wwPDB EM Validation Summary Report (i)

Sep 9, 2026 – 03:33 am BST

PDB ID	:	6ZKL / pdb_00006zkl
EMDB ID	:	EMD-11253
Title	:	Complex I inhibited by rotenone, open1
Authors	:	Kampjut, D.; Sazanov, L.A.
Deposited on	:	2020-06-30
Resolution	:	3.10 Å(reported)
Based on initial model	:	5LNK

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

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

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

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

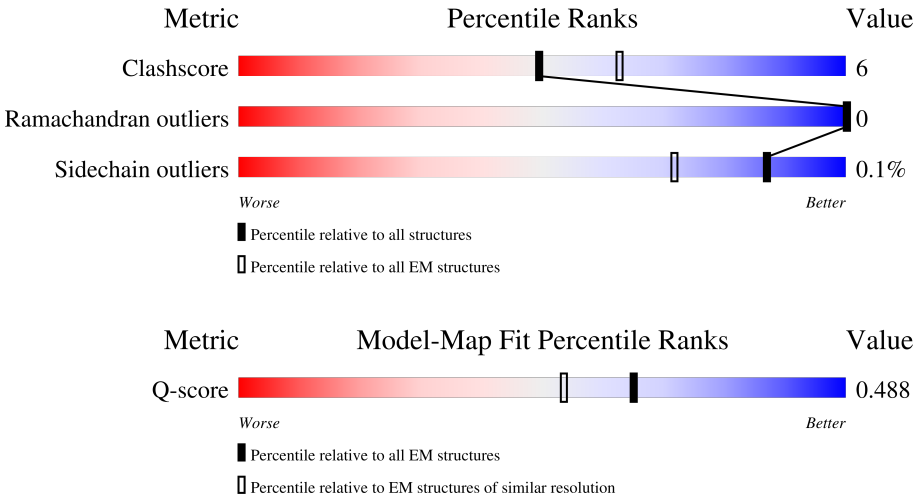
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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.



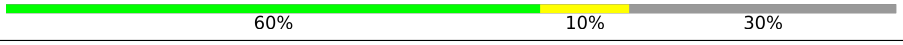
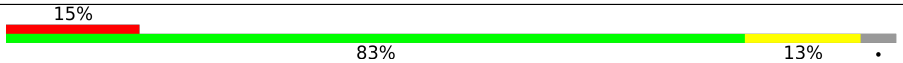
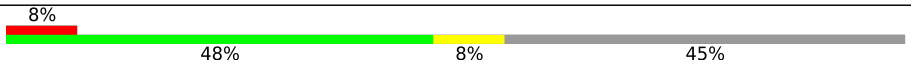
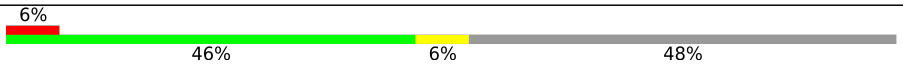
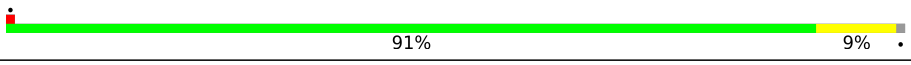
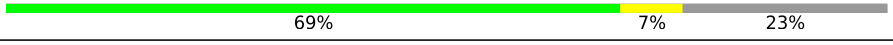
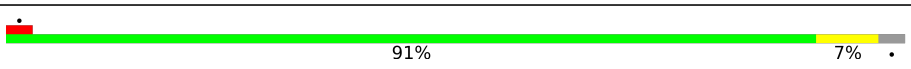
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	1	464	75% 18% 7%
2	2	246	71% 15% 13%
3	3	727	79% 16% 5%
4	4	463	5% 73% 19% 8%

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Mol	Chain	Length	Quality of chain
5	5	266	
6	6	223	
7	9	217	
8	A	115	
9	H	318	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	V	141	
16	W	189	
17	X	157	
17	j	157	
18	Y	172	
19	Z	175	
20	a	109	
21	b	124	
22	c	170	
23	d	380	
24	e	99	
25	f	116	
26	g	140	
27	h	114	
28	i	145	

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Mol	Chain	Length	Quality of chain
29	k	355	79% 11% 10%
30	l	106	84% 15%
31	m	84	86% 10% 5%
32	n	98	15% 72% 8% 19%
33	o	122	7% 75% 23%
34	p	130	23% 86% 12%
35	q	144	85% 12%
36	r	128	64% 13% 23%
37	s	137	7% 74% 15% 11%
38	t	179	12% 83% 16%
39	u	108	5% 52% 8% 40%
40	v	186	9% 69% 15% 17%
41	w	154	5% 55% 11% 34%
42	x	76	59% 5% 36%
43	y	58	7% 78% 9% 14%
44	z	70	90% 10%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	CDL	L	704	X	-	-	-
53	CDL	V	204	X	-	-	-
53	CDL	Y	201	X	-	-	-
53	CDL	o	201	X	-	-	-

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 67492 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 dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	430	3312	2086	593	613	20	0	0

- Molecule 2 is a protein called Mitochondrial complex I, 24 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	213	1655	1058	278	309	10	0	0

- Molecule 3 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	688	5275	3301	922	1011	41	0	0

- Molecule 4 is a protein called Mitochondrial complex I, 49 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	426	3427	2188	590	624	25	0	0

- Molecule 5 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	208	1726	1112	296	315	3	0	0

- Molecule 6 is a protein called Mitochondrial complex I, PSST subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	156	1247	795	225	213	14	0	0

- Molecule 7 is a protein called Mitochondrial complex I, TYKY subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	110	Total	C	N	O	S	0	0
			880	593	128	153	6		

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	314	Total	C	N	O	S	0	0
			2498	1685	380	414	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	166	Total	C	N	O	S	0	0
			1264	851	181	219	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			749	490	112	132	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			4806	3187	746	829	44		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3647	2429	571	607	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	347	Total	C	N	O	S	0	0
			2723	1808	416	459	40		

- Molecule 15 is a protein called Mitochondrial complex I, B14.7 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	140	Total	C	N	O	S	0	0
			1028	656	175	191	6		

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	139	Total	C	N	O	S	0	0
			1155	761	194	198	2		

- Molecule 17 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	87	Total	C	N	O	S	0	0
			701	451	103	142	5		
17	j	82	Total	C	N	O	S	0	0
			660	425	98	132	5		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	171	Total	C	N	O	S	0	0
			1403	889	253	251	10		

- Molecule 19 is a protein called Mitochondrial complex I, PDSW subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	171	Total	C	N	O	S	0	0
			1441	905	266	262	8		

- Molecule 20 is a protein called Mitochondrial complex I, 10 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	a	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

- Molecule 21 is a protein called Mitochondrial complex I, 13 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	b	95	Total	C	N	O	S	0	0
			737	451	139	144	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	126	Total	C	N	O	S	0	0
			1024	646	182	193	3		

- Molecule 23 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	297	Total	C	N	O	S	0	0
			2372	1516	432	419	5		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	86	Total	C	N	O	S	0	0
			691	434	129	126	2		

- Molecule 25 is a protein called Mitochondrial complex I, B13 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	113	Total	C	N	O	S	0	0
			917	595	153	167	2		

- Molecule 26 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	g	114	Total	C	N	O	S	0	0
			969	619	180	166	4		

- Molecule 27 is a protein called Mitochondrial complex I, B14.5a subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	h	96	Total	C	N	O	S	0	0
			769	480	146	140	3		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	i	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	k	320	Total	C	N	O	P	S	0	0
			2596	1659	432	494	1	10		

- Molecule 30 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	l	105	Total	C	N	O	S	0	0
			874	551	164	153	6		

- Molecule 31 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	m	80	Total	C	N	O	S	0	0
			626	411	103	110	2		

- Molecule 32 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	n	79	Total	C	N	O	S	0	0
			634	415	106	111	2		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	o	120	Total	C	N	O	S	0	0
			1004	652	175	172	5		

- Molecule 34 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	p	128	Total	C	N	O	S	0	0
			1059	675	189	194	1		

- Molecule 35 is a protein called Mitochondrial complex I, B16.6 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	q	139	Total	C	N	O	S	0	0
			1142	733	200	200	9		

- Molecule 36 is a protein called Mitochondrial complex I, B17 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	r	99	Total	C	N	O	S	0	0
			846	554	149	142	1		

- Molecule 37 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	s	122	Total	C	N	O	S	0	0
			1047	653	199	186	9		

- Molecule 38 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	t	177	Total	C	N	O	S	0	0
			1520	973	279	262	6		

- Molecule 39 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	u	65	Total	C	N	O	S	0	0
			563	372	93	97	1		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	v	155	Total	C	N	O	S	0	0
			1307	846	213	239	9		

- Molecule 41 is a protein called Mitochondrial complex I, ESSS subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	w	101	Total	C	N	O	S	0	0
			846	542	140	160	4		

- Molecule 42 is a protein called Mitochondrial complex I, KFYI subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	x	49	Total	C	N	O	0	0
			412	271	70	71		

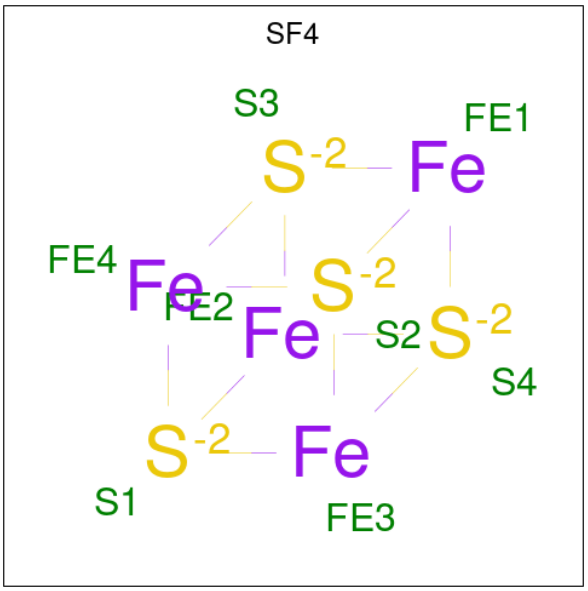
- Molecule 43 is a protein called Mitochondrial complex I, MNLL subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	y	50	Total	C	N	O	0	0
			436	287	77	72		

- Molecule 44 is a protein called Mitochondrial complex I, MWFE subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	z	70	Total	C	N	O	S	0	0
			576	369	106	96	5		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



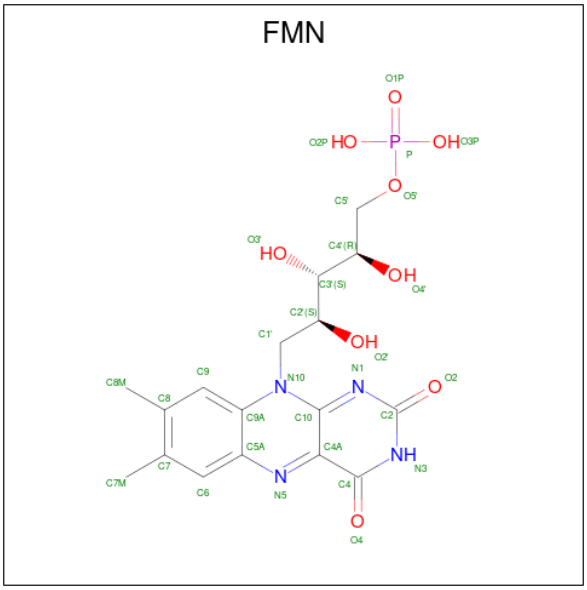
Mol	Chain	Residues	Atoms			AltConf
45	1	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	6	1	Total	Fe	S	0
			8	4	4	

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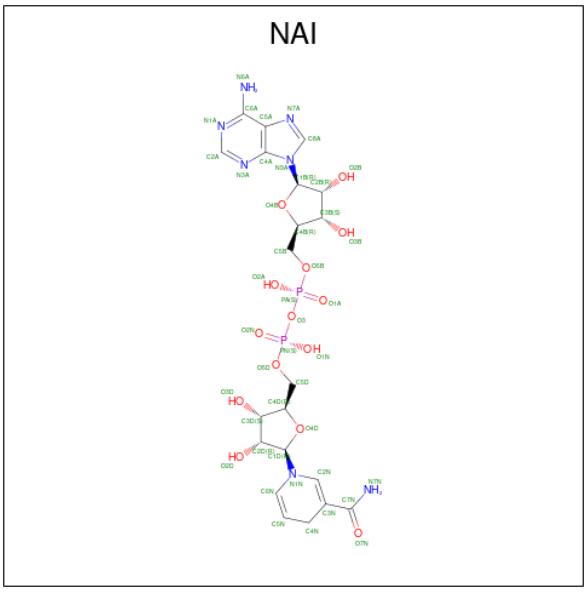
Mol	Chain	Residues	Atoms	AltConf
45	9	1	Total Fe S 8 4 4	0
45	9	1	Total Fe S 8 4 4	0

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



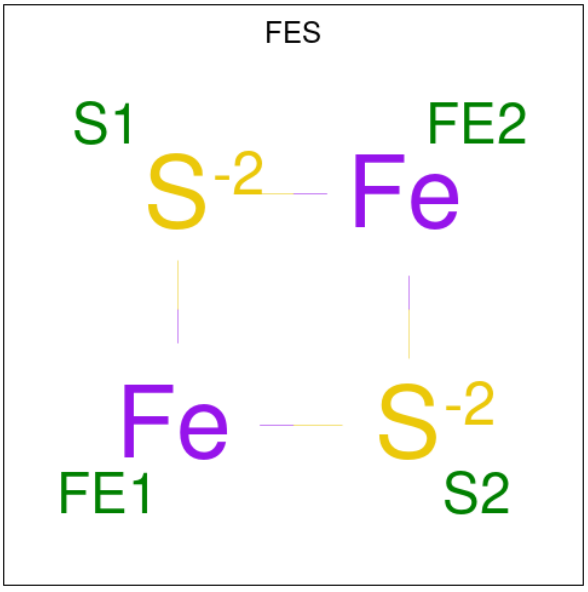
Mol	Chain	Residues	Atoms	AltConf
46	1	1	Total C N O P 31 17 4 9 1	0

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf
47	1	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

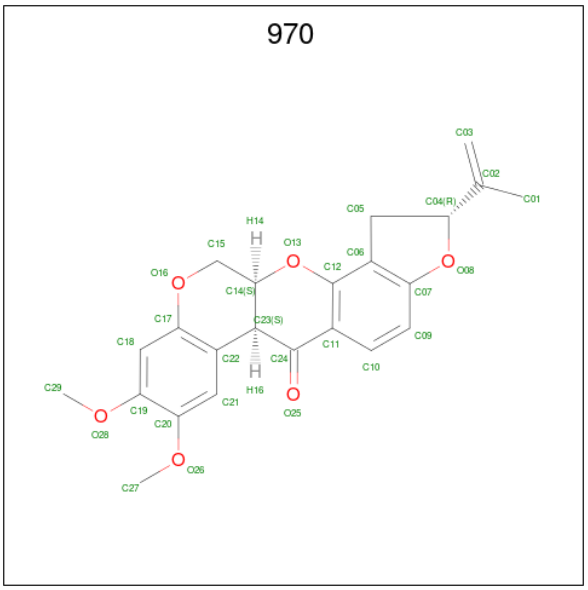


Mol	Chain	Residues	Atoms			AltConf
48	2	1	Total	Fe	S	0
			4	2	2	
48	3	1	Total	Fe	S	0
			4	2	2	

- Molecule 49 is POTASSIUM ION (CCD ID: K) (formula: K).

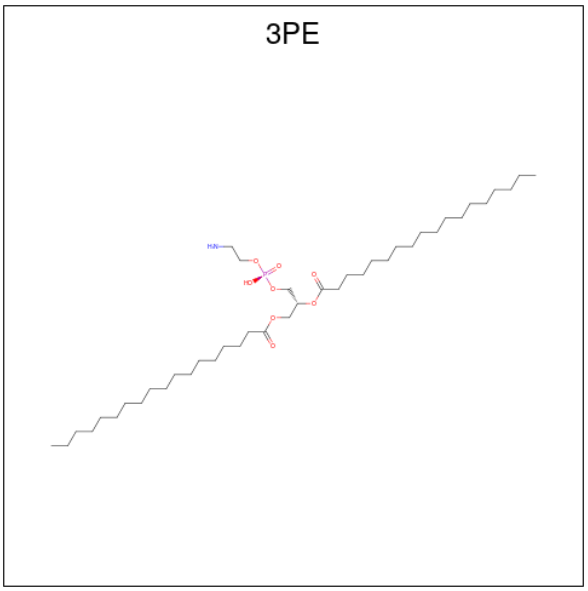
Mol	Chain	Residues	Atoms	AltConf
49	3	1	Total K 1 1	0

- Molecule 50 is (2R,6aS,12aS)-8,9-dimethoxy-2-(prop-1-en-2-yl)-1,2,12,12a-tetrahydrofuro[2',3':7,8][1]benzopyrano[2,3-c][1]benzopyran-6(6aH)-one (CCD ID: 970) (formula: $C_{23}H_{22}O_6$) (labeled as "Ligand of Interest" by depositor).



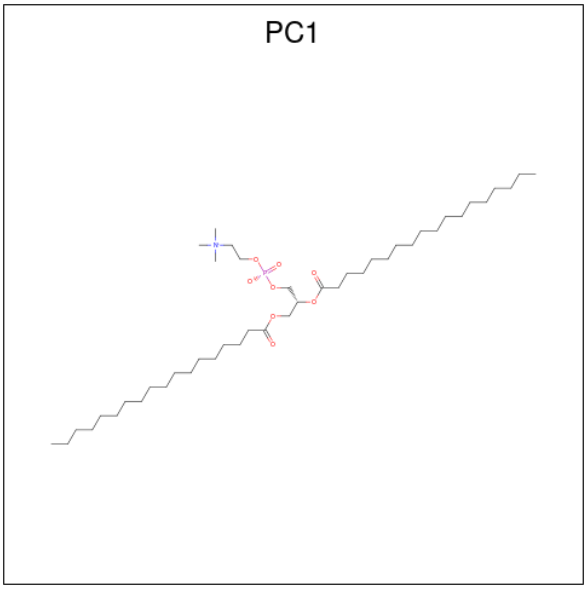
Mol	Chain	Residues	Atoms	AltConf
50	6	1	Total C O 29 23 6	0
50	H	1	Total C O 29 23 6	0

- Molecule 51 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



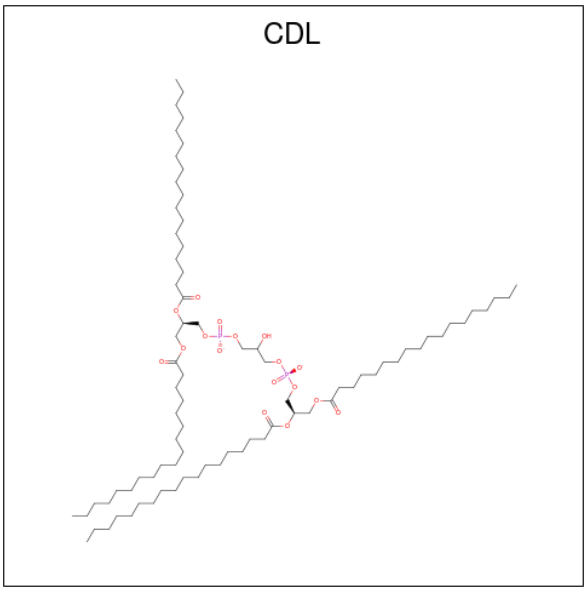
Mol	Chain	Residues	Atoms					AltConf
51	6	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	J	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	K	1	Total	C	N	O	P	0
			40	30	1	8	1	
51	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
51	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	L	1	Total	C	N	O	P	0
			31	21	1	8	1	
51	M	1	Total	C	N	O	P	0
			44	34	1	8	1	
51	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	V	1	Total	C	N	O	P	0
			35	25	1	8	1	
51	V	1	Total	C	N	O	P	0
			37	27	1	8	1	
51	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	l	1	Total	C	N	O	P	0
			31	21	1	8	1	
51	p	1	Total	C	O	P		0
			27	18	8	1		

- Molecule 52 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



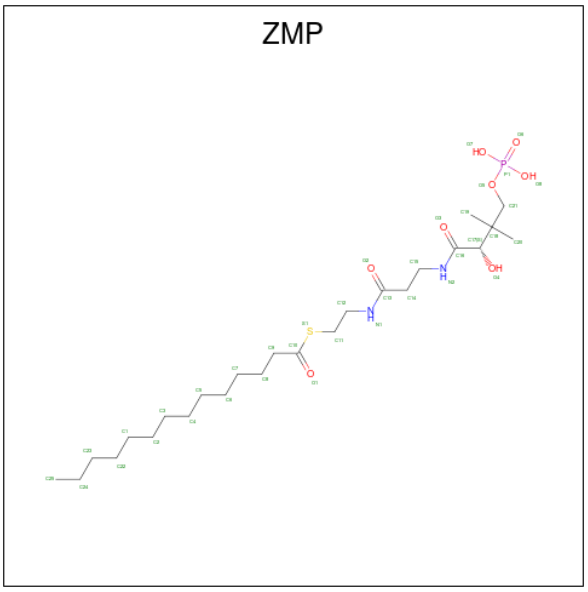
Mol	Chain	Residues	Atoms					AltConf
52	9	1	Total	C	N	O	P	0
			54	44	1	8	1	
52	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
52	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
52	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
52	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
52	w	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 53 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
53	L	1	Total	C	O	P	0
			100	81	17	2	
53	V	1	Total	C	O	P	0
			94	75	17	2	
53	V	1	Total	C	O	P	0
			85	66	17	2	
53	W	1	Total	C	O	P	0
			100	81	17	2	
53	Y	1	Total	C	O	P	0
			100	81	17	2	
53	i	1	Total	C	O	P	0
			58	39	17	2	
53	o	1	Total	C	O	P	0
			75	56	17	2	
53	o	1	Total	C	O	P	0
			90	71	17	2	

- Molecule 54 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).

