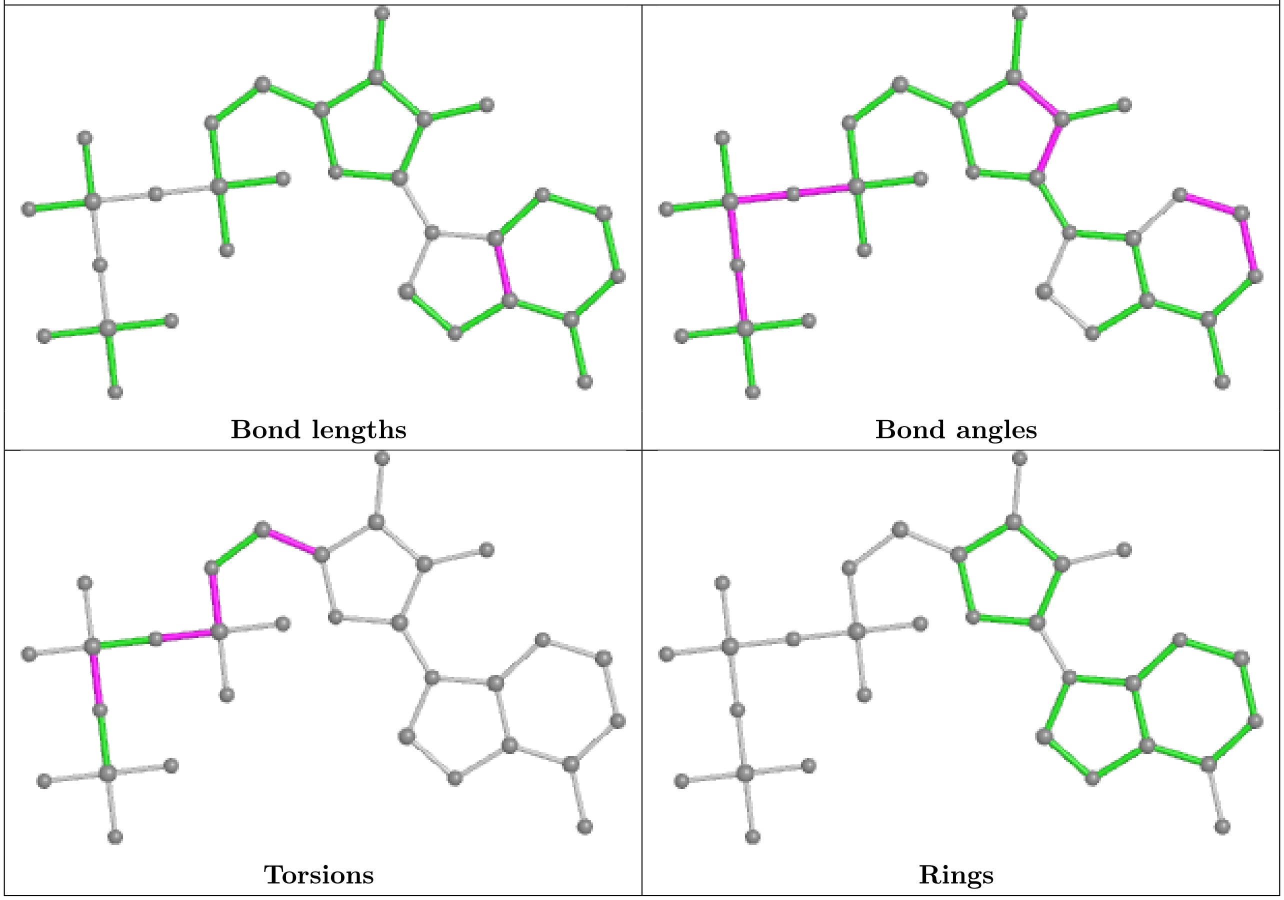
Bond lengths

Bond angles

Torsions

Rings

Ligand ATP O 401



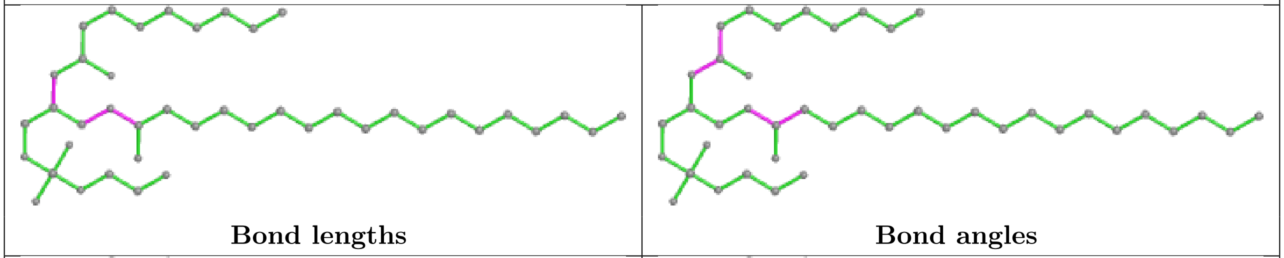
Bond lengths

Bond angles

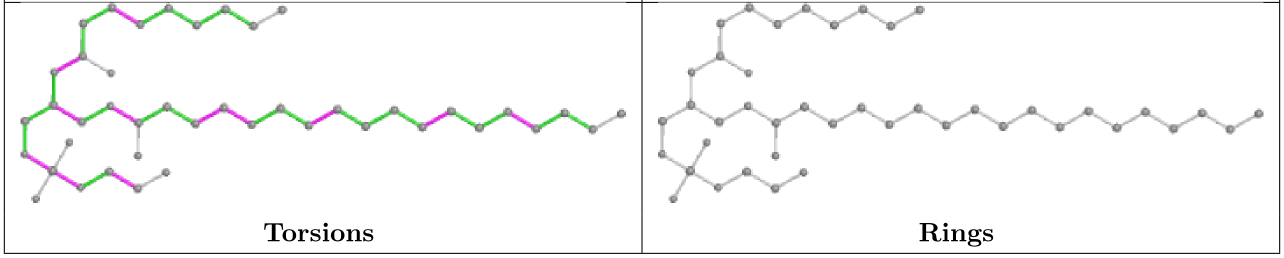
Torsions

Rings

Ligand 3PE M 501

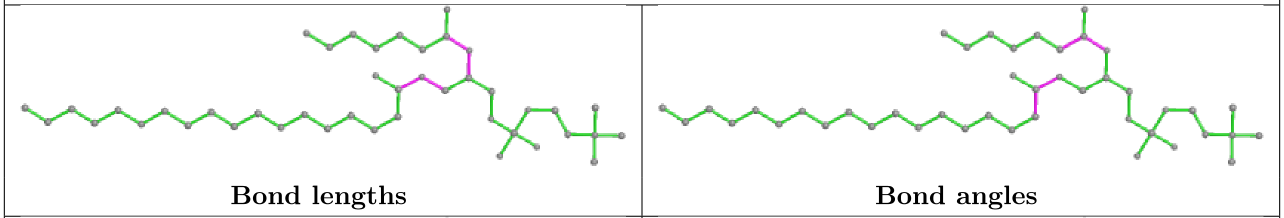


Bond lengths Bond angles

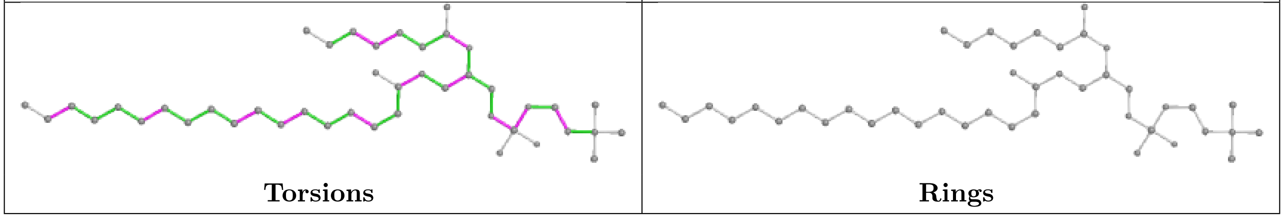


Torsions Rings

Ligand PC1 B 203

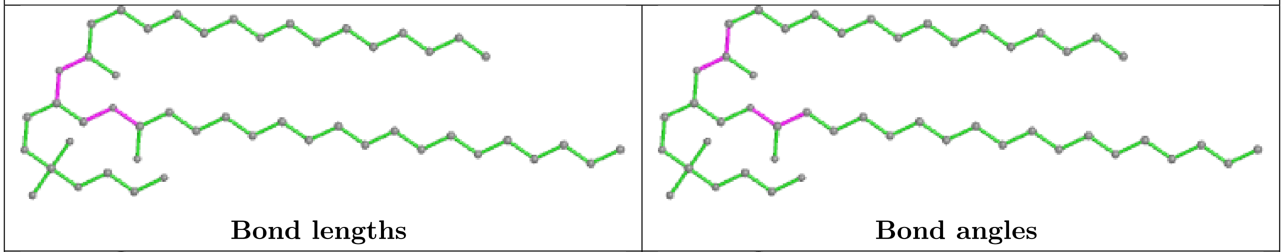


Bond lengths Bond angles

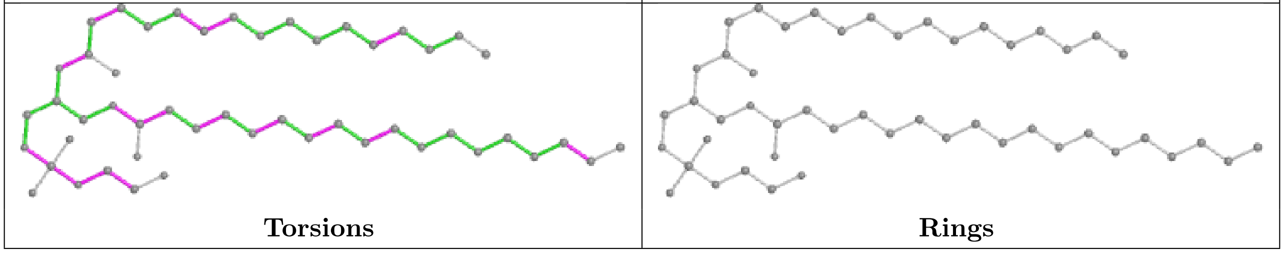


Torsions Rings

Ligand 3PE L 702

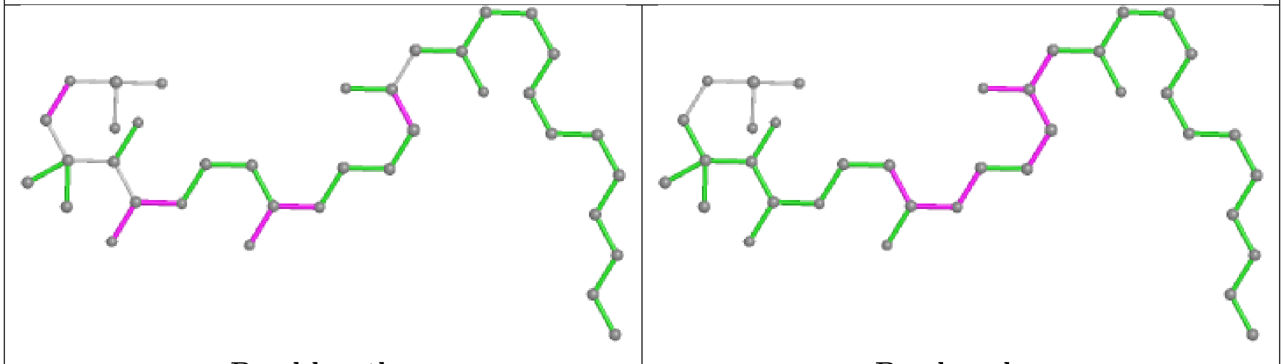


Bond lengths Bond angles



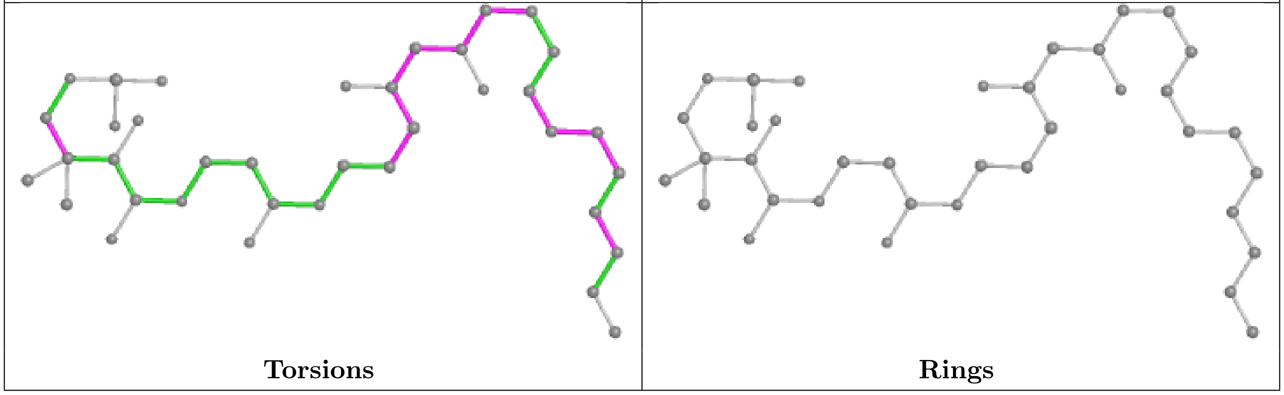
Torsions Rings

Ligand EHZ T 201



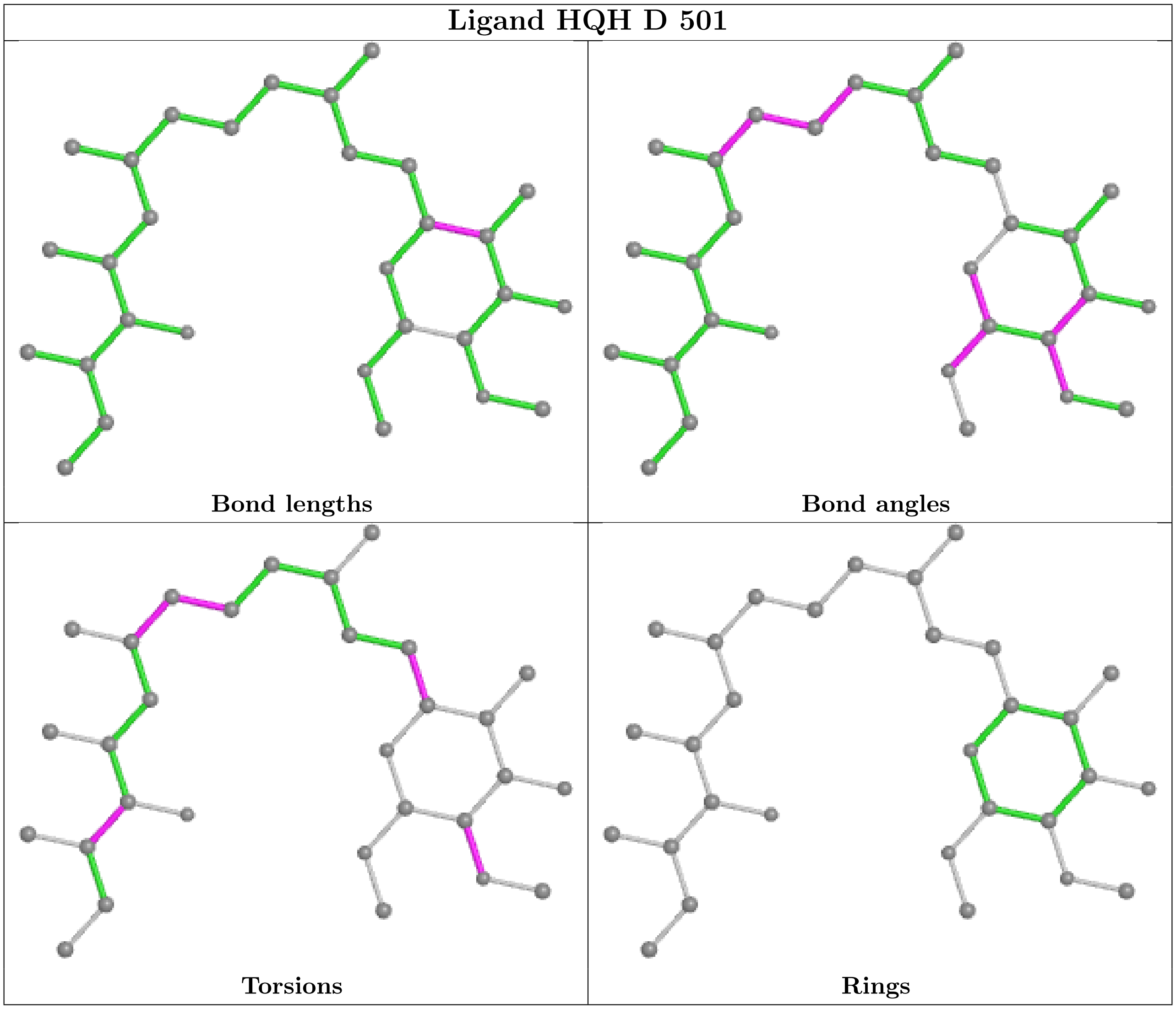
Bond lengths

Bond angles



Torsions

Rings



Ligand HQH D 501

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.

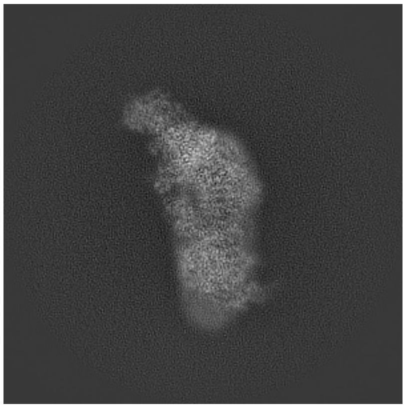
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11424. These allow visual inspection of the internal detail of the map and identification of artifacts.

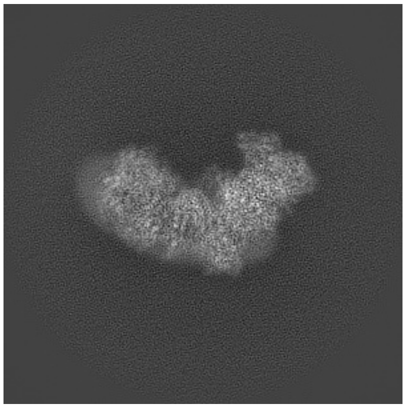
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