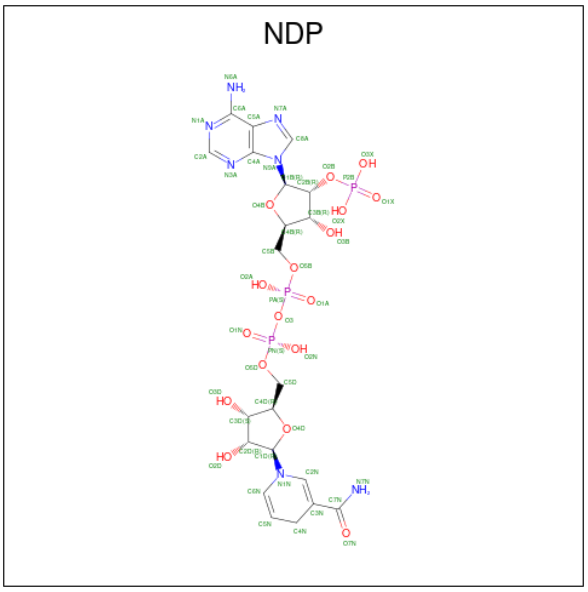


Mol	Chain	Residues	Atoms						AltConf
54	X	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	
54	g	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

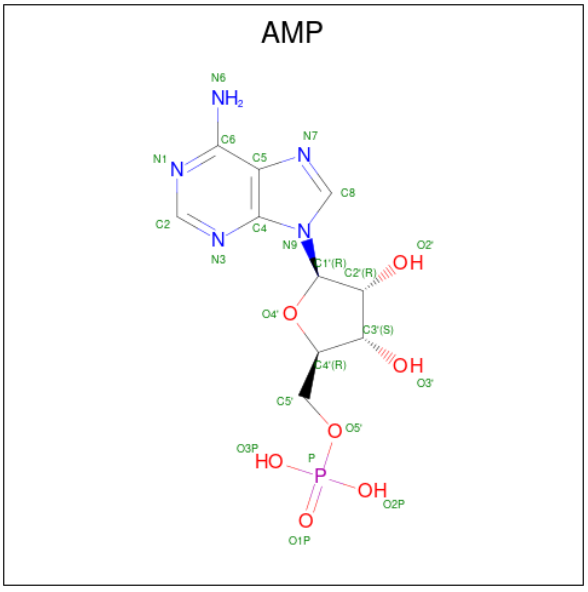
Mol	Chain	Residues	Atoms		AltConf
55	b	1	Total	Zn	0
			1	1	

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



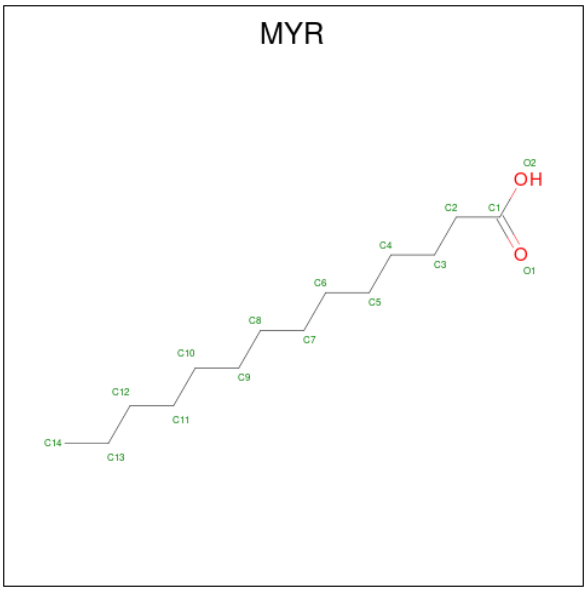
Mol	Chain	Residues	Atoms					AltConf
56	d	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 57 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					AltConf
57	k	1	Total	C	N	O	P	0
			23	10	5	7	1	

- Molecule 58 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



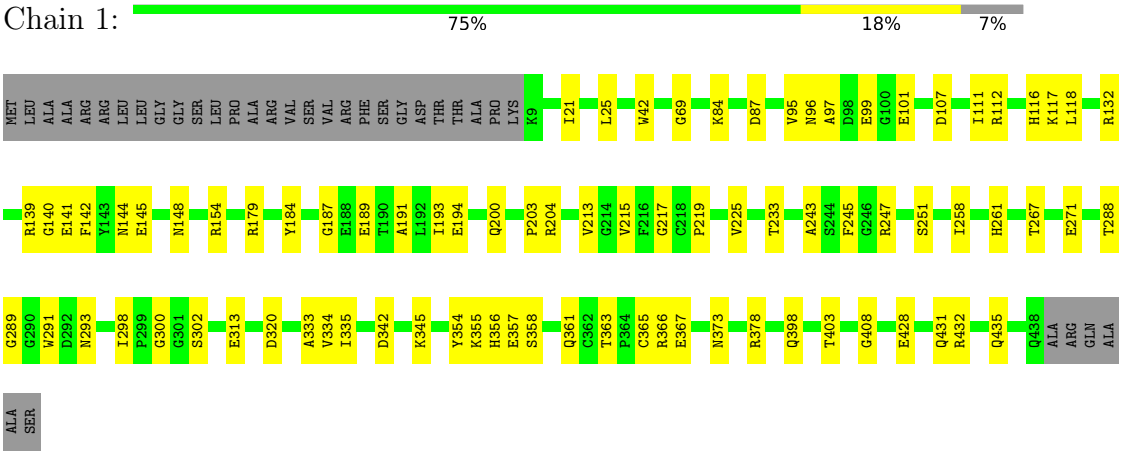
Mol	Chain	Residues	Atoms			AltConf
58	s	1	Total	C	O	0
			15	14	1	

3 Residue-property plots (i)

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

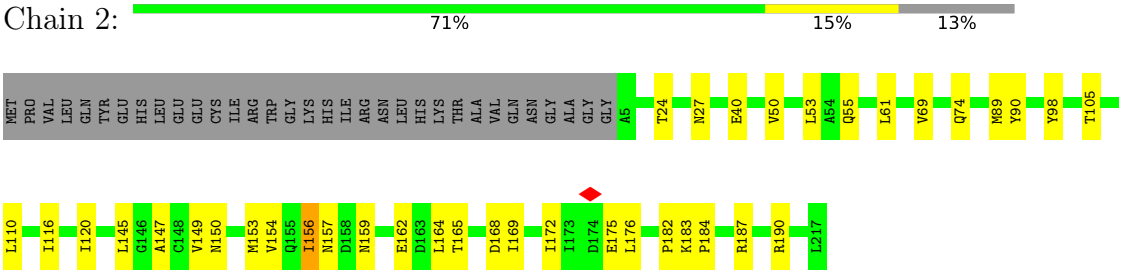
• Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1:



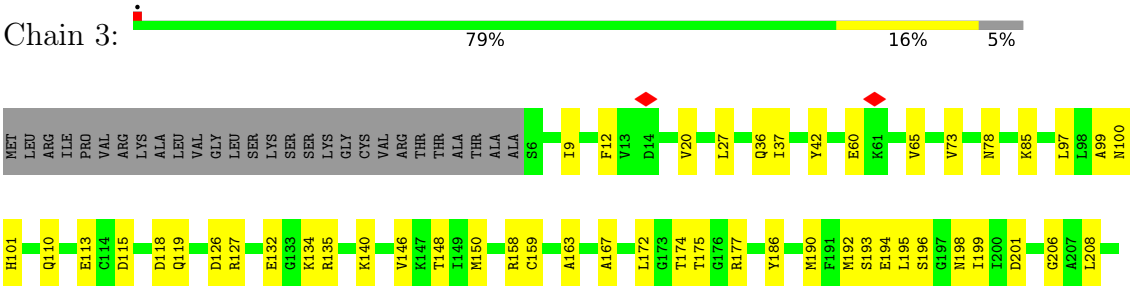
• Molecule 2: Mitochondrial complex I, 24 kDa subunit

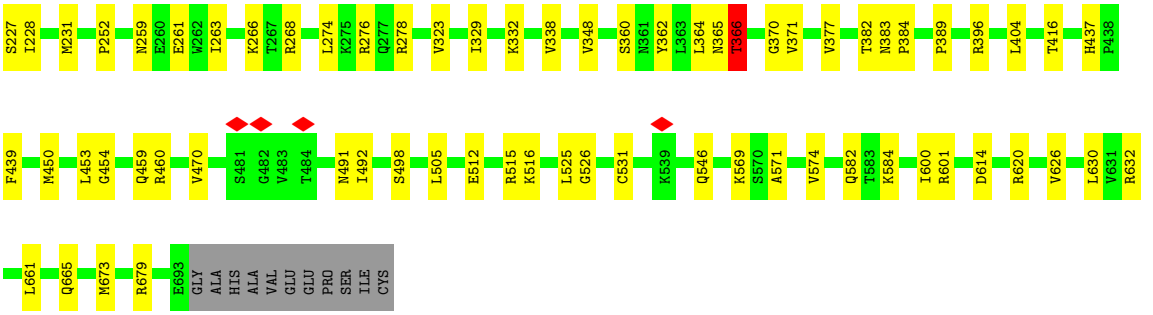
Chain 2:



• Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

Chain 3:

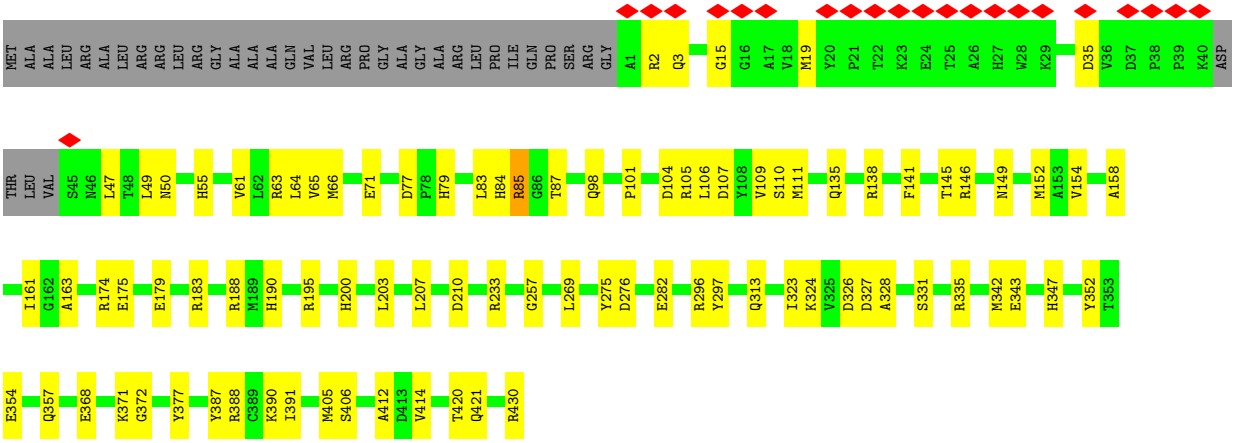




• Molecule 4: Mitochondrial complex I, 49 kDa subunit

Chain 4:

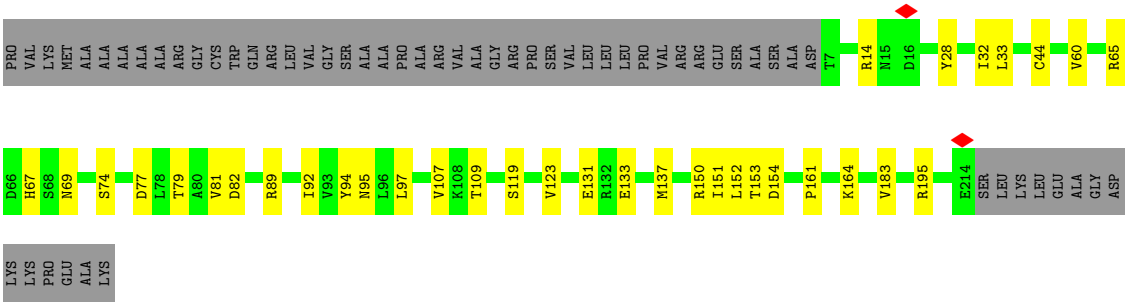




• Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3

Chain 5:

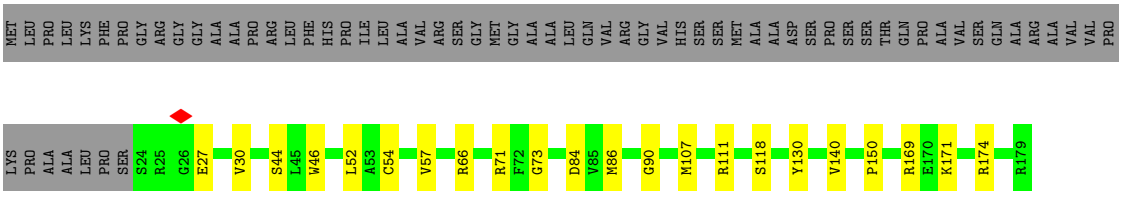




• Molecule 6: Mitochondrial complex I, PSST subunit

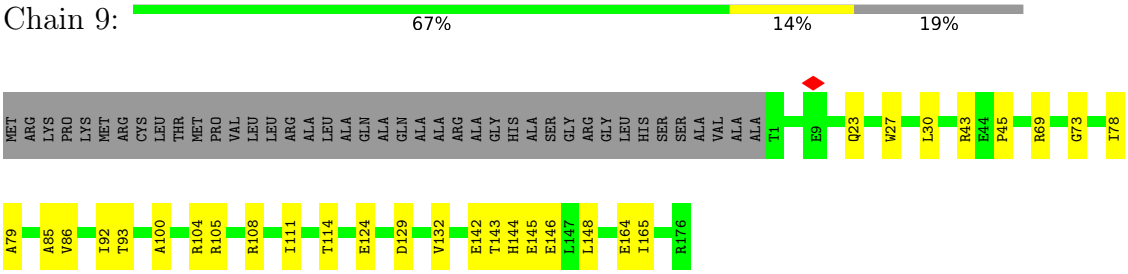
Chain 6:





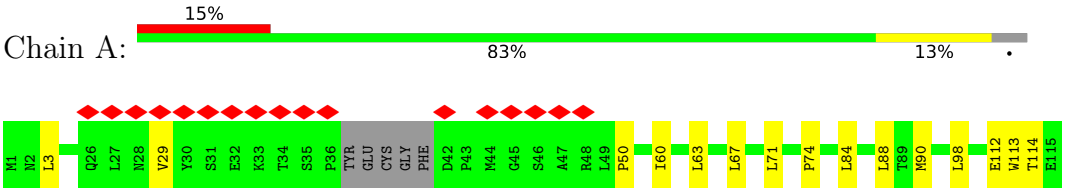
• Molecule 7: Mitochondrial complex I, TYKY subunit

Chain 9:



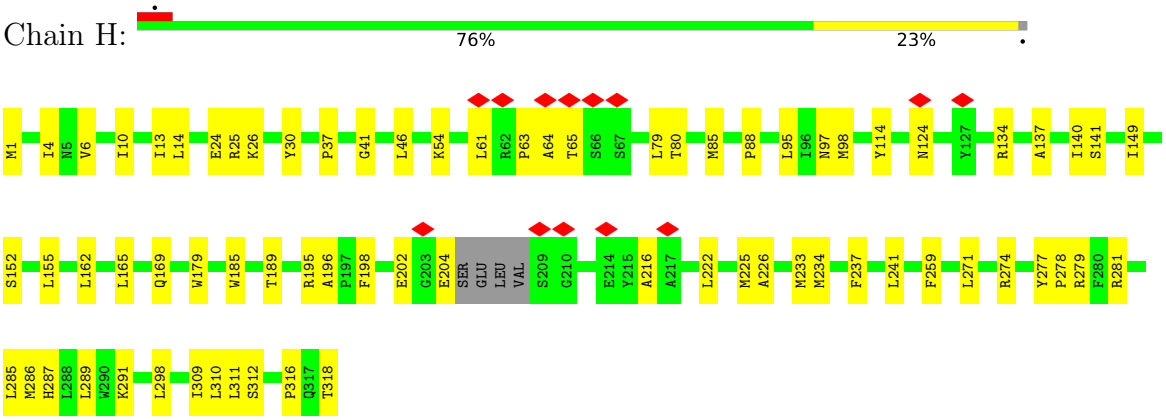
• Molecule 8: NADH-ubiquinone oxidoreductase chain 3

Chain A:



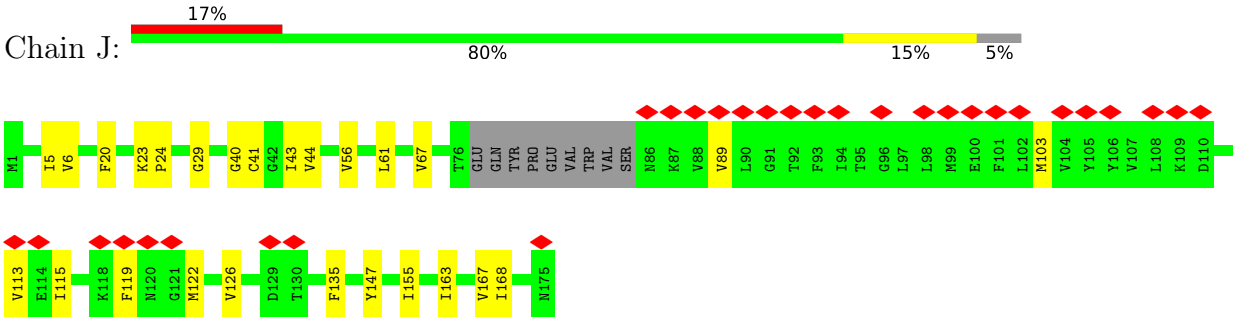
• Molecule 9: NADH-ubiquinone oxidoreductase chain 1

Chain H:



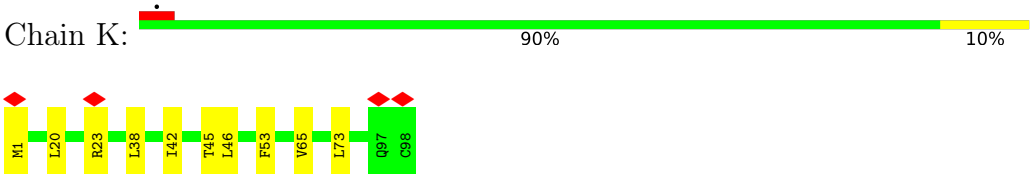
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:



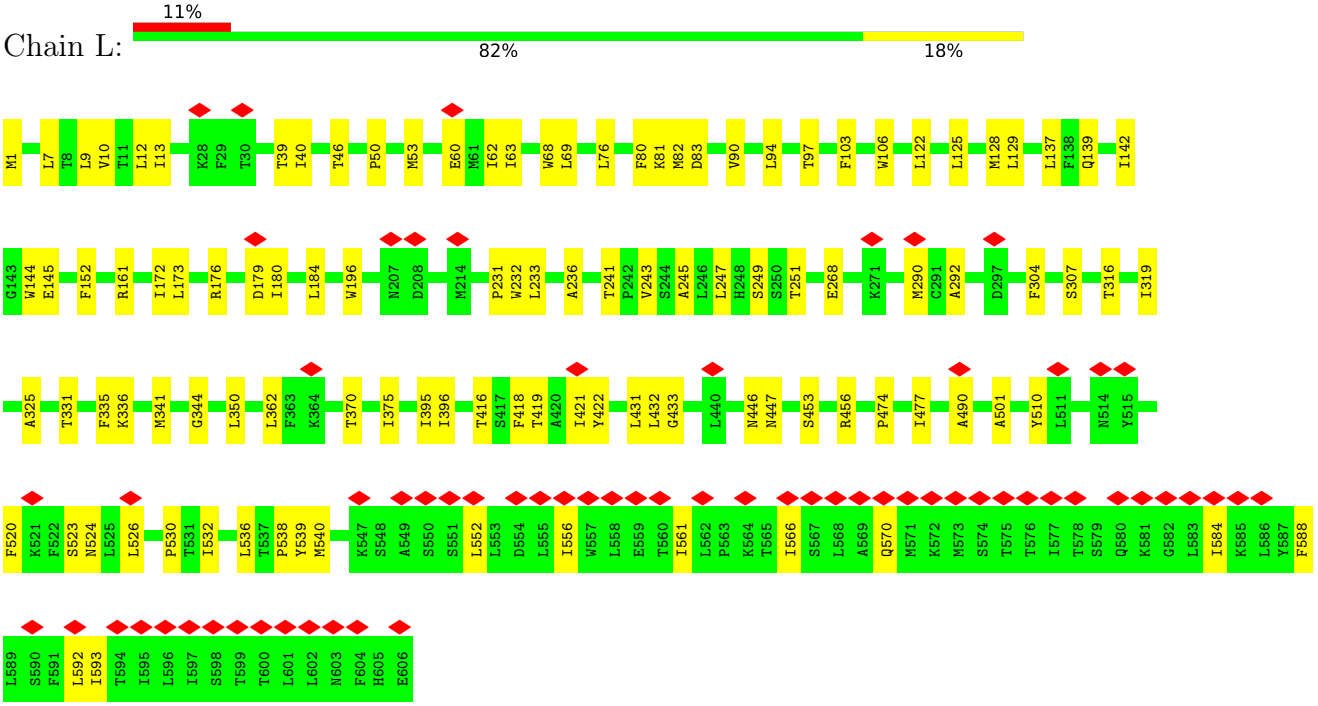
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:



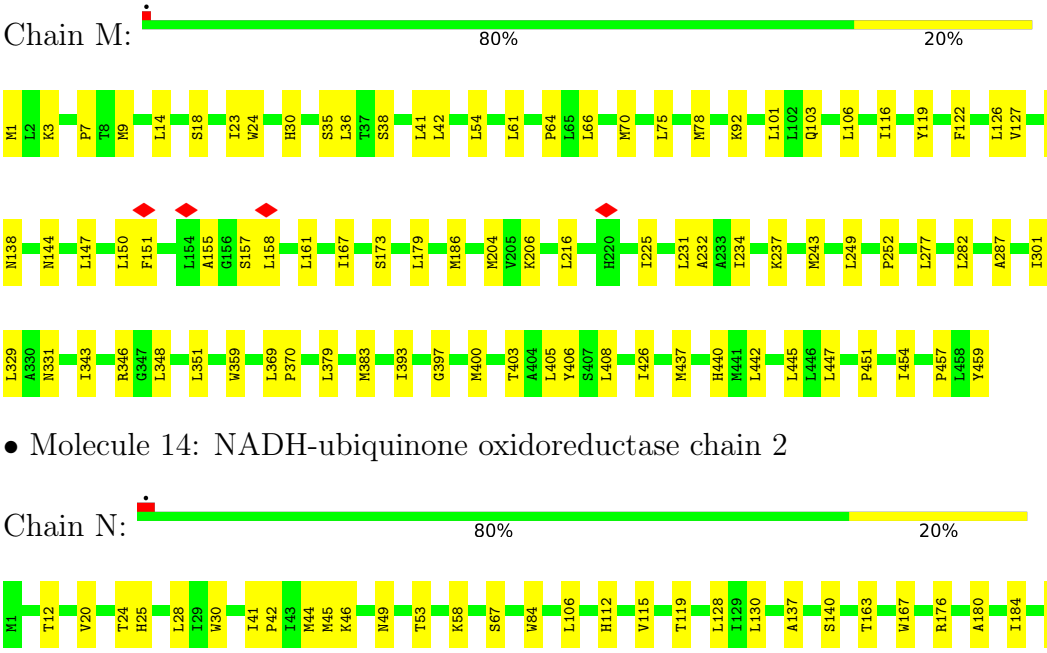
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:



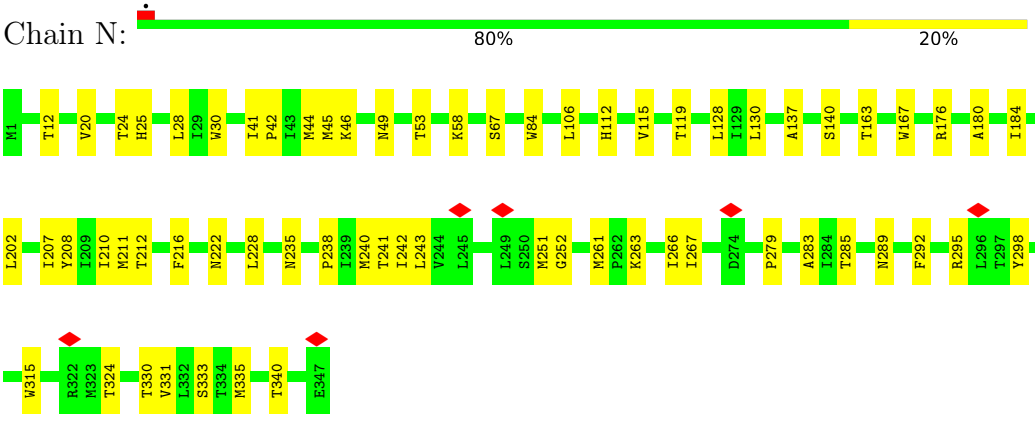
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:



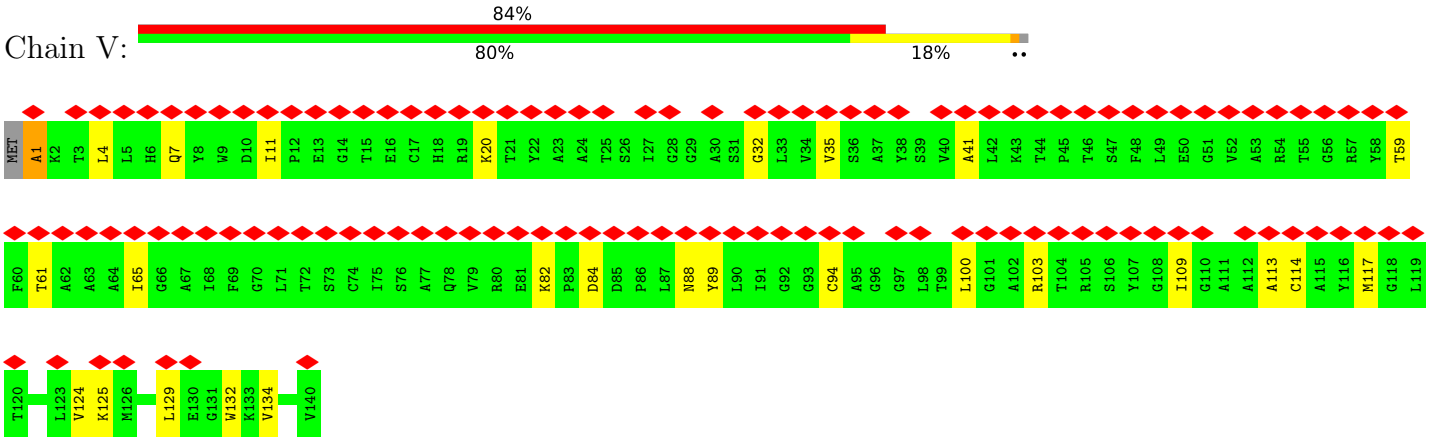
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:



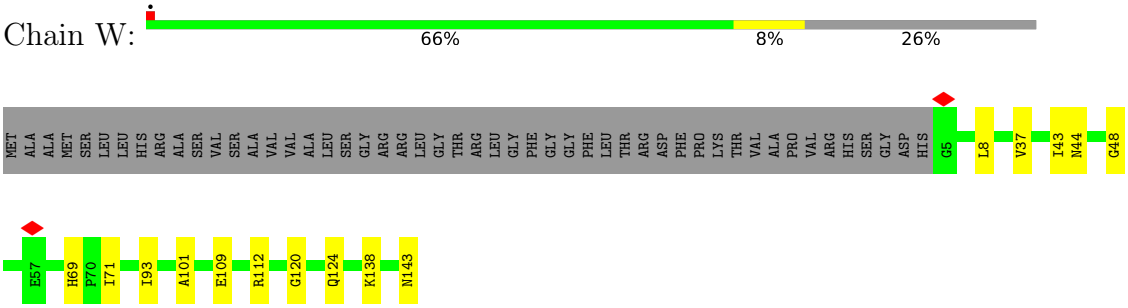
• Molecule 15: Mitochondrial complex I, B14.7 subunit

Chain V:



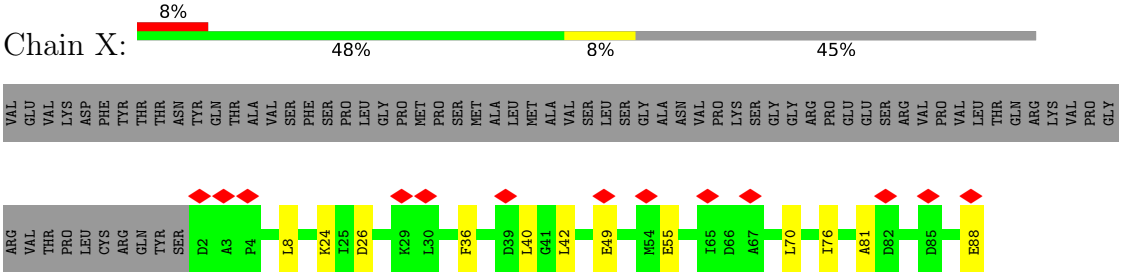
• Molecule 16: NADH:ubiquinone oxidoreductase subunit B5

Chain W:



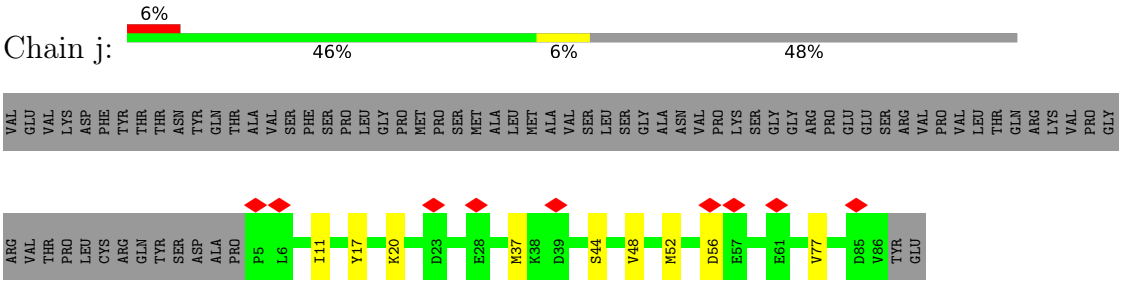
• Molecule 17: Acyl carrier protein

Chain X:



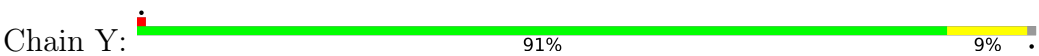
• Molecule 17: Acyl carrier protein

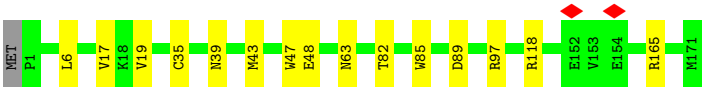
Chain j:



• Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain Y:

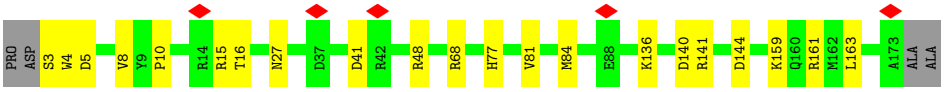




• Molecule 19: Mitochondrial complex I, PDSW subunit

Chain Z:





• Molecule 20: Mitochondrial complex I, 10 kDa subunit

Chain a:



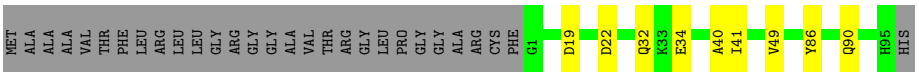




• Molecule 21: Mitochondrial complex I, 13 kDa subunit

Chain b:

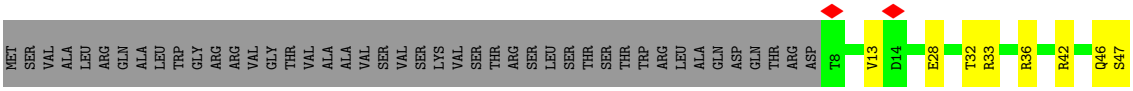


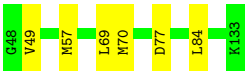


• Molecule 22: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain c:



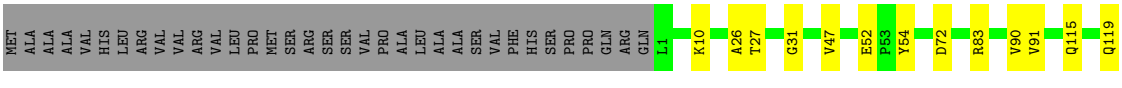




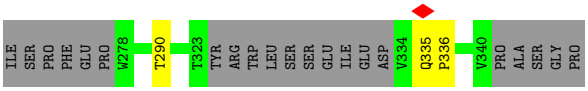
• Molecule 23: NADH:ubiquinone oxidoreductase subunit A9

Chain d:





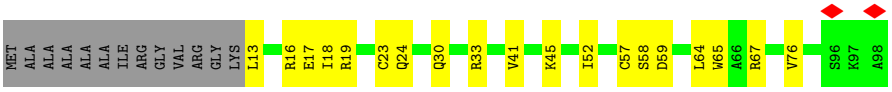




• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain e:

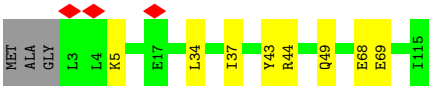




• Molecule 25: Mitochondrial complex I, B13 subunit

Chain f:

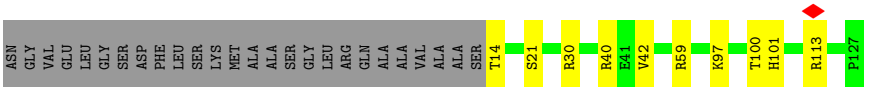




• Molecule 26: NADH:ubiquinone oxidoreductase subunit A6

Chain g:

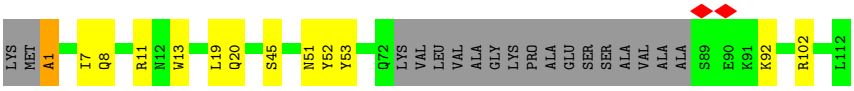




• Molecule 27: Mitochondrial complex I, B14.5a subunit

Chain h:





• Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain i:

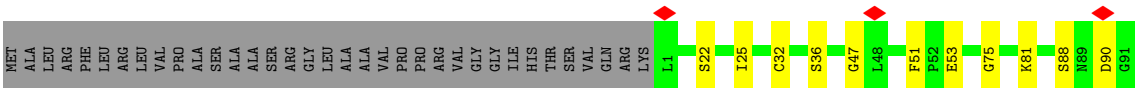


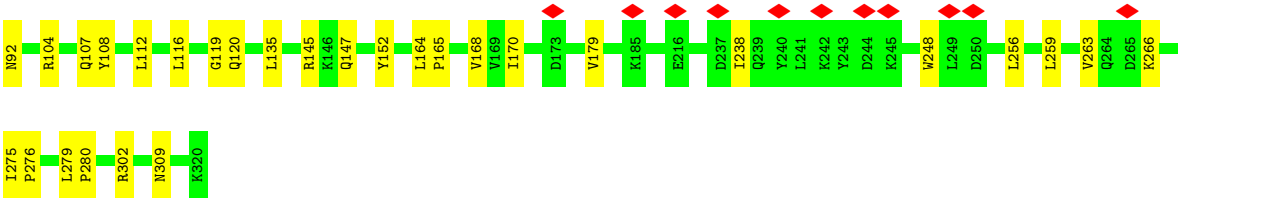


• Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

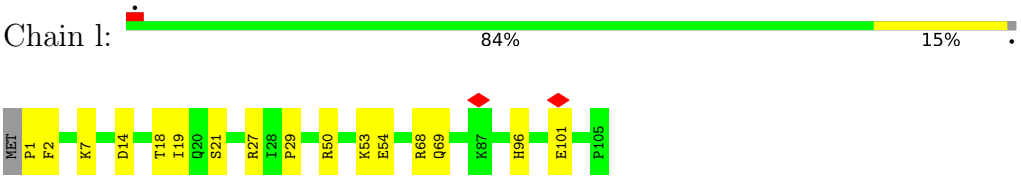
Chain k:



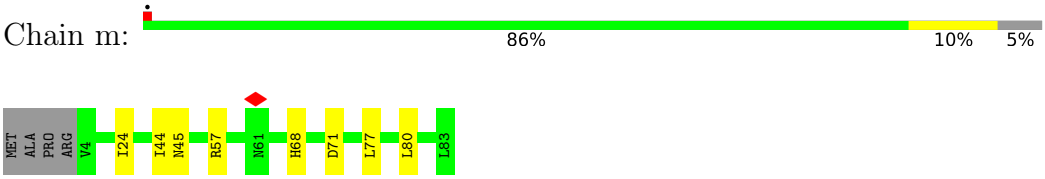




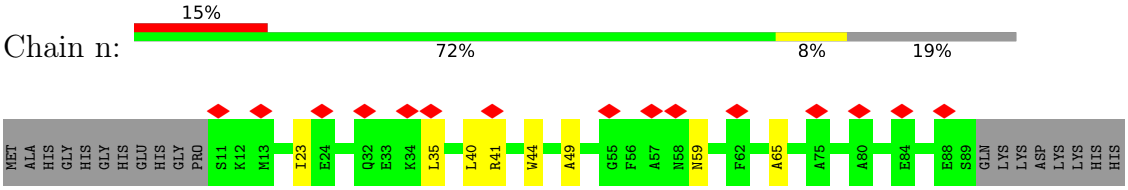
• Molecule 30: NADH:ubiquinone oxidoreductase subunit S5



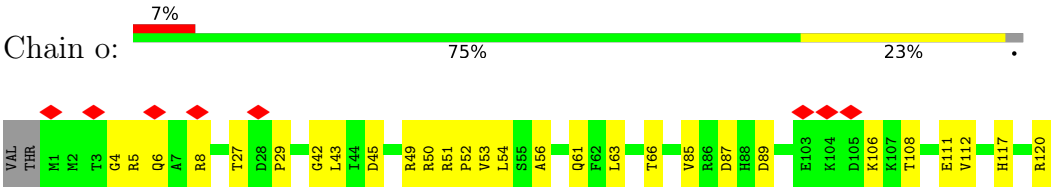
• Molecule 31: NADH:ubiquinone oxidoreductase subunit A3