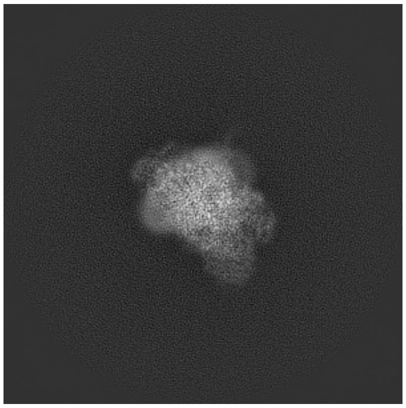
6.1.1 Primary map



X

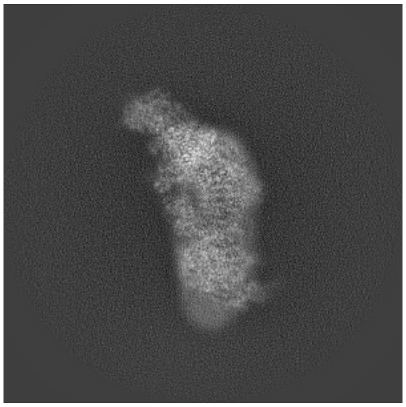


Y

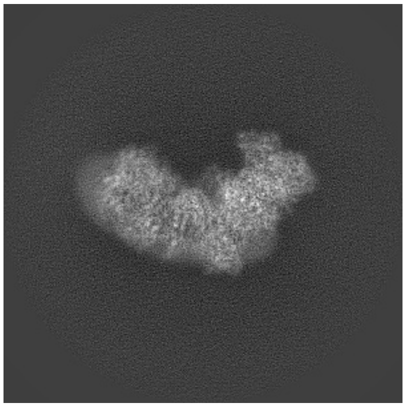


Z

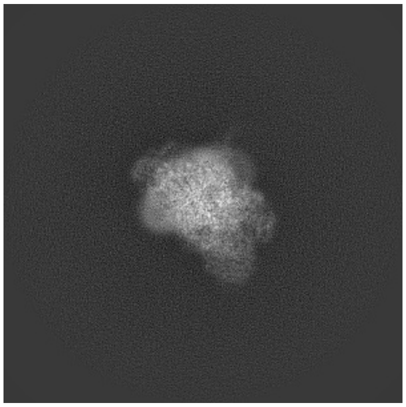
6.1.2 Raw map



X



Y

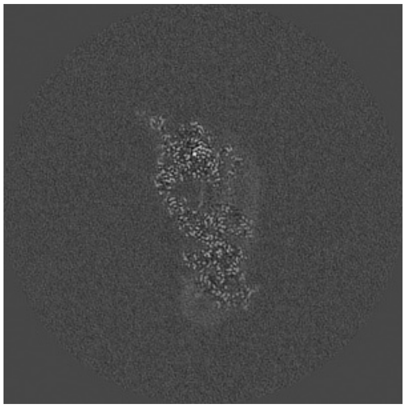


Z

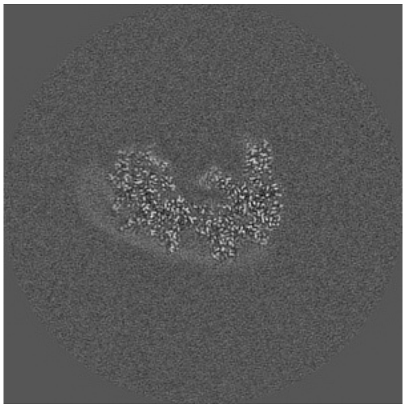
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

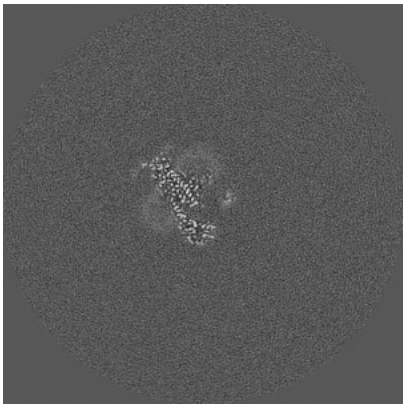
6.2.1 Primary map



X Index: 225

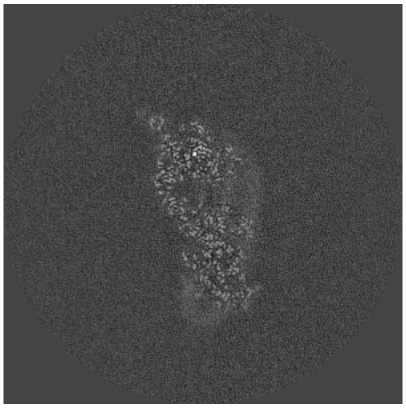


Y Index: 225

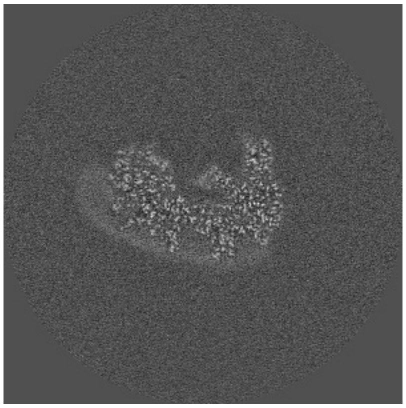


Z Index: 225

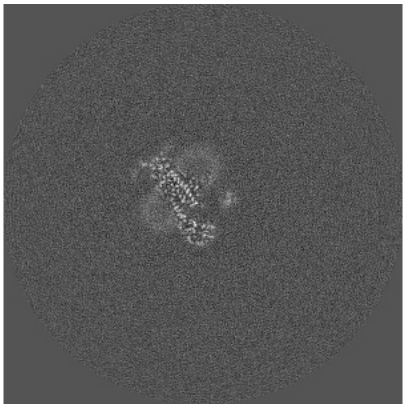
6.2.2 Raw map



X Index: 225



Y Index: 225

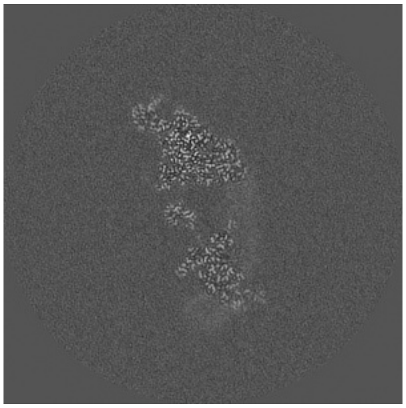


Z Index: 225

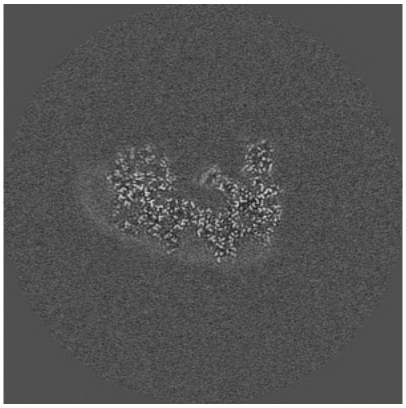
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

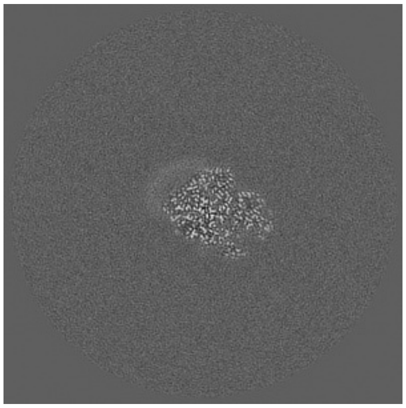
6.3.1 Primary map



X Index: 237

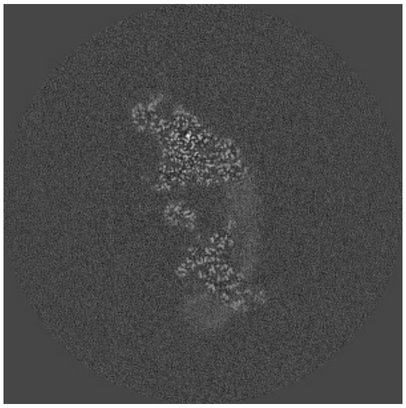


Y Index: 227

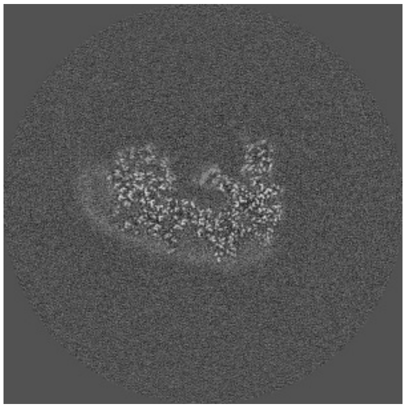


Z Index: 286

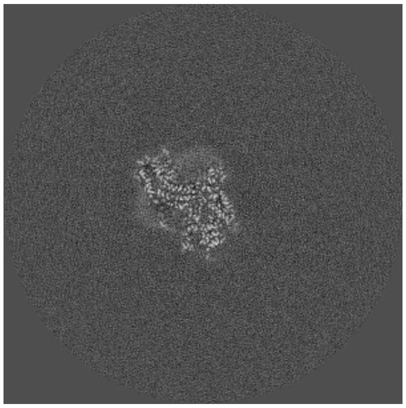
6.3.2 Raw map



X Index: 237



Y Index: 227



Z Index: 252

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

6.4 Orthogonal surface views

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0241. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X