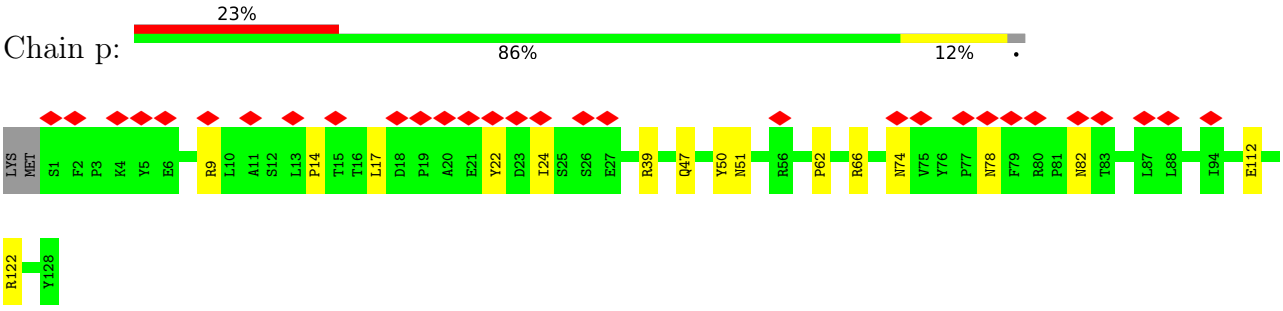
• Molecule 32: NADH:ubiquinone oxidoreductase subunit B3



• Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2



• Molecule 34: NADH:ubiquinone oxidoreductase subunit B4



• Molecule 35: Mitochondrial complex I, B16.6 subunit

Chain q:

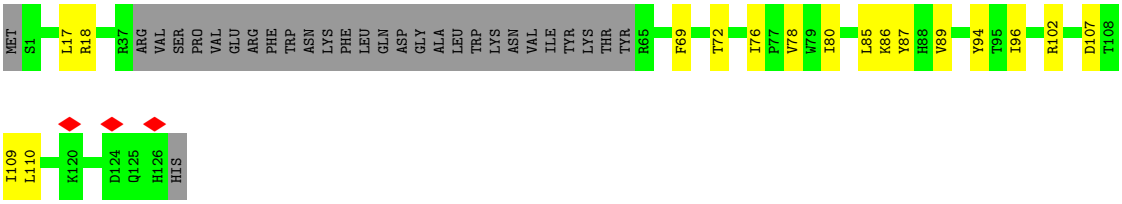




• Molecule 36: Mitochondrial complex I, B17 subunit

Chain r:

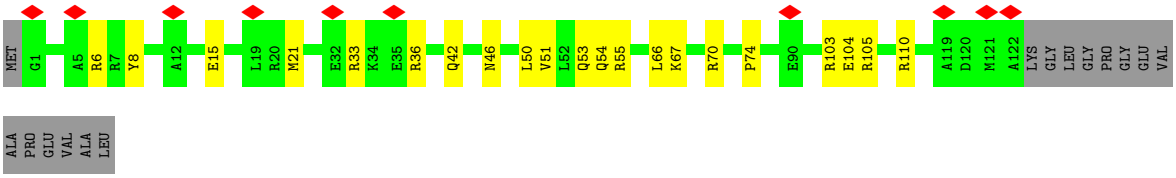




• Molecule 37: NADH:ubiquinone oxidoreductase subunit B7

Chain s:

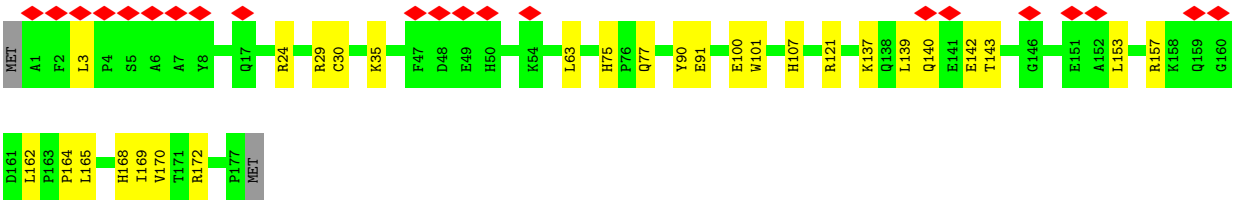




• Molecule 38: NADH:ubiquinone oxidoreductase subunit B9

Chain t:

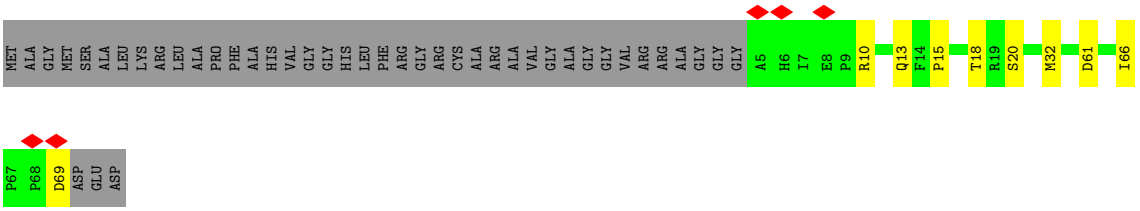




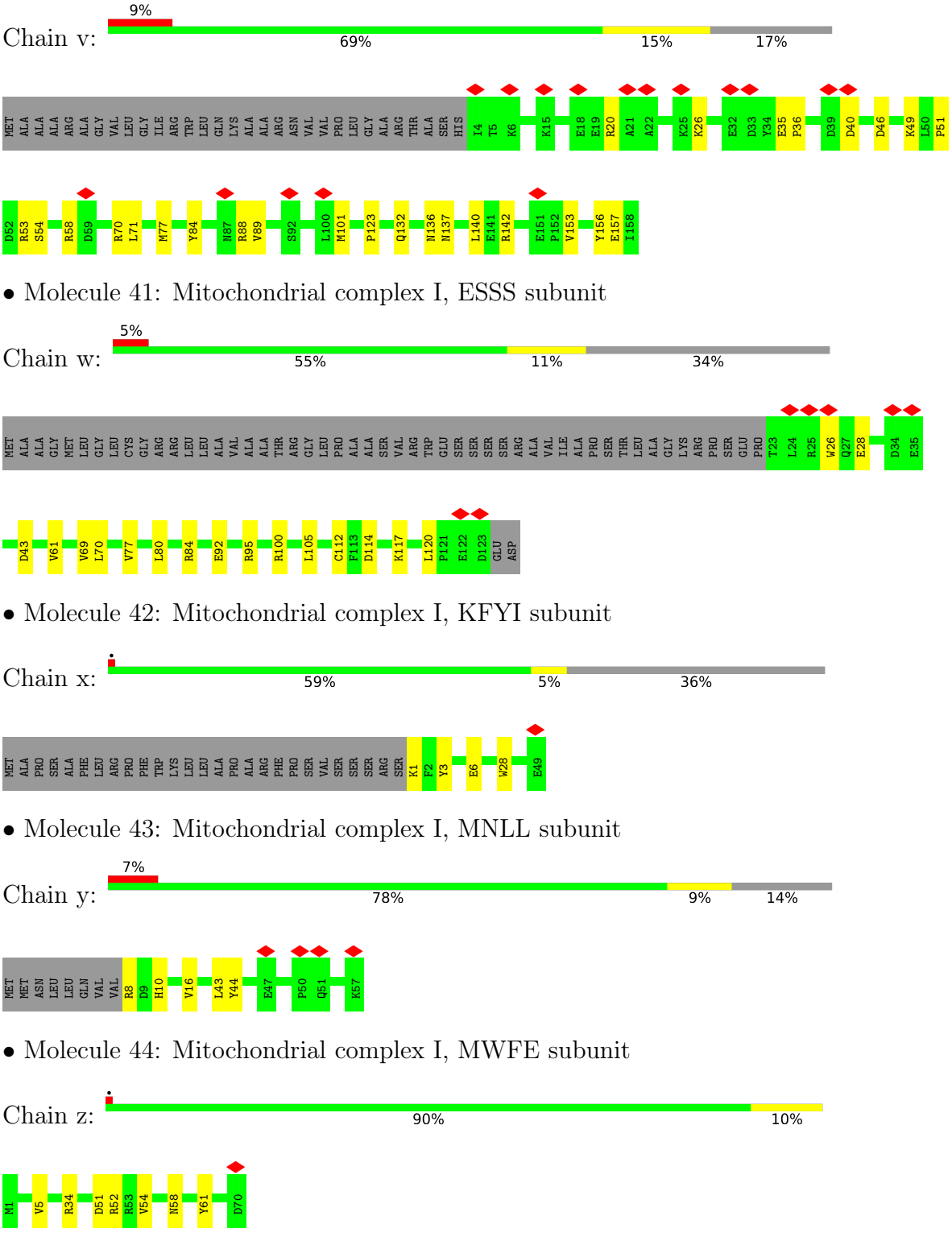
• Molecule 39: NADH:ubiquinone oxidoreductase subunit B2

Chain u:





• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial


Chain v:
9%
69%
15%
17%
MET ALA ALA ALA ARG ALA GLY VAL LEU GLY ILE ARG TRP LEU GLN LYS ALA ALA ARG ASN VAL VAL PRO LEU GLY ALA ARG THR ALA SER HIS I4 T5 K6 K15 E18 E19 R20 A21 A22 K25 K26 E32 D33 Y34 E35 P36 D39 D40 D46 K49 L50 P51
D52 R53 S54 R58 D59 R70 L71 M77 Y84 N87 R88 V89 S92 L100 M101 P123 Q132 N136 N137 L140 E141 R142 E151 P152 V153 Y156 E157 I158
• Molecule 41: Mitochondrial complex I, ESSS subunit
Chain w:
5%
55%
11%
34%
MET ALA ALA GLY MET LEU GLY LEU CYS GLY ARG ARG LEU LEU ALA VAL ALA ALA THR ARG GLY LEU PRO ALA ALA SER VAL ARG TRP GLU SER SER SER SER ARG ALA VAL ILE ALA PRO SER THR LEU ALA GLY LYS ARG PRO SER GLU PRO T23 L24 R25 W26 Q27 E28 D34 E35
D43 V61 V69 L70 V77 L80 R84 E92 R95 R100 L105 C112 F113 D114 K117 L120 P121 E122 D123 GLU ASP
• Molecule 42: Mitochondrial complex I, KFYI subunit
Chain x:
59%
5%
36%
MET ALA PRO SER ALA PHE LEU ARG PRO PHE TRP LYS LEU LEU ALA PRO ALA ARG PHE PRO SER VAL SER SER SER ARG SER K1 F2 Y3 E6 W28 E49
• Molecule 43: Mitochondrial complex I, MNLL subunit
Chain y:
7%
78%
9%
14%
MET MET ASN LEU LEU GLN VAL VAL R8 D9 H10 V16 L43 Y44 E47 P50 Q51 K57
• Molecule 44: Mitochondrial complex I, MWFE subunit
Chain z:
90%
10%
M1 V5 R34 D51 R52 R53 V54 N58 Y61 D70

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21296	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.467	Depositor
Minimum map value	-0.150	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	172.943, 190.98, 289.65298	wwPDB
Map dimensions	273, 180, 163	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZMP, CDL, ZN, SEP, FES, SF4, AMP, PC1, AYA, 970, FME, 3PE, MYR, K, NAI, 2MR, NDP, FMN

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	1	0.27	0/3386	0.56	0/4575
2	2	0.26	0/1695	0.59	2/2306 (0.1%)
3	3	0.25	0/5362	0.54	3/7266 (0.0%)
4	4	0.28	0/3504	0.53	0/4746
5	5	0.25	0/1776	0.54	0/2417
6	6	0.29	0/1278	0.56	0/1728
7	9	0.28	0/1445	0.56	0/1956
8	A	0.26	0/902	0.63	2/1234 (0.2%)
9	H	0.30	0/2572	0.60	0/3517
10	J	0.26	0/1293	0.57	0/1748
11	K	0.29	0/749	0.58	0/1014
12	L	0.27	0/4924	0.58	0/6698
13	M	0.27	0/3731	0.57	0/5085
14	N	0.29	0/2787	0.57	0/3795
15	V	0.21	0/1041	0.45	0/1412
16	W	0.22	0/1188	0.50	0/1607
17	X	0.19	0/713	0.45	0/963
17	j	0.21	0/670	0.50	0/902
18	Y	0.22	0/1440	0.53	0/1942
19	Z	0.20	0/1475	0.48	0/1989
20	a	0.17	0/383	0.43	0/518
21	b	0.20	0/749	0.45	0/1009
22	c	0.23	0/1047	0.44	0/1415
23	d	0.22	0/2424	0.48	0/3276
24	e	0.20	0/702	0.47	0/945
25	f	0.21	0/937	0.51	0/1271
26	g	0.24	0/993	0.52	0/1336
27	h	0.23	0/779	0.53	0/1053
28	i	0.21	0/1250	0.43	0/1698
29	k	0.19	0/2646	0.44	0/3579
30	l	0.24	0/896	0.56	0/1200

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	m	0.22	0/647	0.48	0/890
32	n	0.19	0/653	0.41	0/882
33	o	0.21	0/1035	0.45	0/1398
34	p	0.18	0/1085	0.48	0/1467
35	q	0.22	0/1171	0.49	0/1579
36	r	0.21	0/874	0.54	0/1188
37	s	0.19	0/1072	0.48	0/1436
38	t	0.19	0/1573	0.54	0/2130
39	u	0.19	0/590	0.46	0/810
40	v	0.19	0/1361	0.48	0/1861
41	w	0.23	0/872	0.51	0/1185
42	x	0.16	0/425	0.38	0/576
43	y	0.21	0/449	0.54	0/605
44	z	0.24	0/591	0.49	0/795
All	All	0.24	0/67135	0.53	7/91002 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	3	0	2
4	4	0	1
8	A	0	2
All	All	0	5

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	338	VAL	N-CA-C	-6.95	106.23	112.90
3	3	366	THR	CA-C-N	5.77	132.56	121.54
3	3	366	THR	C-N-CA	5.77	132.56	121.54
2	2	156	ILE	CA-C-N	5.65	132.34	121.54
2	2	156	ILE	C-N-CA	5.65	132.34	121.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	259	ASN	Peptide
3	3	366	THR	Peptide
4	4	275	TYR	Peptide
8	A	113	TRP	Peptide
8	A	29	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3312	0	3269	54	0
2	2	1655	0	1668	23	0
3	3	5275	0	5300	73	0
4	4	3427	0	3365	64	0
5	5	1726	0	1676	24	0
6	6	1247	0	1259	15	0
7	9	1414	0	1370	24	0
8	A	880	0	920	13	0
9	H	2498	0	2609	51	0
10	J	1264	0	1294	22	0
11	K	749	0	793	12	0
12	L	4806	0	4945	82	0
13	M	3647	0	3849	66	0
14	N	2723	0	2930	45	0
15	V	1028	0	1036	16	0
16	W	1155	0	1177	12	0
17	X	701	0	692	9	0
17	j	660	0	663	5	0
18	Y	1403	0	1392	11	0
19	Z	1441	0	1419	17	0
20	a	371	0	344	6	0
21	b	737	0	710	6	0
22	c	1024	0	1023	12	0
23	d	2372	0	2407	18	0
24	e	691	0	706	12	0
25	f	917	0	958	7	0
26	g	969	0	980	8	0
27	h	769	0	780	12	0
28	i	1209	0	1182	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	k	2596	0	2559	22	0
30	l	874	0	869	14	0
31	m	626	0	635	6	0
32	n	634	0	616	6	0
33	o	1004	0	995	22	0
34	p	1059	0	1062	13	0
35	q	1142	0	1137	15	0
36	r	846	0	864	16	0
37	s	1047	0	1015	19	0
38	t	1520	0	1477	23	0
39	u	563	0	509	7	0
40	v	1307	0	1207	18	0
41	w	846	0	792	16	0
42	x	412	0	411	4	0
43	y	436	0	437	5	0
44	z	576	0	570	5	0
45	1	8	0	0	1	0
45	3	16	0	0	1	0
45	6	8	0	0	1	0
45	9	16	0	0	0	0
46	1	31	0	19	2	0
47	1	44	0	27	5	0
48	2	4	0	0	1	0
48	3	4	0	0	0	0
49	3	1	0	0	0	0
50	6	29	0	0	0	0
50	H	29	0	0	0	0
51	6	51	0	82	1	0
51	A	51	0	82	0	0
51	J	51	0	82	3	0
51	K	40	0	54	1	0
51	L	122	0	172	3	0
51	M	44	0	65	2	0
51	N	51	0	82	2	0
51	V	72	0	92	2	0
51	i	51	0	82	1	0
51	l	31	0	36	0	0
51	p	27	0	27	0	0
52	9	54	0	88	2	0
52	A	83	0	117	1	0
52	L	54	0	88	4	0
52	M	54	0	88	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	w	54	0	88	4	0
53	L	100	0	156	7	0
53	V	179	0	261	10	0
53	W	100	0	156	8	0
53	Y	100	0	156	7	0
53	i	58	0	60	1	0
53	o	165	0	230	11	0
54	X	31	0	34	1	0
54	g	34	0	40	0	0
55	b	1	0	0	0	0
56	d	48	0	26	1	0
57	k	23	0	12	0	0
58	s	15	0	27	0	0
All	All	67492	0	68400	776	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 776 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:50:ASN:HD21	4:4:63:ARG:HH21	1.35	0.71
24:e:19:ARG:HB2	24:e:65:TRP:HB2	1.73	0.69
7:9:43:ARG:HG2	27:h:11:ARG:HD2	1.73	0.69
37:s:33:ARG:HH12	37:s:103:ARG:HH22	1.41	0.67
9:H:237:PHE:O	9:H:241:LEU:HB2	1.94	0.66