Y

Z

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

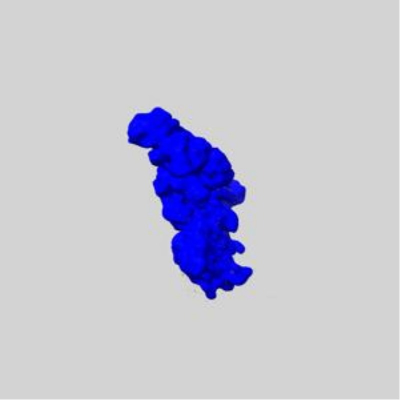
6.5 Mask visualisation ⓘ

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

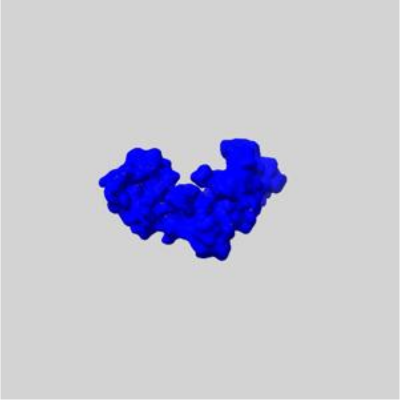
A mask typically either:

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

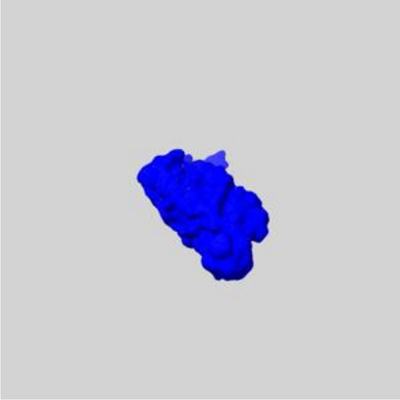
6.5.1 emd_11424_msk_1.map ⓘ



X



Y

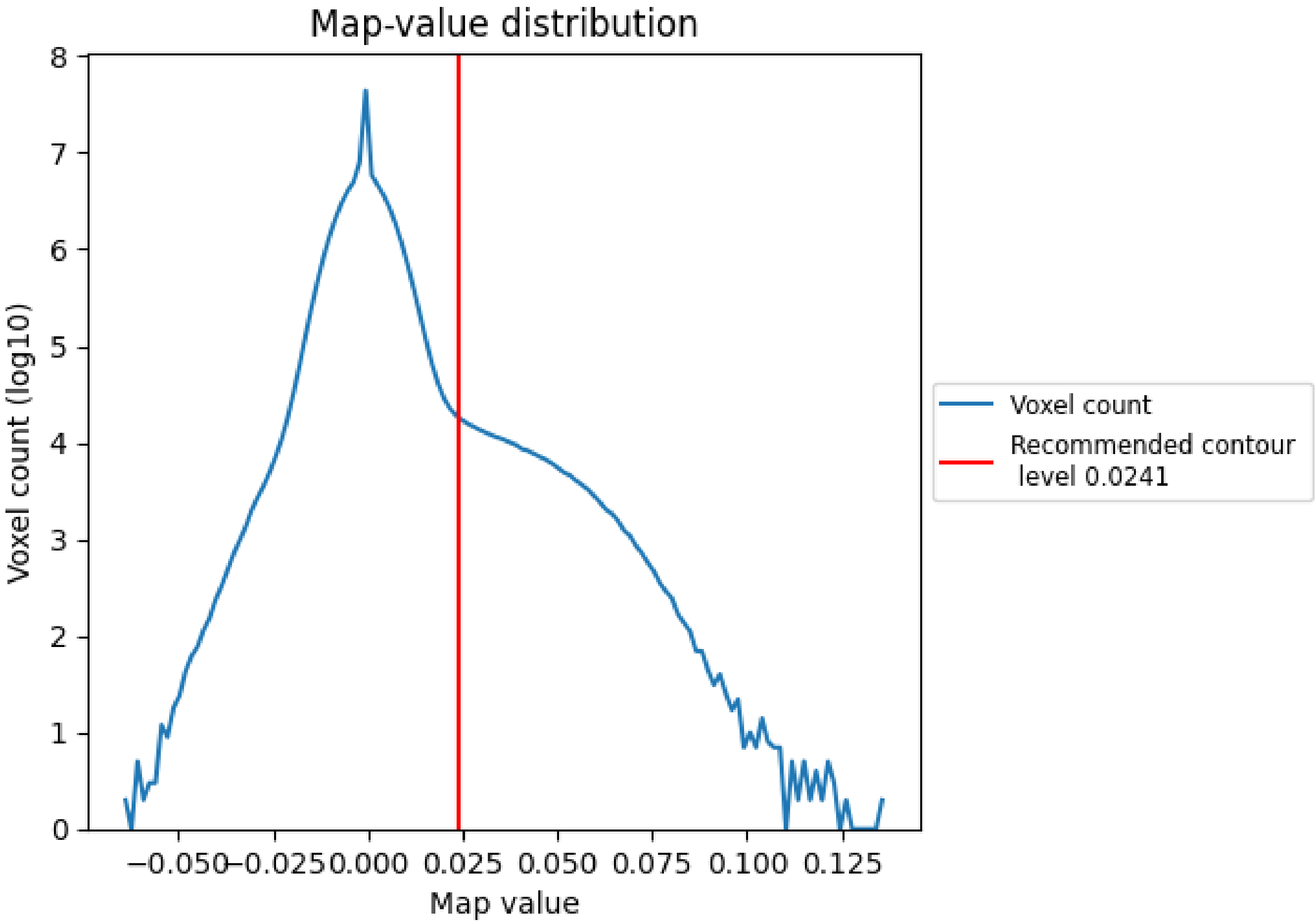


Z

7 Map analysis ⓘ

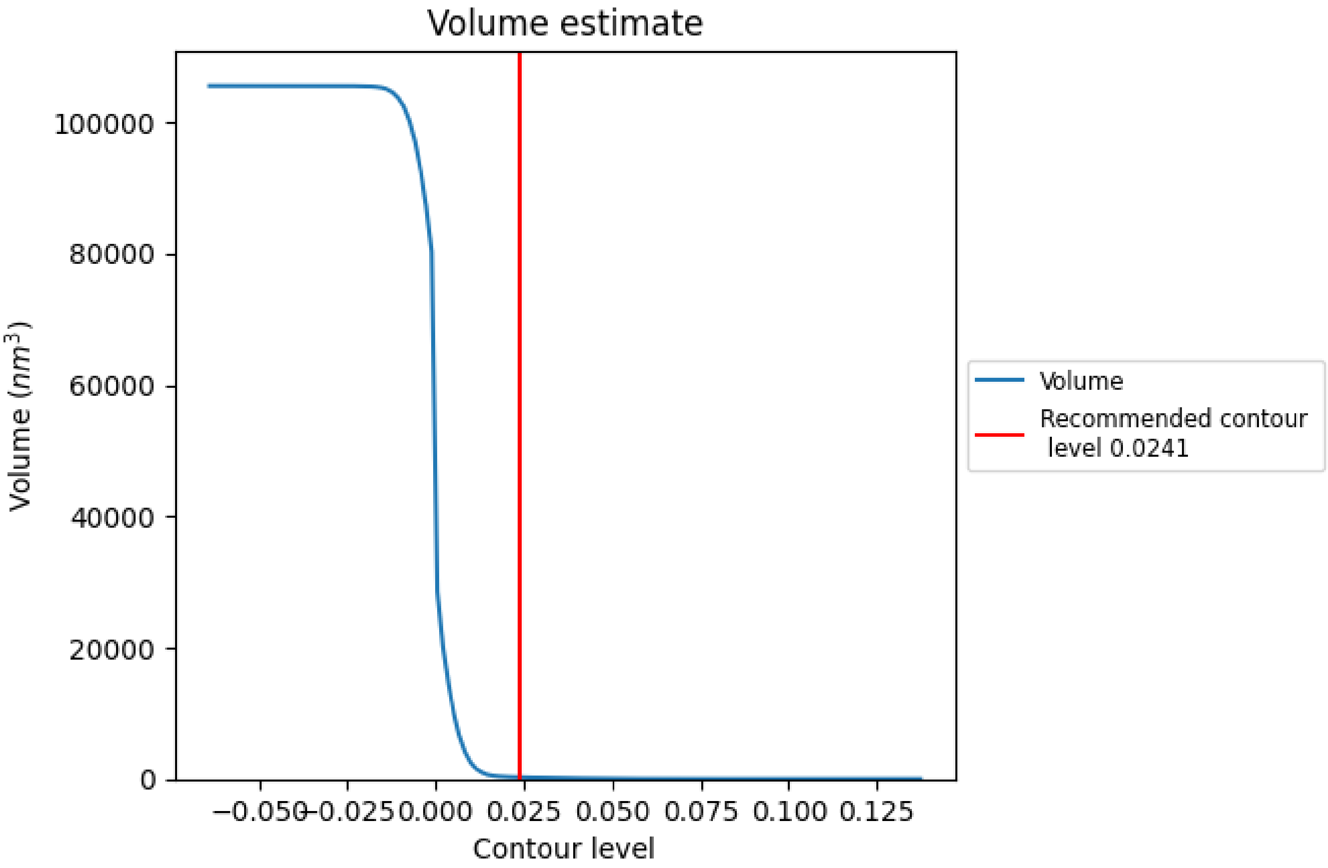
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

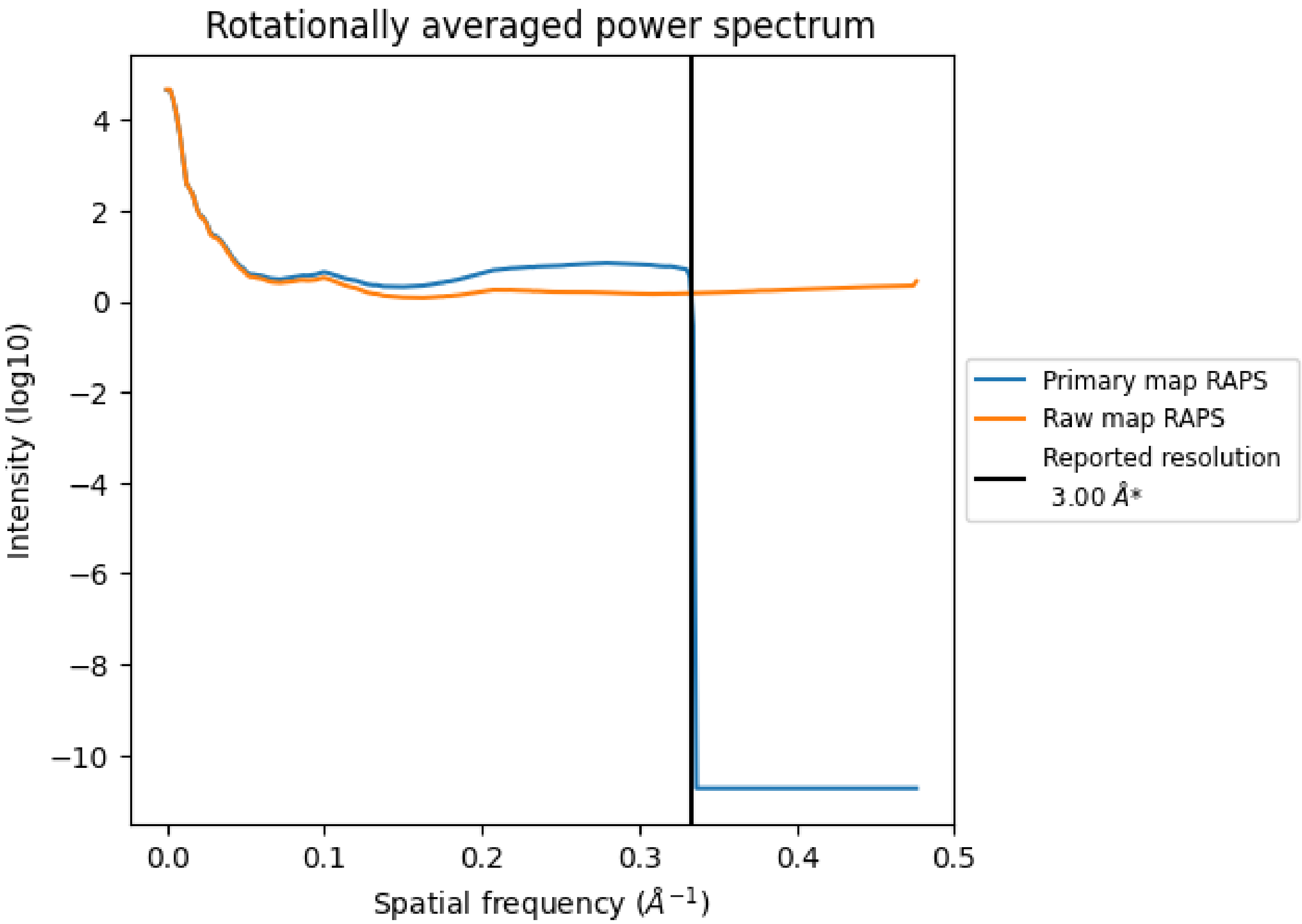
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 258 nm^3; this corresponds to an approximate mass of 233 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 ⓘ