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	428/464 (92%)	407 (95%)	21 (5%)	0	100	100
2	2	211/246 (86%)	194 (92%)	17 (8%)	0	100	100
3	3	686/727 (94%)	657 (96%)	29 (4%)	0	100	100
4	4	421/463 (91%)	409 (97%)	12 (3%)	0	100	100
5	5	206/266 (77%)	199 (97%)	7 (3%)	0	100	100
6	6	154/223 (69%)	146 (95%)	8 (5%)	0	100	100
7	9	174/217 (80%)	167 (96%)	7 (4%)	0	100	100
8	A	106/115 (92%)	96 (91%)	10 (9%)	0	100	100
9	H	310/318 (98%)	297 (96%)	13 (4%)	0	100	100
10	J	162/175 (93%)	154 (95%)	8 (5%)	0	100	100
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	604/606 (100%)	573 (95%)	31 (5%)	0	100	100
13	M	457/459 (100%)	444 (97%)	13 (3%)	0	100	100
14	N	345/347 (99%)	335 (97%)	10 (3%)	0	100	100
15	V	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
16	W	137/189 (72%)	136 (99%)	1 (1%)	0	100	100
17	X	85/157 (54%)	83 (98%)	2 (2%)	0	100	100
17	j	80/157 (51%)	78 (98%)	2 (2%)	0	100	100
18	Y	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
19	Z	169/175 (97%)	164 (97%)	5 (3%)	0	100	100
20	a	42/109 (38%)	42 (100%)	0	0	100	100
21	b	93/124 (75%)	91 (98%)	2 (2%)	0	100	100
22	c	124/170 (73%)	120 (97%)	4 (3%)	0	100	100
23	d	289/380 (76%)	281 (97%)	8 (3%)	0	100	100
24	e	84/99 (85%)	82 (98%)	2 (2%)	0	100	100
25	f	111/116 (96%)	108 (97%)	3 (3%)	0	100	100
26	g	112/140 (80%)	107 (96%)	5 (4%)	0	100	100
27	h	92/114 (81%)	86 (94%)	6 (6%)	0	100	100
28	i	143/145 (99%)	142 (99%)	1 (1%)	0	100	100
29	k	317/355 (89%)	302 (95%)	15 (5%)	0	100	100
30	l	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
31	m	78/84 (93%)	73 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	n	77/98 (79%)	75 (97%)	2 (3%)	0	100	100
33	o	118/122 (97%)	118 (100%)	0	0	100	100
34	p	126/130 (97%)	121 (96%)	5 (4%)	0	100	100
35	q	137/144 (95%)	135 (98%)	2 (2%)	0	100	100
36	r	95/128 (74%)	89 (94%)	6 (6%)	0	100	100
37	s	120/137 (88%)	114 (95%)	6 (5%)	0	100	100
38	t	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
39	u	63/108 (58%)	58 (92%)	5 (8%)	0	100	100
40	v	153/186 (82%)	144 (94%)	9 (6%)	0	100	100
41	w	99/154 (64%)	93 (94%)	6 (6%)	0	100	100
42	x	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
43	y	48/58 (83%)	46 (96%)	2 (4%)	0	100	100
44	z	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
All	All	8052/9247 (87%)	7740 (96%)	312 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	344/368 (94%)	344 (100%)	0	100	100
2	2	183/210 (87%)	183 (100%)	0	100	100
3	3	578/608 (95%)	578 (100%)	0	100	100
4	4	366/391 (94%)	366 (100%)	0	100	100
5	5	189/230 (82%)	189 (100%)	0	100	100
6	6	132/181 (73%)	131 (99%)	1 (1%)	73	81
7	9	151/179 (84%)	150 (99%)	1 (1%)	76	82
8	A	99/103 (96%)	99 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	H	274/278 (99%)	273 (100%)	1 (0%)	84 86
10	J	135/144 (94%)	135 (100%)	0	100 100
11	K	86/86 (100%)	86 (100%)	0	100 100
12	L	538/538 (100%)	538 (100%)	0	100 100
13	M	411/411 (100%)	411 (100%)	0	100 100
14	N	315/315 (100%)	315 (100%)	0	100 100
15	V	101/102 (99%)	100 (99%)	1 (1%)	68 79
16	W	122/160 (76%)	122 (100%)	0	100 100
17	X	80/141 (57%)	80 (100%)	0	100 100
17	j	76/141 (54%)	76 (100%)	0	100 100
18	Y	154/155 (99%)	154 (100%)	0	100 100
19	Z	155/157 (99%)	155 (100%)	0	100 100
20	a	43/93 (46%)	43 (100%)	0	100 100
21	b	79/97 (81%)	79 (100%)	0	100 100
22	c	113/150 (75%)	113 (100%)	0	100 100
23	d	255/326 (78%)	255 (100%)	0	100 100
24	e	76/82 (93%)	76 (100%)	0	100 100
25	f	101/102 (99%)	101 (100%)	0	100 100
26	g	107/124 (86%)	107 (100%)	0	100 100
27	h	84/96 (88%)	84 (100%)	0	100 100
28	i	131/131 (100%)	131 (100%)	0	100 100
29	k	283/309 (92%)	283 (100%)	0	100 100
30	l	94/95 (99%)	94 (100%)	0	100 100
31	m	69/72 (96%)	69 (100%)	0	100 100
32	n	61/76 (80%)	61 (100%)	0	100 100
33	o	107/109 (98%)	107 (100%)	0	100 100
34	p	114/116 (98%)	113 (99%)	1 (1%)	70 80
35	q	119/122 (98%)	119 (100%)	0	100 100
36	r	95/122 (78%)	95 (100%)	0	100 100
37	s	110/120 (92%)	110 (100%)	0	100 100
38	t	159/161 (99%)	159 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	u	59/84 (70%)	59 (100%)	0	100	100
40	v	140/160 (88%)	140 (100%)	0	100	100
41	w	92/130 (71%)	92 (100%)	0	100	100
42	x	44/67 (66%)	44 (100%)	0	100	100
43	y	46/54 (85%)	46 (100%)	0	100	100
44	z	59/59 (100%)	59 (100%)	0	100	100
All	All	7129/7955 (90%)	7124 (100%)	5 (0%)	87	90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	6	54	CYS
7	9	78	ILE
9	H	259	PHE
15	V	134	VAL
34	p	24	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
30	l	100	GLN
43	y	13	HIS
33	o	12	GLN
40	v	55	GLN
12	L	546	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

7 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	$\#\|Z\| > 2$
27	AYA	h	1	27	6,7,8	1.26	1 (16%)	5,8,10	1.15	1 (20%)
13	FME	M	1	13	8,9,10	0.94	0	7,9,11	1.07	0
12	FME	L	1	12	8,9,10	0.92	0	7,9,11	1.83	2 (28%)
29	SEP	k	36	29	8,9,10	1.54	1 (12%)	8,12,14	1.72	2 (25%)
4	2MR	4	85	4	10,12,13	2.42	3 (30%)	5,13,15	1.19	1 (20%)
11	FME	K	1	11	8,9,10	0.94	0	7,9,11	0.87	0
15	AYA	V	1	15	6,7,8	1.15	0	5,8,10	2.17	2 (40%)

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
27	AYA	h	1	27	-	0/4/6/8	-
13	FME	M	1	13	-	2/7/9/11	-
12	FME	L	1	12	-	1/7/9/11	-
29	SEP	k	36	29	-	4/5/8/10	-
4	2MR	4	85	4	-	3/10/13/15	-
11	FME	K	1	11	-	3/7/9/11	-
15	AYA	V	1	15	-	2/4/6/8	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	85	2MR	CZ-NE	5.07	1.45	1.34
4	4	85	2MR	CZ-NH2	4.86	1.44	1.33
29	k	36	SEP	P-O1P	3.36	1.61	1.50
27	h	1	AYA	CA-N	-2.40	1.44	1.46
4	4	85	2MR	CQ1-NH1	-2.18	1.42	1.46

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	1	FME	CA-N-CN	3.63	128.40	122.82
29	k	36	SEP	OG-CB-CA	3.56	111.61	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	V	1	AYA	CB-CA-N	3.34	113.33	109.61
15	V	1	AYA	CA-N-CT	2.96	125.83	121.52
12	L	1	FME	C-CA-N	2.88	114.94	109.73

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	K	1	FME	O1-CN-N-CA
11	K	1	FME	O-C-CA-CB
12	L	1	FME	CA-CB-CG-SD
13	M	1	FME	CB-CA-N-CN
13	M	1	FME	C-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	h	1	AYA	1	0
13	M	1	FME	1	0
4	4	85	2MR	1	0
11	K	1	FME	1	0
15	V	1	AYA	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 47 ligands modelled in this entry, 2 are monoatomic - leaving 45 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	$\#\|Z\|>2$
46	FMN	1	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.29	7 (14%)
45	SF4	9	402	7	0,12,12	-	-	-		
52	PC1	M	502	-	53,53,53	0.29	0	59,61,61	0.32	0
53	CDL	i	202	-	57,57,99	0.36	0	63,69,111	0.28	0
56	NDP	d	401	-	49,52,52	0.37	0	66,80,80	0.37	0
45	SF4	9	403	7	0,12,12	-	-	-		
51	3PE	J	201	-	50,50,50	0.31	0	53,55,55	0.44	1 (1%)
51	3PE	L	702	-	50,50,50	0.30	0	53,55,55	0.34	0
51	3PE	i	201	-	50,50,50	0.30	0	53,55,55	0.29	0
53	CDL	L	704	-	99,99,99	0.26	0	105,111,111	0.25	0
45	SF4	3	801	3	0,12,12	-	-	-		
53	CDL	o	201	-	74,74,99	0.30	0	80,86,111	0.48	1 (1%)
51	3PE	K	101	-	39,39,50	0.34	0	42,44,55	0.31	0
47	NAI	1	503	-	45,48,48	0.40	0	60,73,73	1.68	3 (5%)
53	CDL	W	201	-	99,99,99	0.28	0	105,111,111	0.25	0
52	PC1	w	801	-	53,53,53	0.29	0	59,61,61	0.38	0
52	PC1	A	401	-	45,45,53	0.31	0	51,53,61	0.33	0
45	SF4	3	802	3	0,12,12	-	-	-		
53	CDL	V	203	-	93,93,99	0.26	0	99,105,111	0.26	0
50	970	H	501	-	33,33,33	0.30	0	48,50,50	0.69	1 (2%)
51	3PE	M	501	-	43,43,50	0.33	0	46,48,55	0.46	0
52	PC1	L	703	-	53,53,53	0.30	0	59,61,61	0.61	2 (3%)
52	PC1	9	401	-	53,53,53	0.31	0	59,61,61	0.49	1 (1%)
53	CDL	Y	201	-	99,99,99	0.27	0	105,111,111	0.36	1 (0%)
45	SF4	1	501	1	0,12,12	-	-	-		
53	CDL	o	202	-	89,89,99	0.28	0	95,101,111	0.40	0
48	FES	3	803	3	0,4,4	-	-	-		
51	3PE	V	201	-	34,34,50	0.35	0	37,39,55	0.29	0
51	3PE	L	701	-	39,39,50	0.34	0	42,44,55	0.33	0
51	3PE	p	201	-	26,26,50	0.47	0	30,31,55	0.56	1 (3%)
45	SF4	6	502	6	0,12,12	-	-	-		
51	3PE	A	403	-	50,50,50	0.32	0	53,55,55	0.44	1 (1%)
51	3PE	L	705	-	30,30,50	0.42	0	33,35,55	0.82	3 (9%)
51	3PE	V	202	-	36,36,50	0.35	0	39,41,55	0.32	0
53	CDL	V	204	-	84,84,99	0.29	0	90,96,111	0.26	0
52	PC1	A	402	-	36,36,53	0.36	0	42,44,61	0.60	1 (2%)
57	AMP	k	501	-	25,25,25	1.41	4 (16%)	38,38,38	2.12	7 (18%)
51	3PE	l	501	-	30,30,50	0.38	0	33,35,55	0.38	0
58	MYR	s	201	37	14,14,15	0.23	0	13,13,15	0.19	0
50	970	6	501	-	33,33,33	0.26	0	48,50,50	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	FES	2	300	2	0,4,4	-	-	-		
54	ZMP	g	201	-	27,33,36	0.68	1 (3%)	32,40,45	1.12	3 (9%)
51	3PE	N	401	-	50,50,50	0.32	0	53,55,55	0.54	2 (3%)
51	3PE	6	503	-	50,50,50	0.31	0	53,55,55	0.31	0
54	ZMP	X	101	17	24,30,36	0.83	1 (4%)	29,37,45	0.92	1 (3%)

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
46	FMN	1	502	-	-	6/18/18/18	0/3/3/3
53	CDL	i	202	-	-	16/68/68/110	-
52	PC1	M	502	-	-	19/57/57/57	-
45	SF4	9	402	7	-	-	0/6/5/5
56	NDP	d	401	-	-	5/34/77/77	0/5/5/5
45	SF4	9	403	7	-	-	0/6/5/5
51	3PE	J	201	-	-	17/54/54/54	-
51	3PE	L	702	-	-	10/54/54/54	-
53	CDL	L	704	-	1/1/9/9	33/110/110/110	-
51	3PE	i	201	-	-	15/54/54/54	-
45	SF4	3	801	3	-	-	0/6/5/5
53	CDL	o	201	-	2/2/9/9	18/85/85/110	-
51	3PE	K	101	-	-	6/43/43/54	-
47	NAI	1	503	-	-	9/29/72/72	0/5/5/5
53	CDL	W	201	-	-	30/110/110/110	-
52	PC1	w	801	-	-	17/57/57/57	-
52	PC1	A	401	-	-	11/49/49/57	-
53	CDL	V	203	-	-	32/104/104/110	-
45	SF4	3	802	3	-	-	0/6/5/5
50	970	H	501	-	-	4/8/41/41	0/5/5/5
51	3PE	M	501	-	-	11/47/47/54	-
52	PC1	L	703	-	-	16/57/57/57	-
52	PC1	9	401	-	-	20/57/57/57	-
53	CDL	Y	201	-	1/1/9/9	29/110/110/110	-
45	SF4	1	501	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	CDL	o	202	-	-	23/100/100/110	-
48	FES	3	803	3	-	-	0/1/1/1
51	3PE	V	201	-	-	6/38/38/54	-
51	3PE	L	701	-	-	15/43/43/54	-
51	3PE	p	201	-	-	6/27/27/54	-
45	SF4	6	502	6	-	-	0/6/5/5
51	3PE	A	403	-	-	19/54/54/54	-
51	3PE	L	705	-	-	16/34/34/54	-
51	3PE	V	202	-	-	12/40/40/54	-
53	CDL	V	204	-	1/1/9/9	35/95/95/110	-
52	PC1	A	402	-	-	12/40/40/57	-
57	AMP	k	501	-	-	9/10/26/26	0/3/3/3
51	3PE	l	501	-	-	6/34/34/54	-
58	MYR	s	201	37	-	2/11/12/13	-
50	970	6	501	-	-	4/8/41/41	0/5/5/5
48	FES	2	300	2	-	-	0/1/1/1
54	ZMP	g	201	-	-	6/38/40/43	-
51	3PE	N	401	-	-	14/54/54/54	-
51	3PE	6	503	-	-	12/54/54/54	-
54	ZMP	X	101	17	-	13/35/37/43	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	k	501	AMP	C5-C4	4.87	1.48	1.39
46	1	502	FMN	C4A-N5	3.33	1.37	1.30
54	X	101	ZMP	C9-C10	2.88	1.53	1.50
57	k	501	AMP	C5-C6	2.72	1.48	1.41
54	g	201	ZMP	C9-C10	2.45	1.53	1.50

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	1	503	NAI	O5B-PA-O1A	-9.81	70.75	109.07
47	1	503	NAI	O2A-PA-O1A	-7.64	74.46	112.24
57	k	501	AMP	C5-C4-N3	-7.43	117.05	126.75
57	k	501	AMP	N3-C4-N9	5.90	136.81	127.08
57	k	501	AMP	C2-N3-C4	4.32	121.95	111.75

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
53	L	704	CDL	CB4
53	V	204	CDL	CB4
53	Y	201	CDL	CB4
53	o	201	CDL	CB4
53	o	201	CDL	CA4

5 of 534 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	1	502	FMN	C5'-O5'-P-O2P
46	1	502	FMN	C5'-O5'-P-O3P
47	1	503	NAI	C5B-O5B-PA-O2A
47	1	503	NAI	C5D-O5D-PN-O1N
47	1	503	NAI	C5D-O5D-PN-O2N

There are no ring outliers.

30 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	1	502	FMN	2	0
52	M	502	PC1	4	0
53	i	202	CDL	1	0
56	d	401	NDP	1	0
51	J	201	3PE	3	0
51	L	702	3PE	2	0
51	i	201	3PE	1	0
53	L	704	CDL	7	0
45	3	801	SF4	1	0
53	o	201	CDL	2	0
51	K	101	3PE	1	0
47	1	503	NAI	5	0
53	W	201	CDL	8	0
52	w	801	PC1	4	0
52	A	401	PC1	1	0
53	V	203	CDL	5	0
51	M	501	3PE	2	0
52	L	703	PC1	4	0
52	9	401	PC1	2	0
53	Y	201	CDL	7	0
45	1	501	SF4	1	0
53	o	202	CDL	9	0

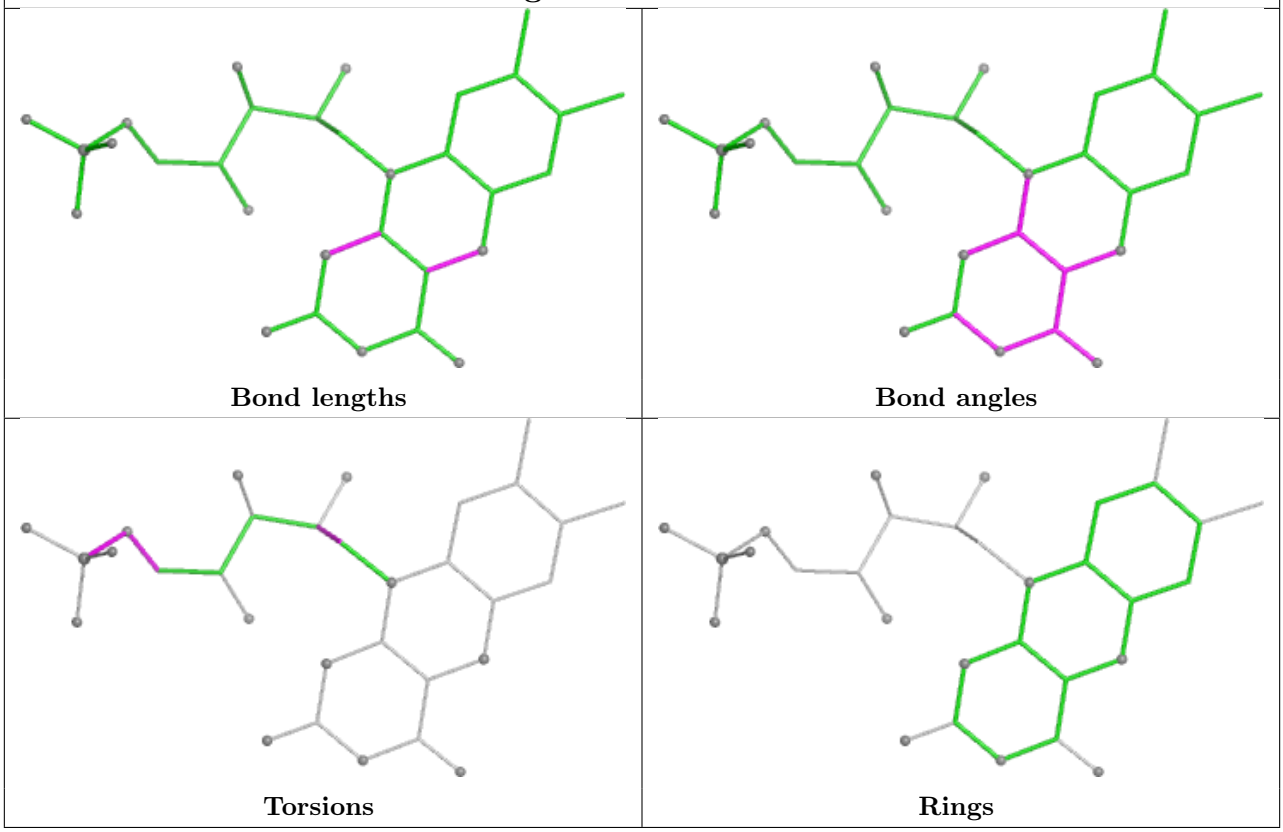
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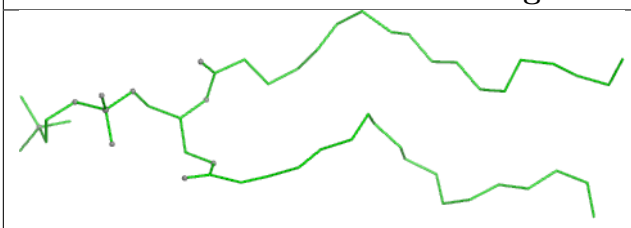
Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	L	701	3PE	1	0
45	6	502	SF4	1	0
51	V	202	3PE	2	0
53	V	204	CDL	8	0
48	2	300	FES	1	0
51	N	401	3PE	2	0
51	6	503	3PE	1	0
54	X	101	ZMP	1	0

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

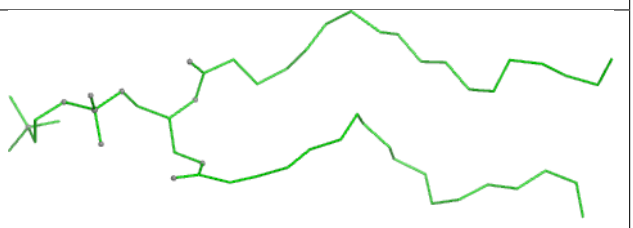
Ligand FMN 1 502



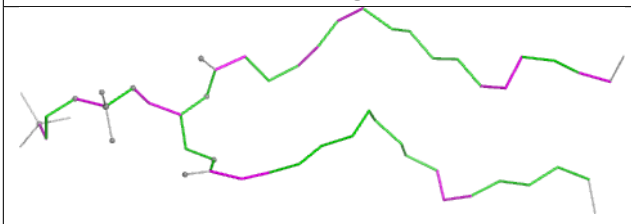
Ligand PC1 M 502



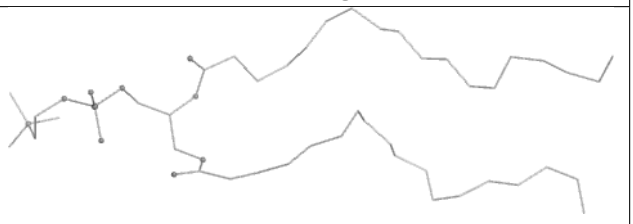
Bond lengths



Bond angles

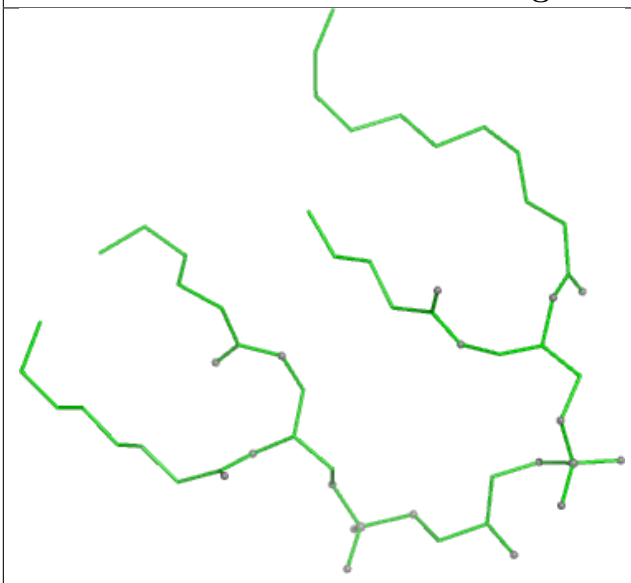


Torsions

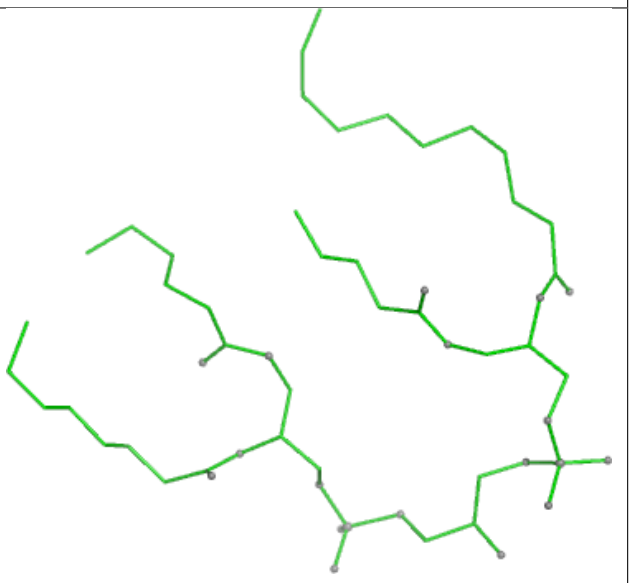


Rings

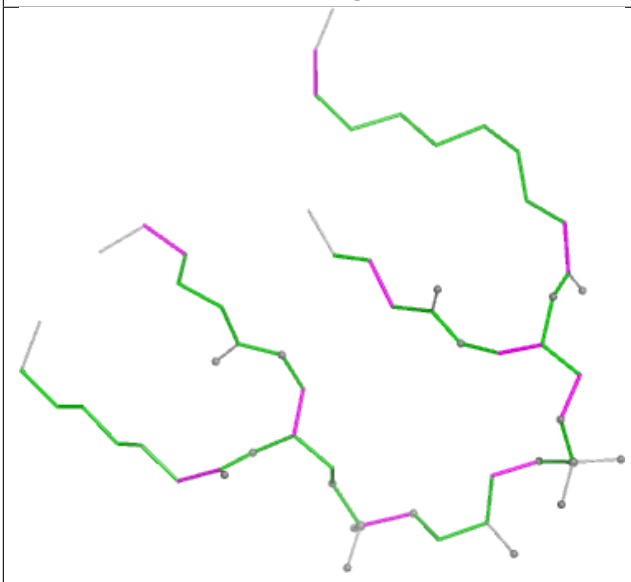
Ligand CDL i 202



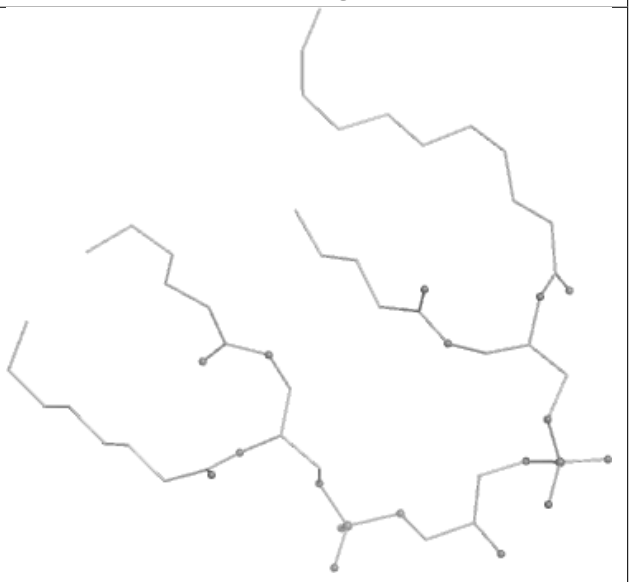
Bond lengths



Bond angles

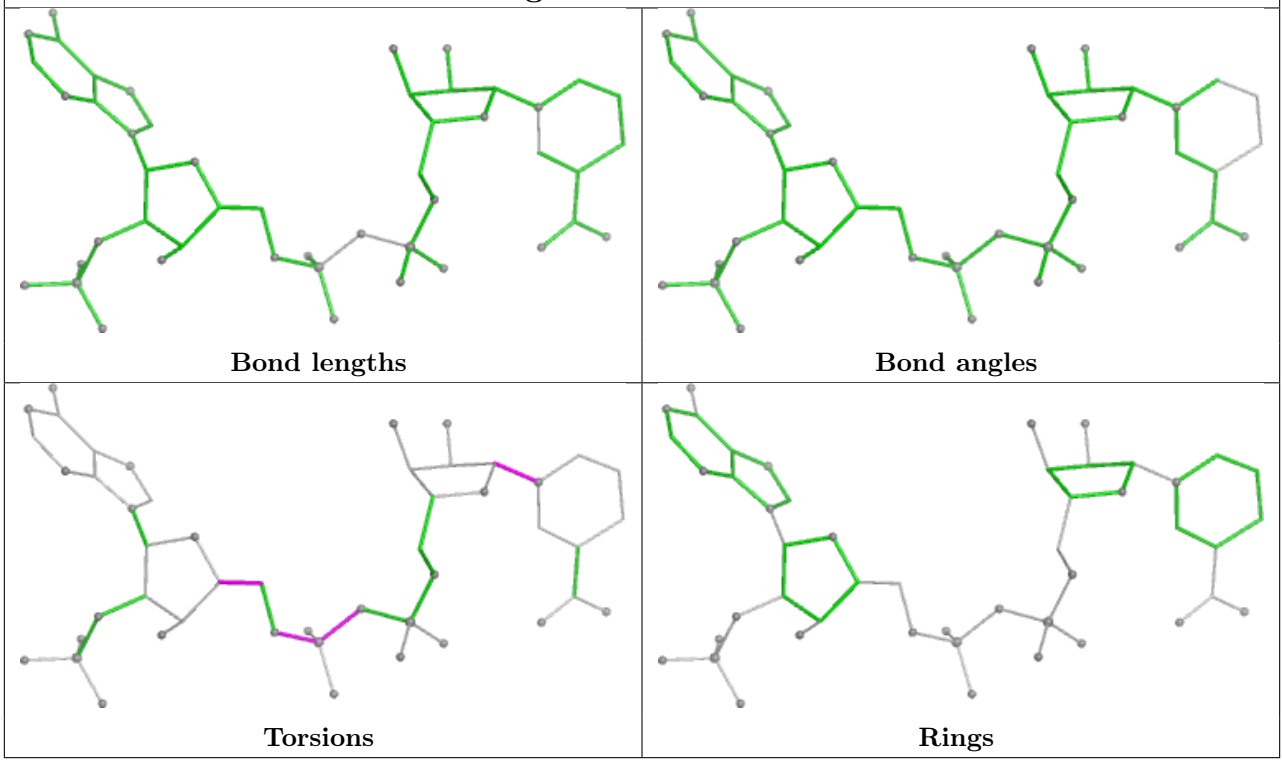


Torsions



Rings

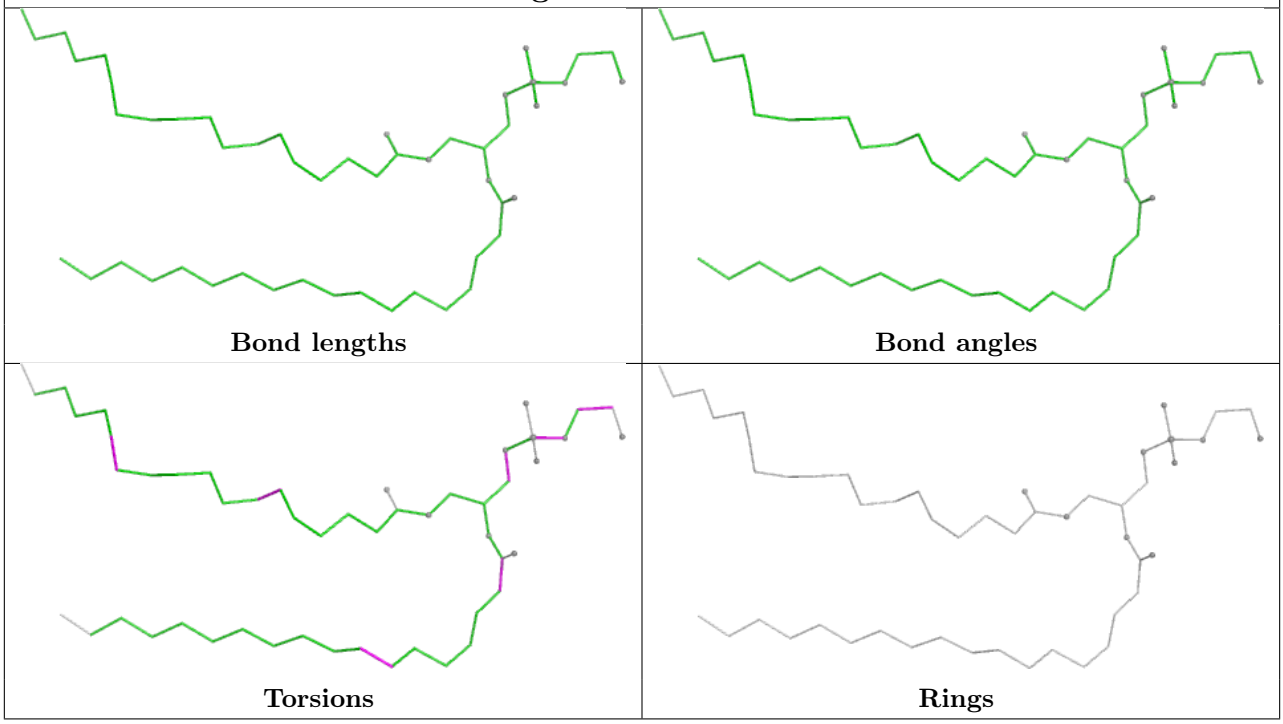
Ligand NDP d 401



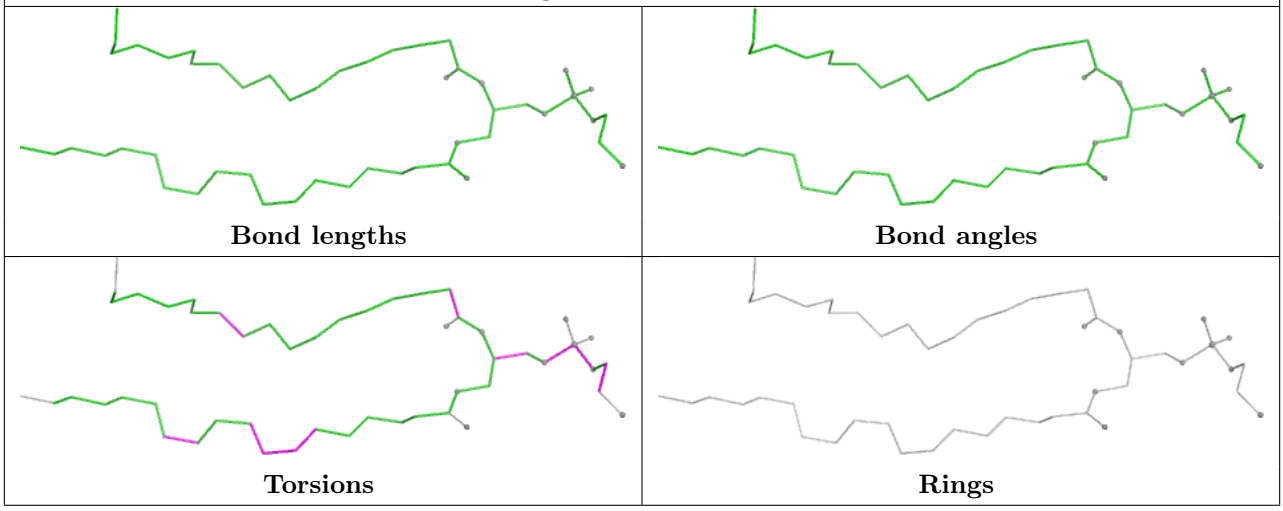
Ligand 3PE J 201



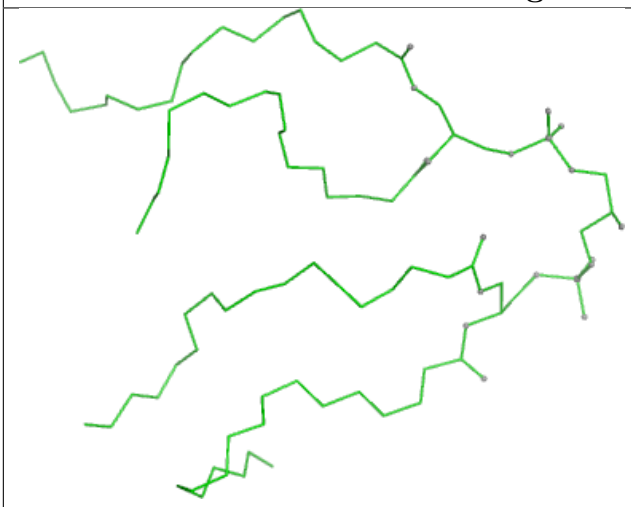
Ligand 3PE L 702



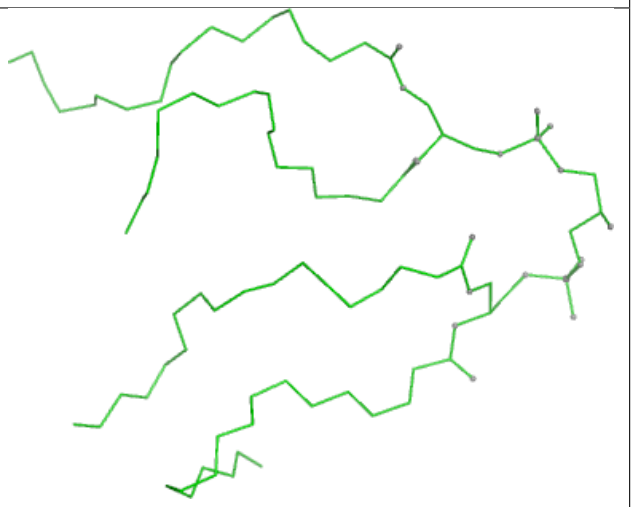
Ligand 3PE i 201



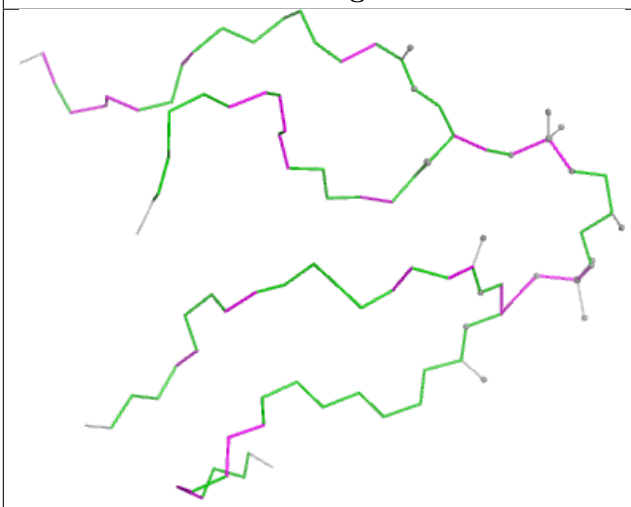