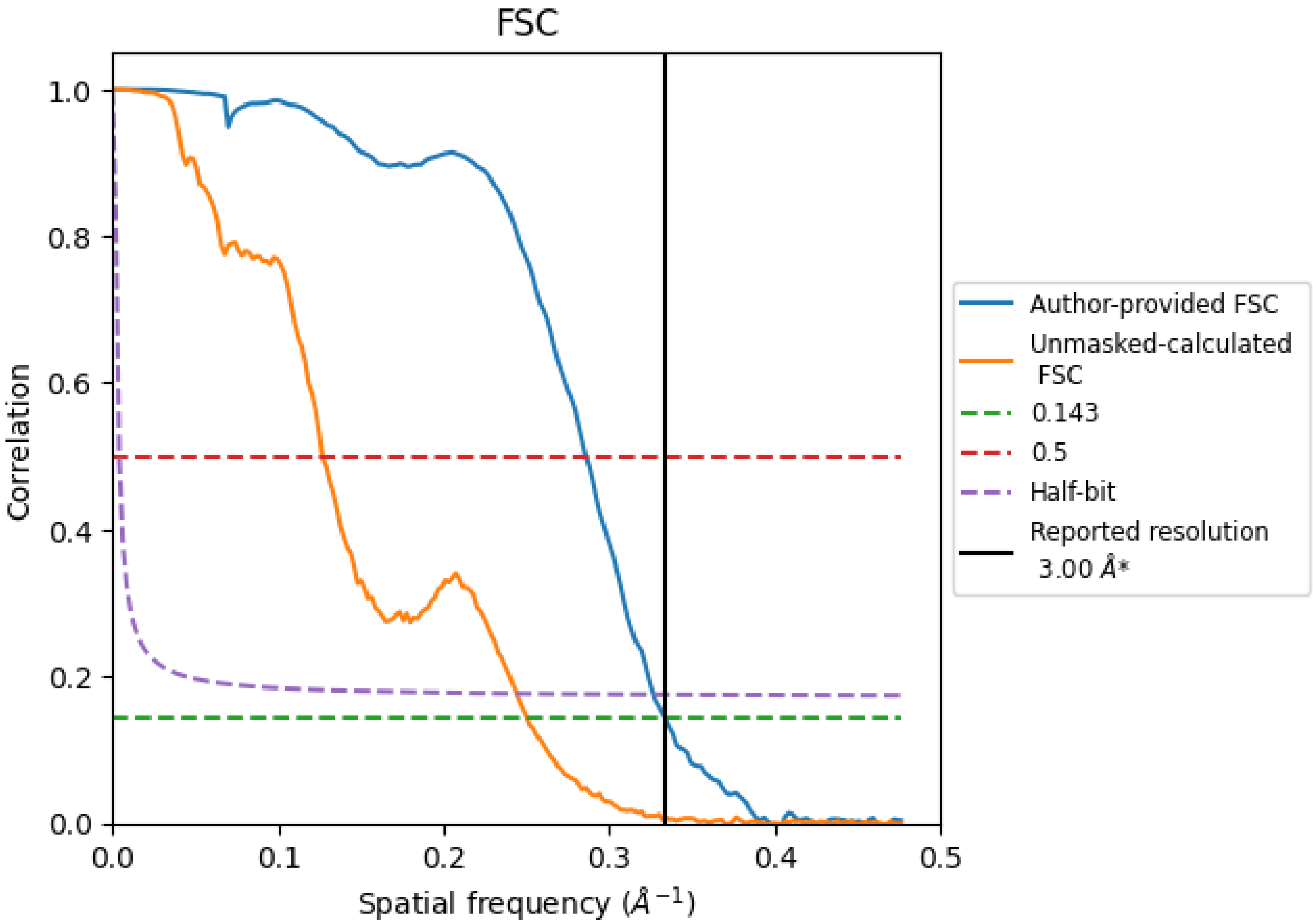


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

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 0.333 Å^{-1}

8.2 Resolution estimates ⓘ

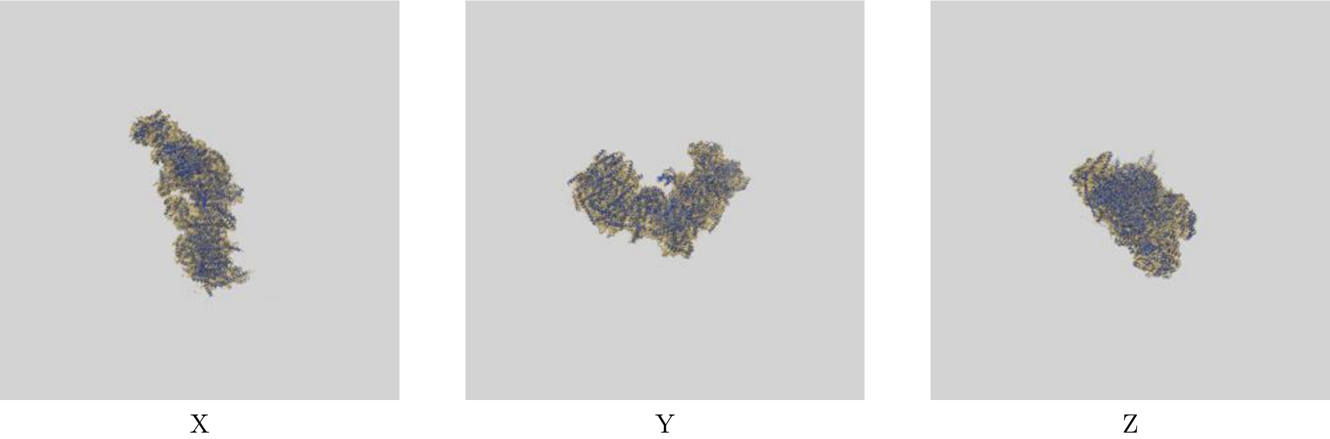
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.00	3.50	3.06
Unmasked-calculated*	3.99	7.89	4.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.99 differs from the reported value 3.0 by more than 10 %

9 Map-model fit (i)

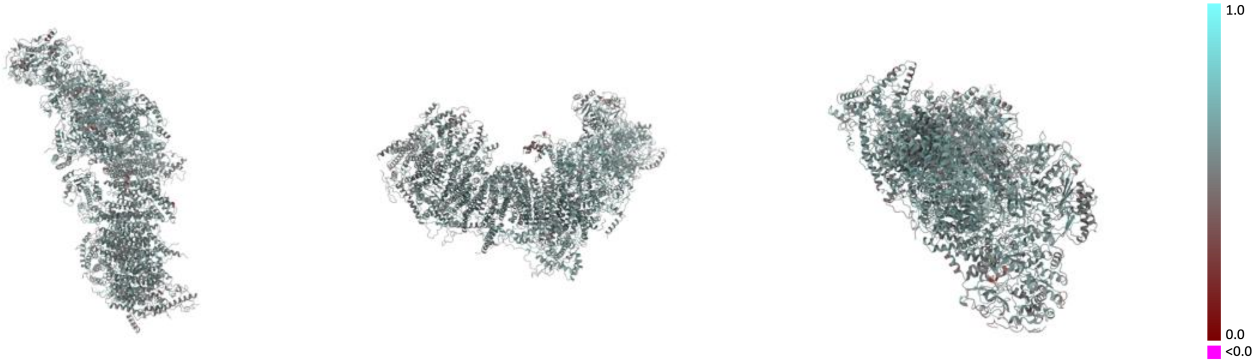
This section contains information regarding the fit between EMDB map EMD-11424 and PDB model 6ZTQ. Per-residue inclusion information can be found in section 3 on page 19.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.0241 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