Ligand CDL L 704



Bond lengths



Bond angles

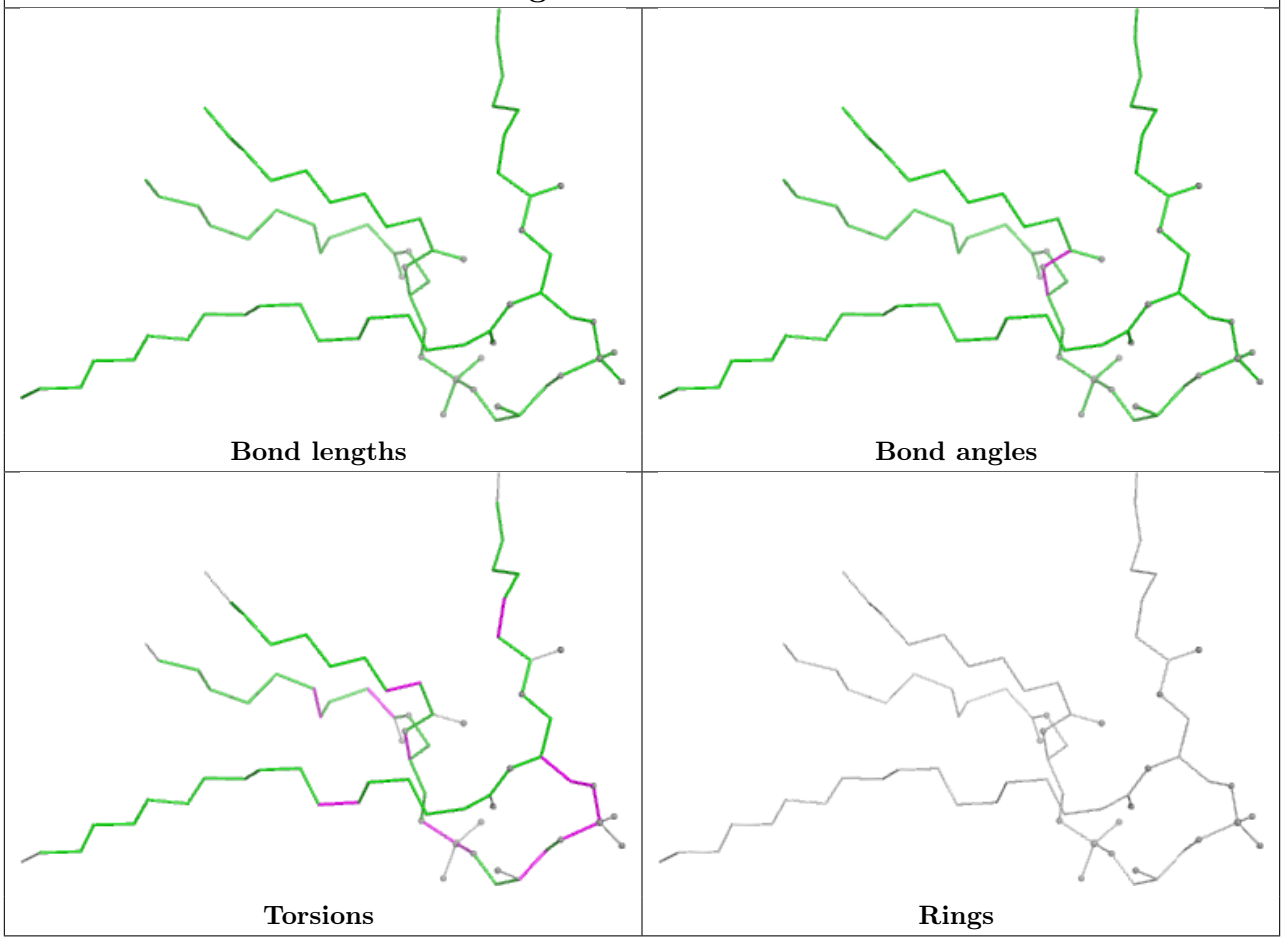


Torsions

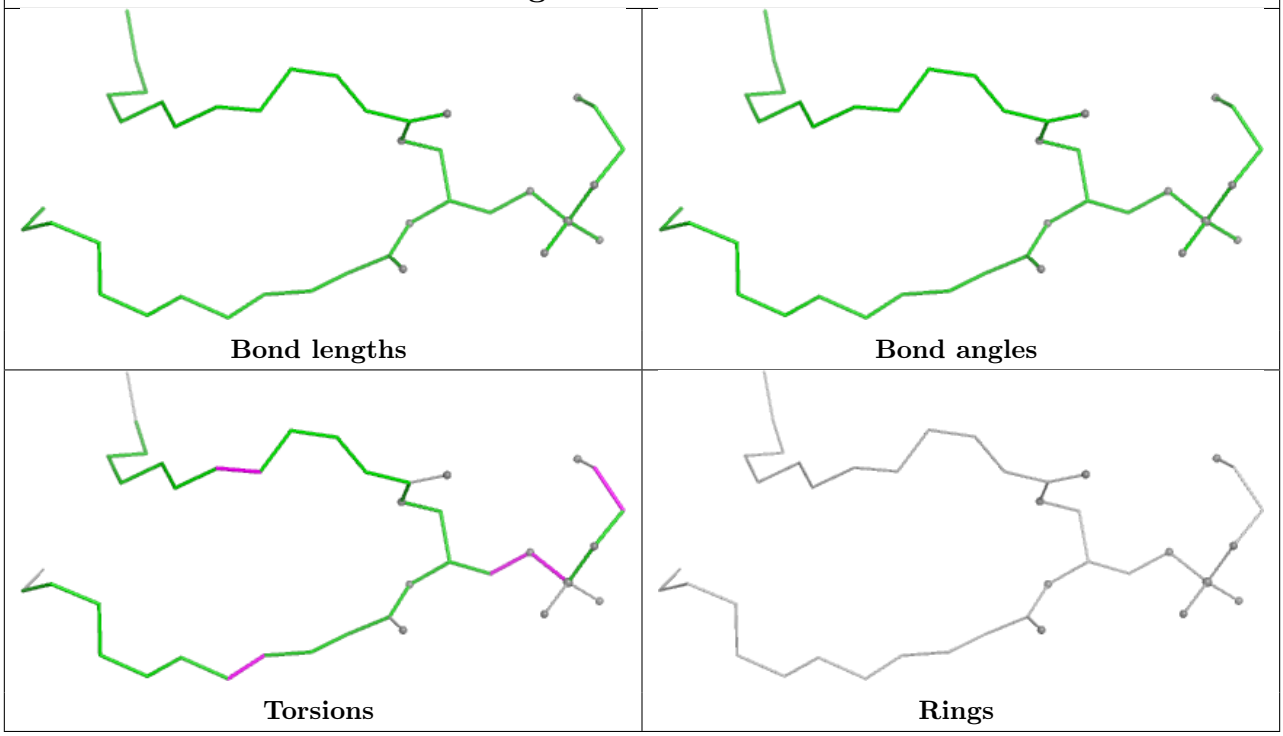


Rings

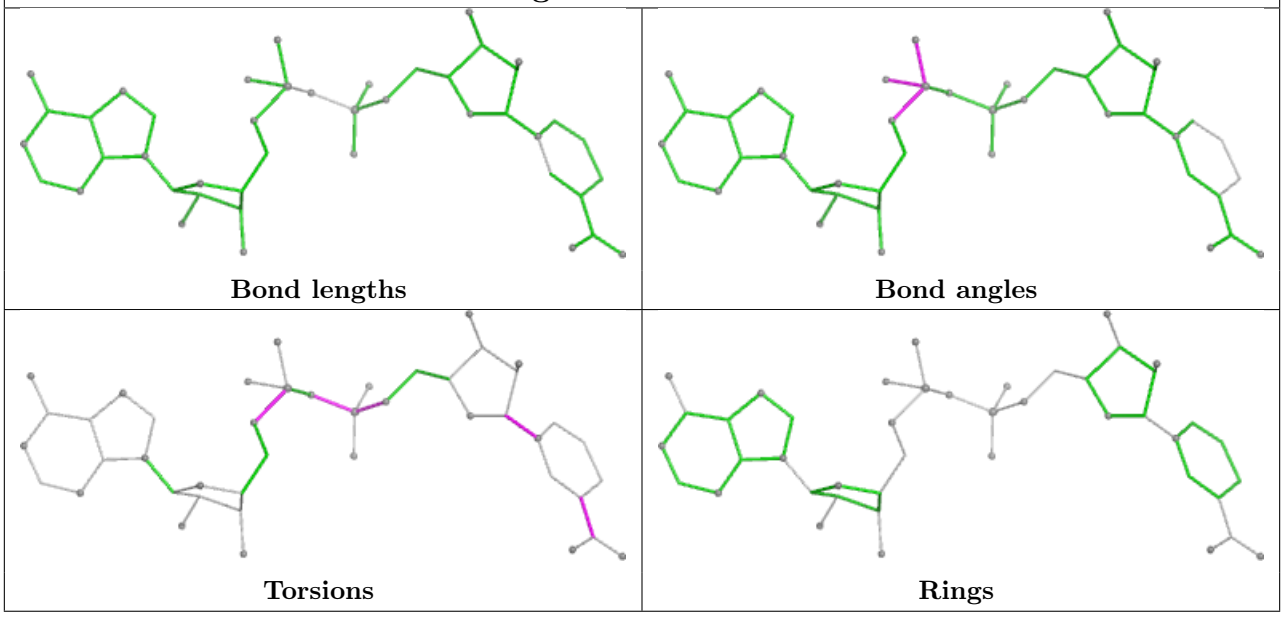
Ligand CDL o 201



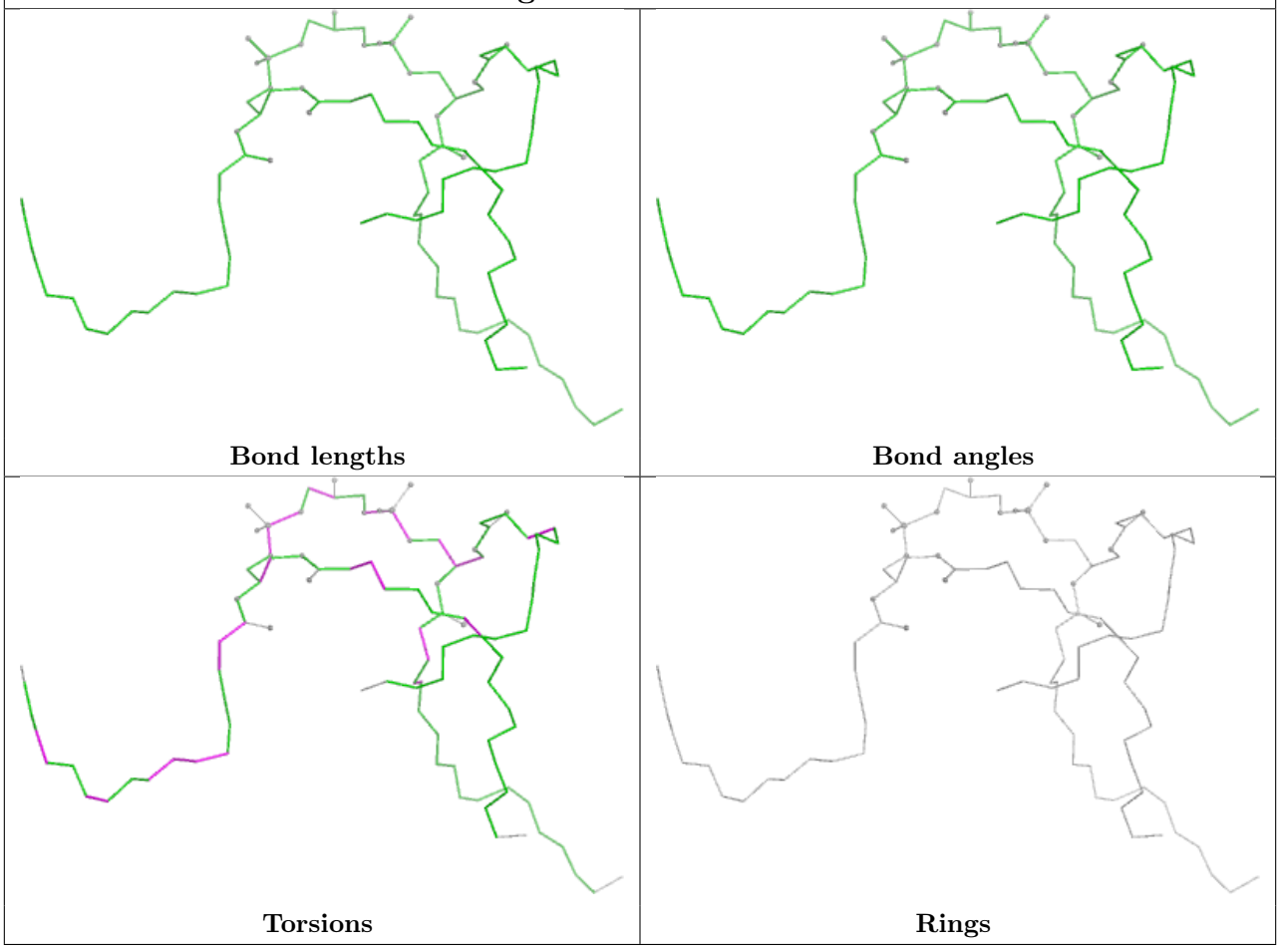
Ligand 3PE K 101



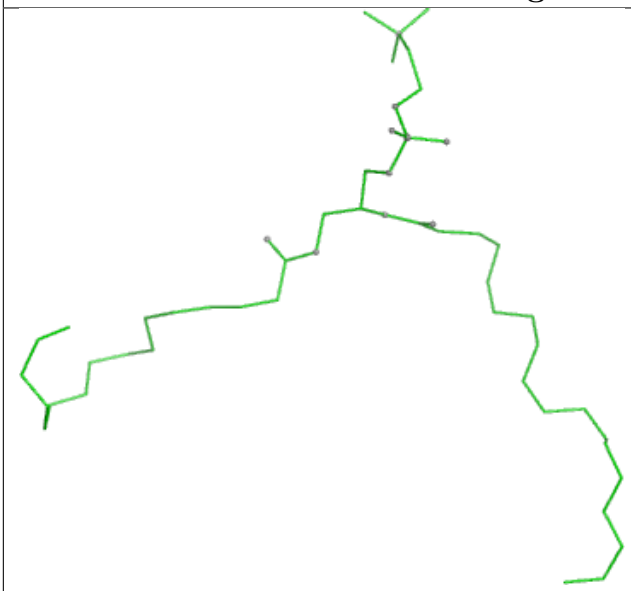
Ligand NAI 1 503



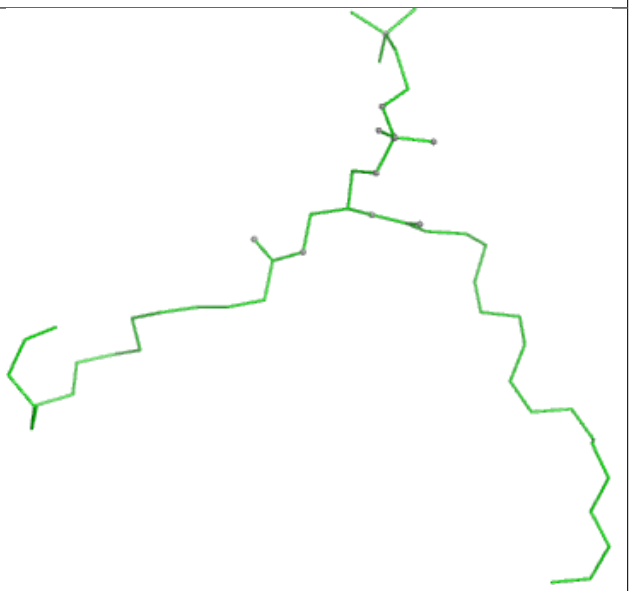
Ligand CDL W 201



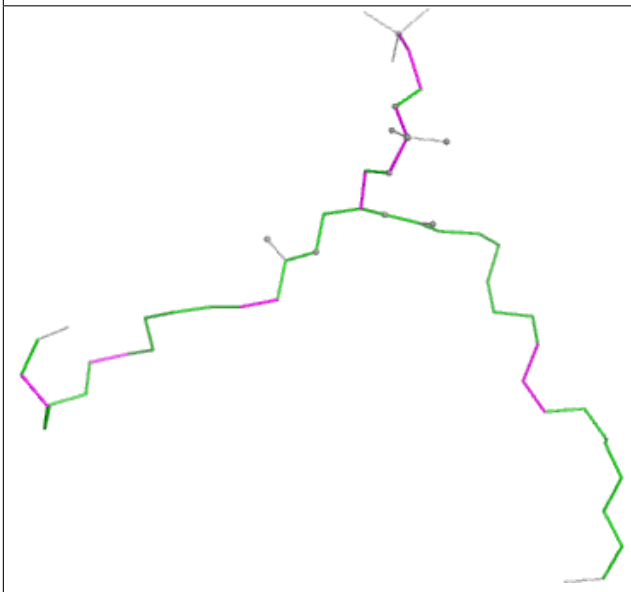
Ligand PC1 w 801



Bond lengths



Bond angles

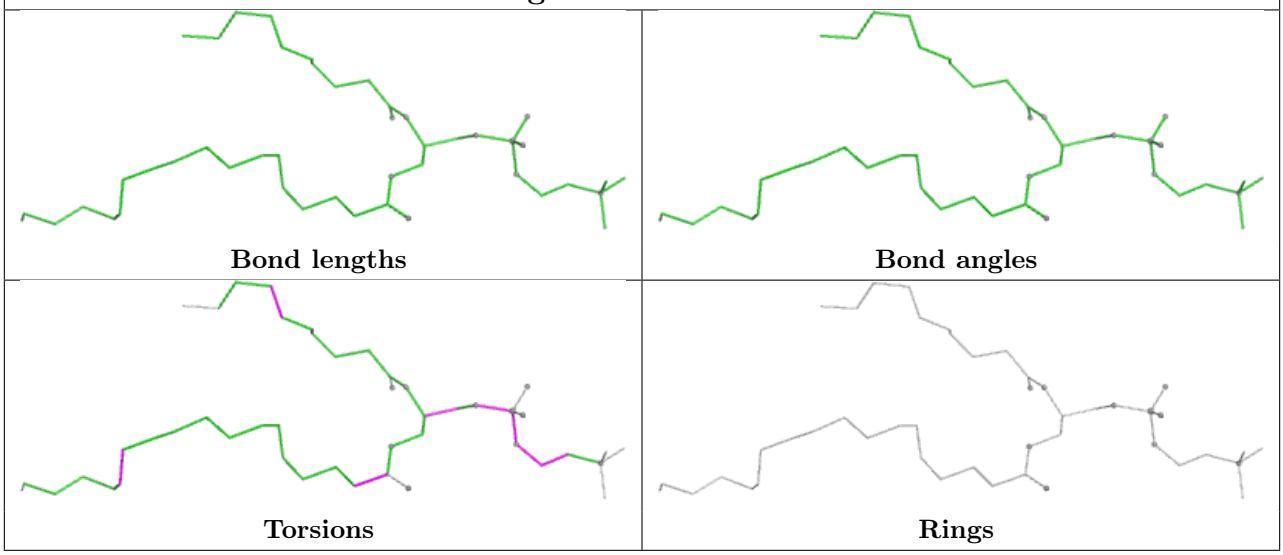


Torsions

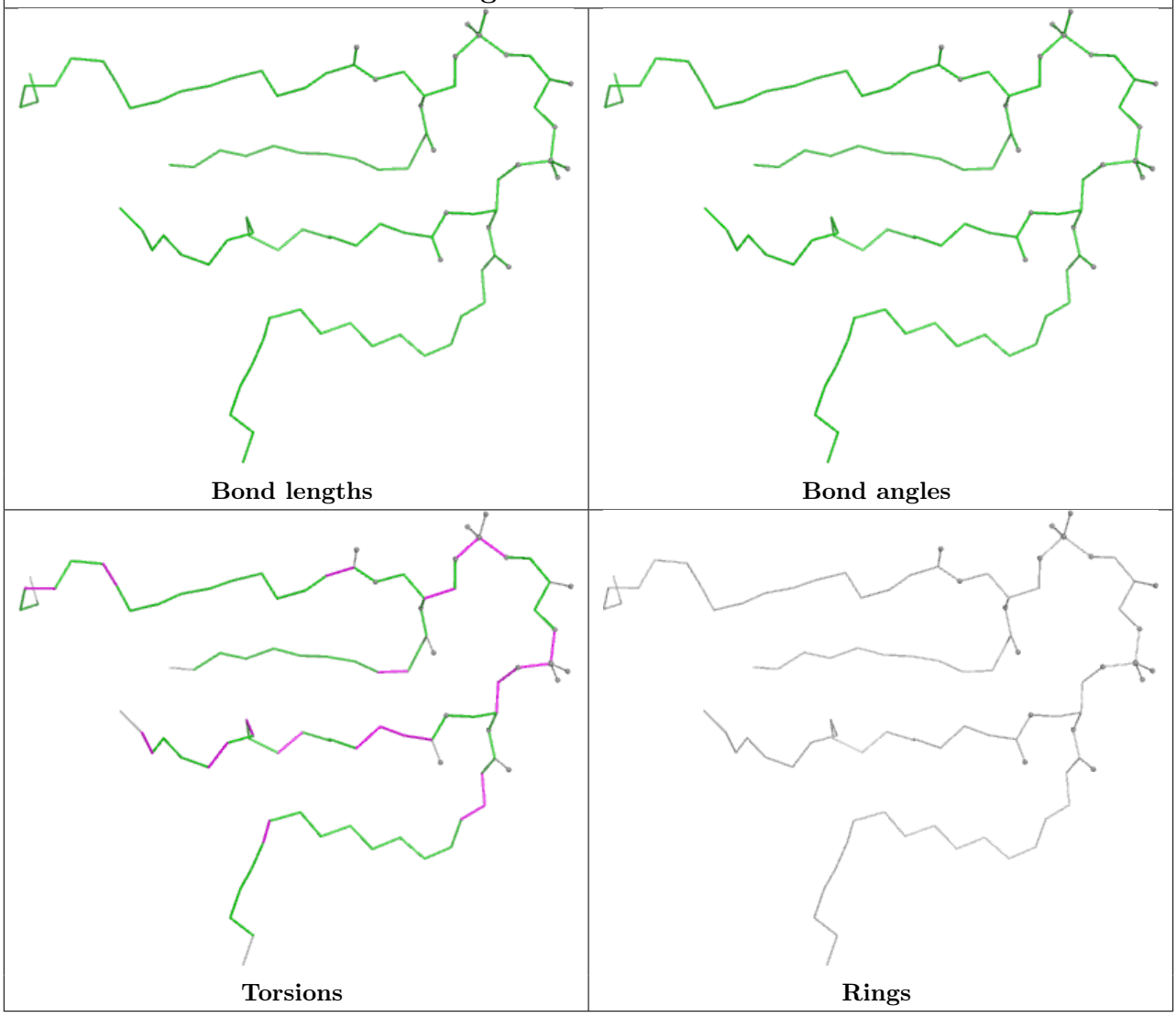


Rings

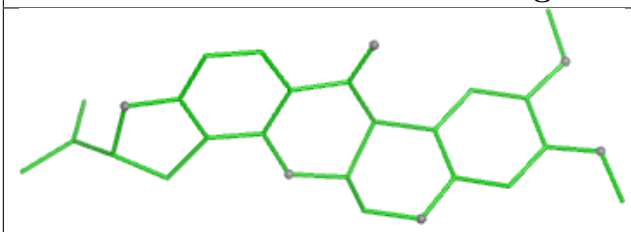
Ligand PC1 A 401



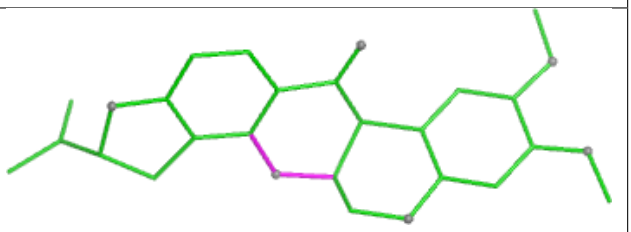
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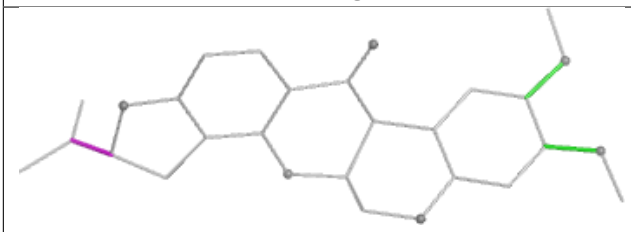
Ligand 970 H 501