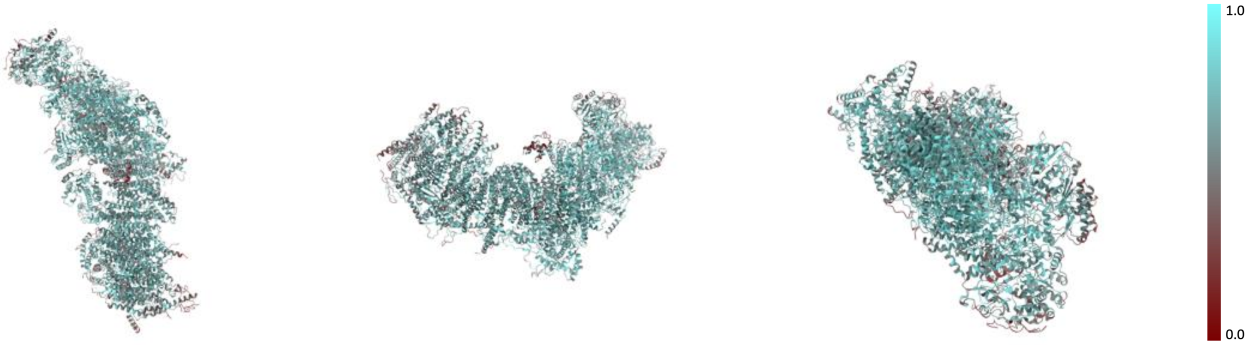
9.2 Q-score mapped to coordinate model



X Y Z

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

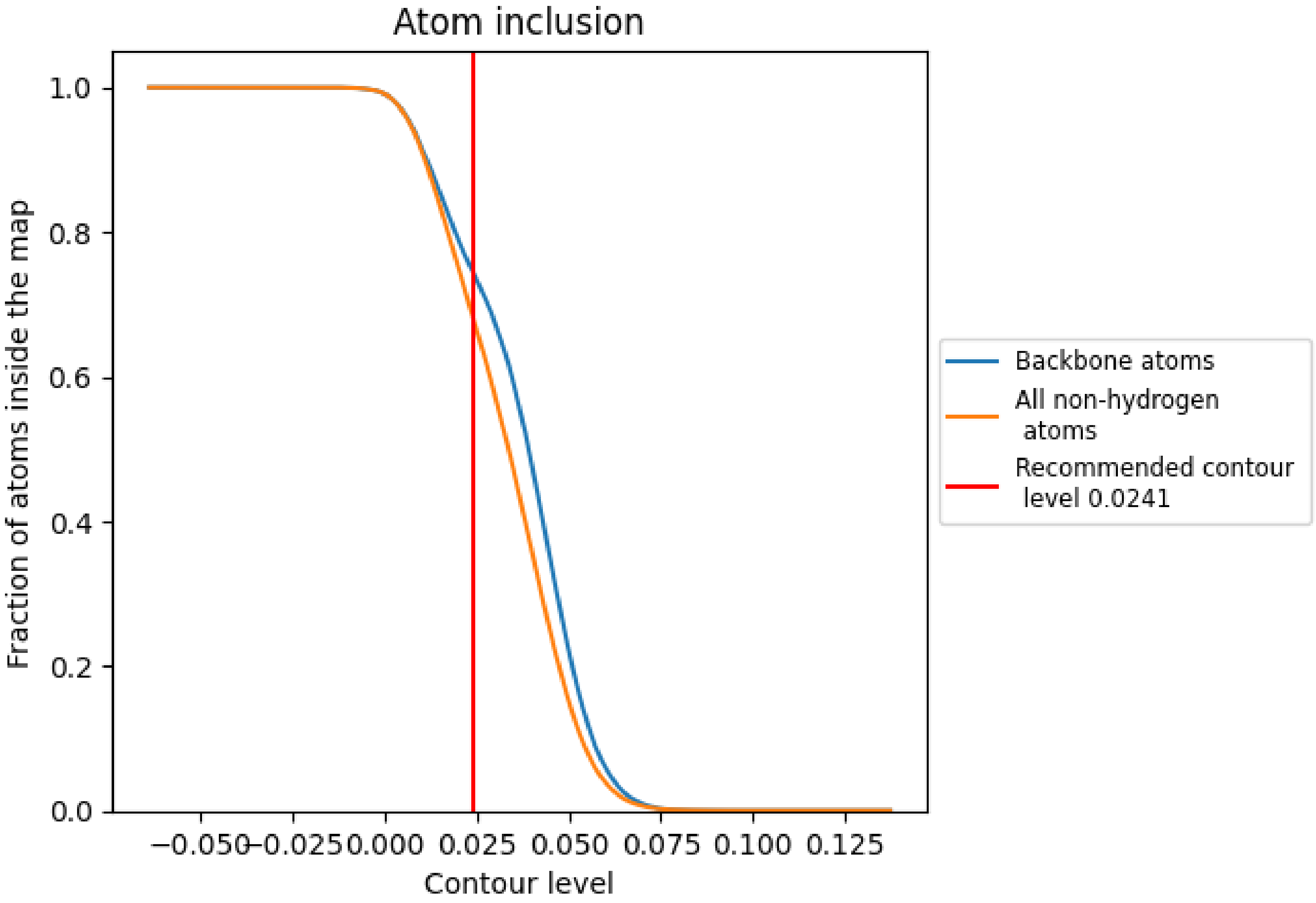
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0241).

9.4 Atom inclusion ⓘ



At the recommended contour level, 74% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0241) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6792	0.5530
A	0.7086	0.5620
B	0.7818	0.5930
C	0.7833	0.5950
D	0.7652	0.5850
E	0.6006	0.5170
F	0.6401	0.5310
G	0.6865	0.5520
H	0.7512	0.5790
I	0.7708	0.5830
J	0.6576	0.5470
K	0.7376	0.5730
L	0.6689	0.5420
M	0.7362	0.5730
N	0.7233	0.5750
O	0.7172	0.5610
P	0.7155	0.5630
Q	0.7062	0.5610
R	0.6938	0.5650
S	0.5648	0.5100
T	0.3639	0.4550
U	0.5505	0.5110
V	0.6652	0.5430
W	0.6865	0.5600
X	0.6728	0.5450
Y	0.6200	0.5360
Z	0.6650	0.5450
a	0.7430	0.5680
b	0.6397	0.5500
c	0.6047	0.5100
d	0.6536	0.5630
e	0.6877	0.5520
f	0.5553	0.5320
g	0.6550	0.5460
h	0.6791	0.5660

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Chain	Atom inclusion	Q-score
i	0.5590	0.5290
j	0.5249	0.5110
k	0.5034	0.5050
l	0.6452	0.5480
m	0.6380	0.5340
n	0.6345	0.5290
o	0.4838	0.4780
p	0.6347	0.5330
q	0.7099	0.5710
r	0.6641	0.5520
s	0.5940	0.5260