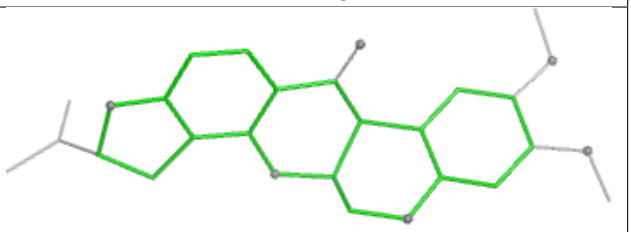
Bond lengths



Bond angles

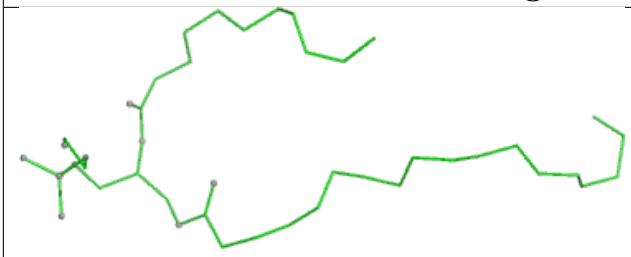


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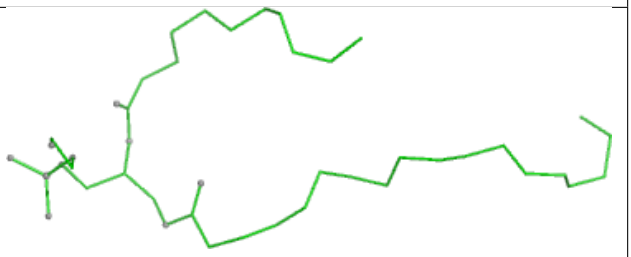


Rings

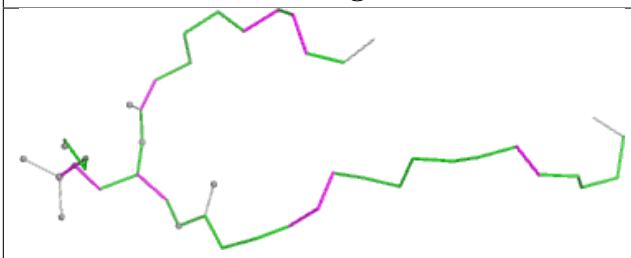
Ligand 3PE M 501



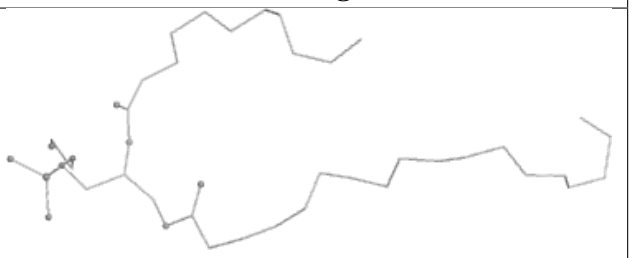
Bond lengths



Bond angles

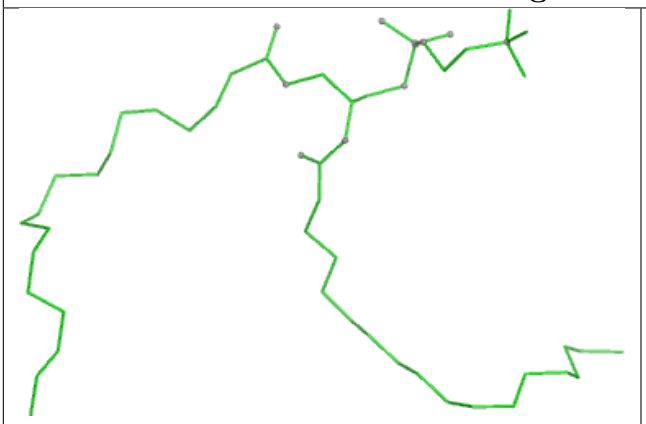


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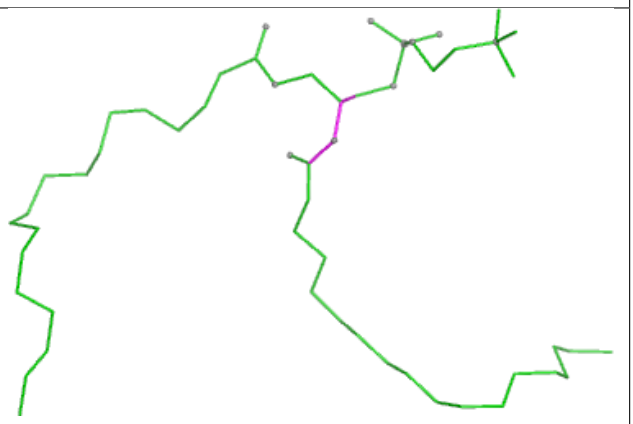


Rings

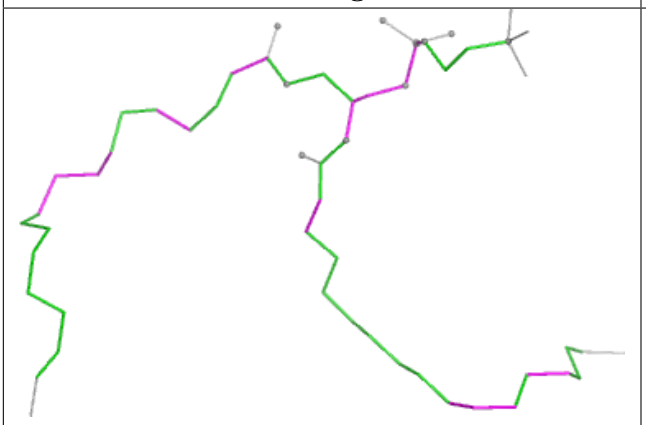
Ligand PC1 L 703



Bond lengths



Bond angles



Torsions



Rings

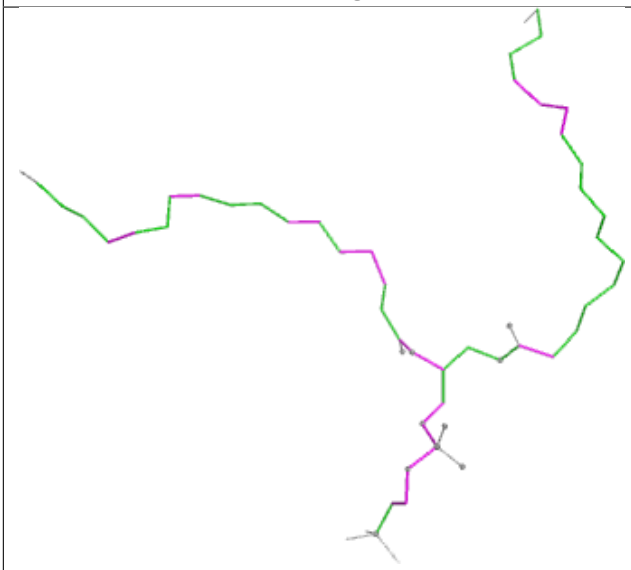
Ligand PC1 9 401



Bond lengths



Bond angles

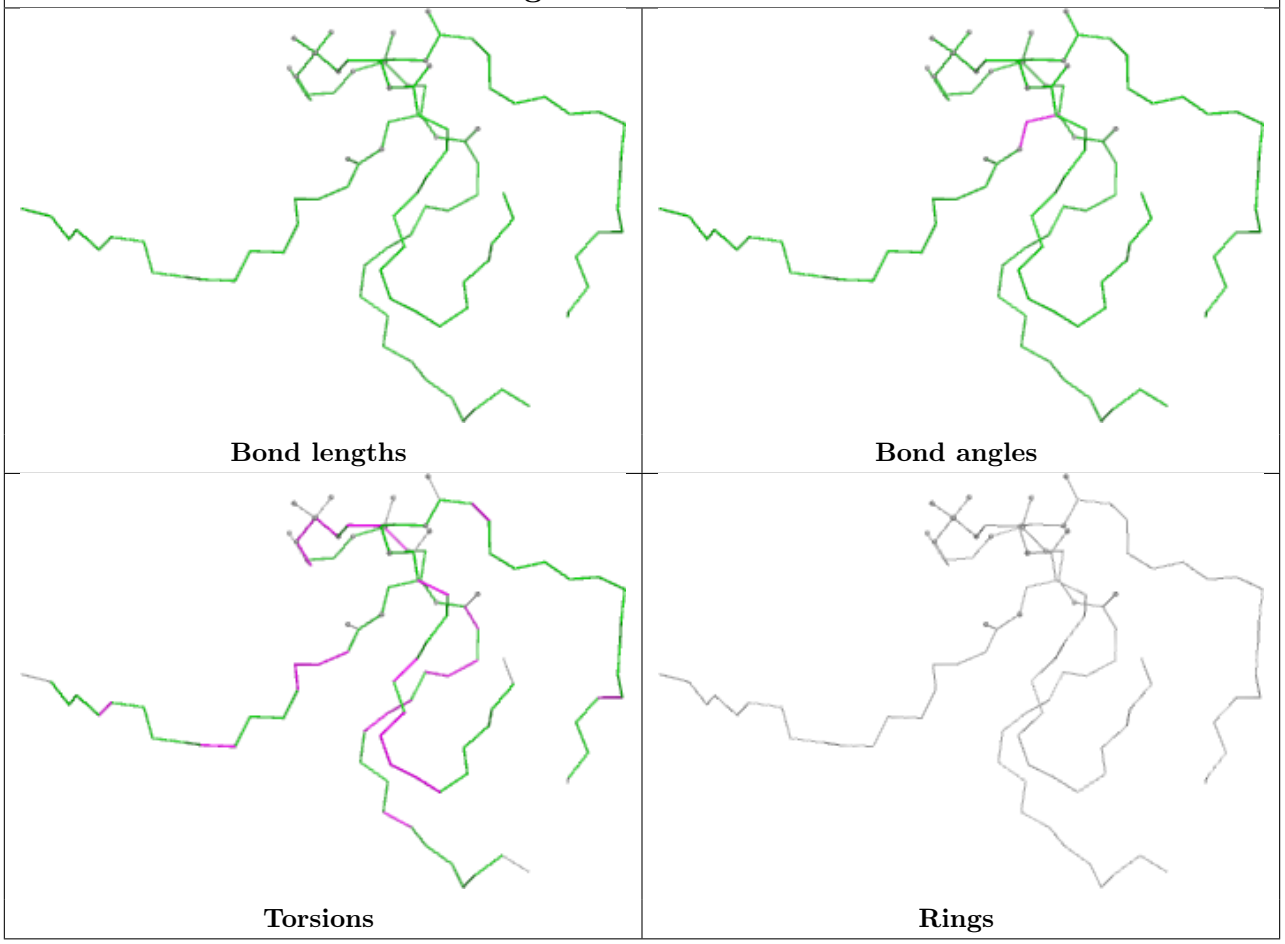


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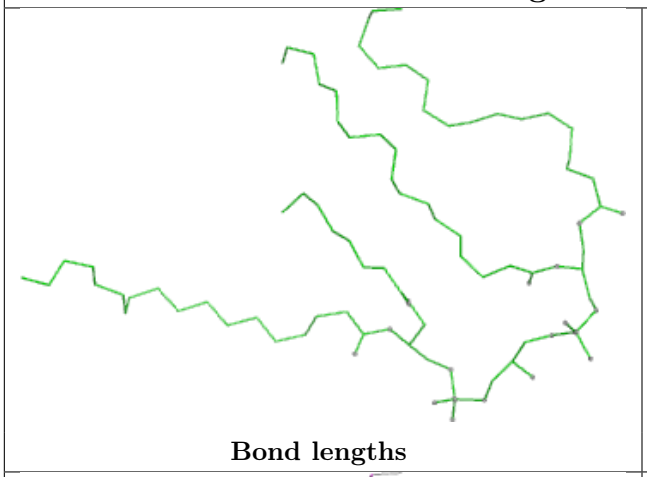


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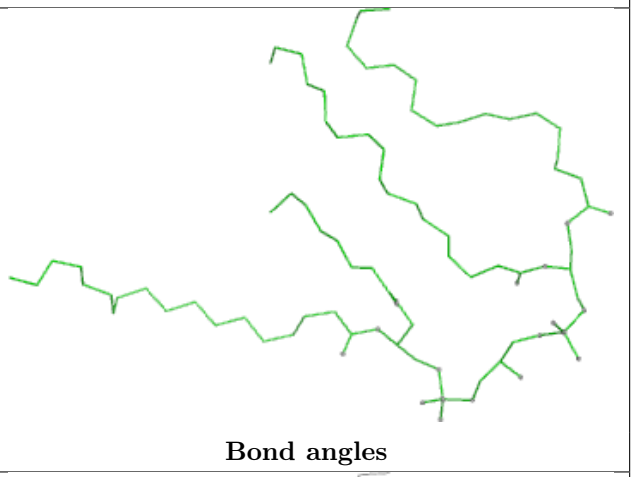
Ligand CDL Y 201



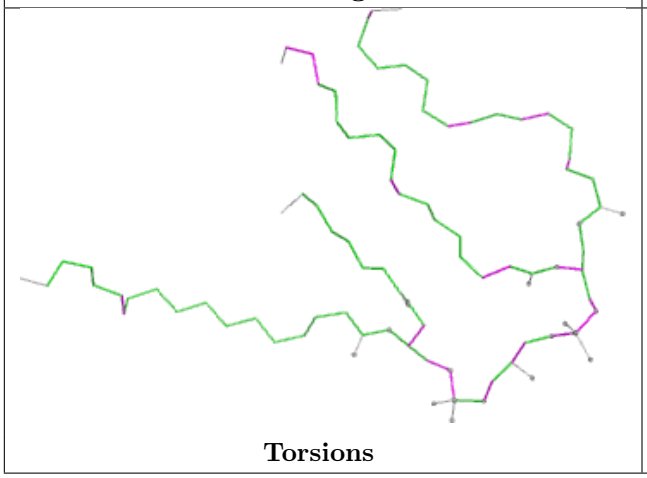
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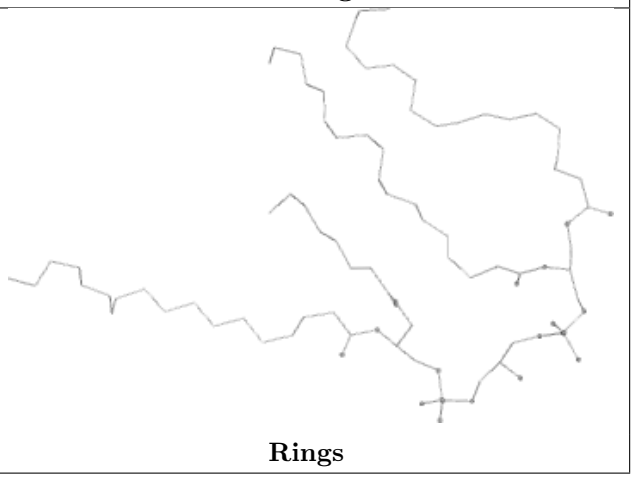
Bond lengths



Bond angles

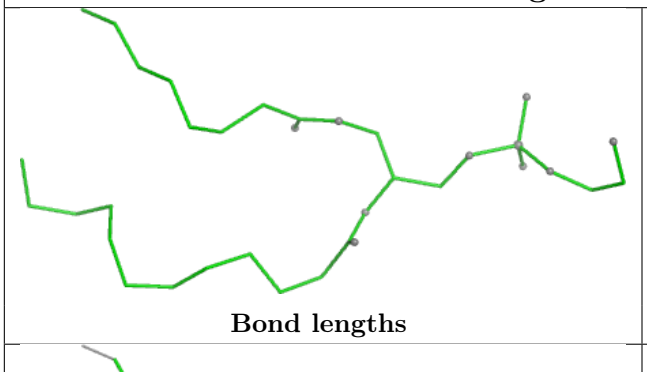


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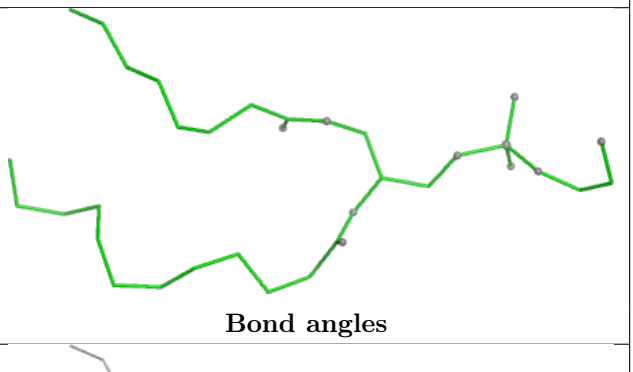


Rings

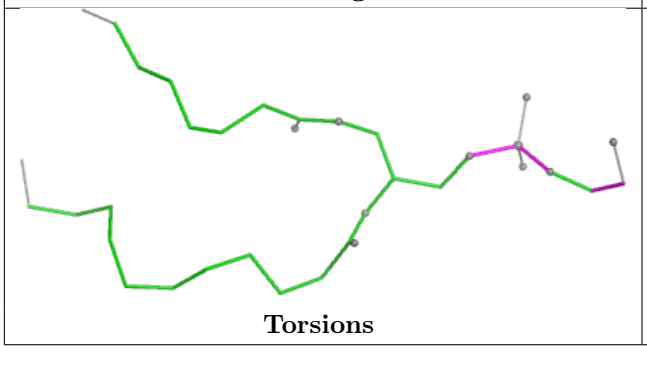
Ligand 3PE V 201



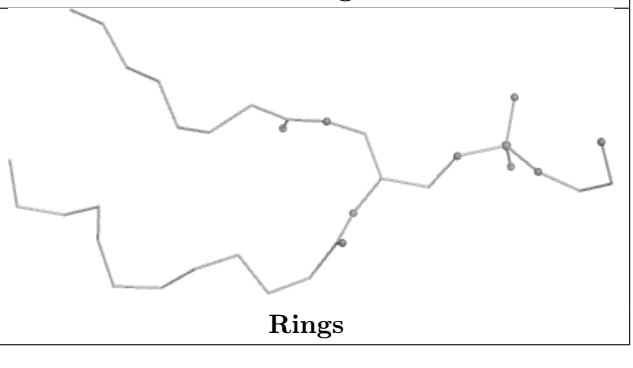
Bond lengths



Bond angles

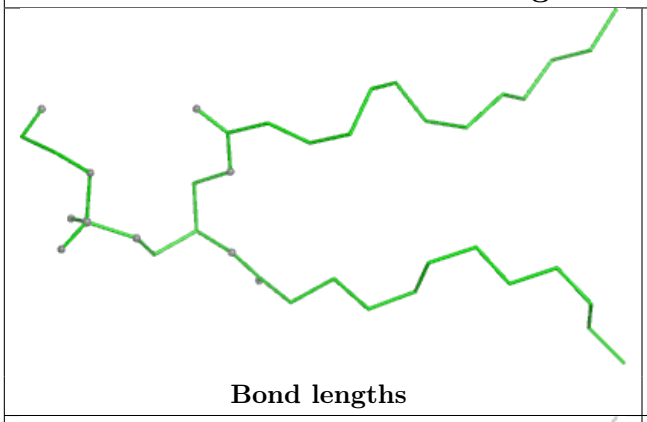


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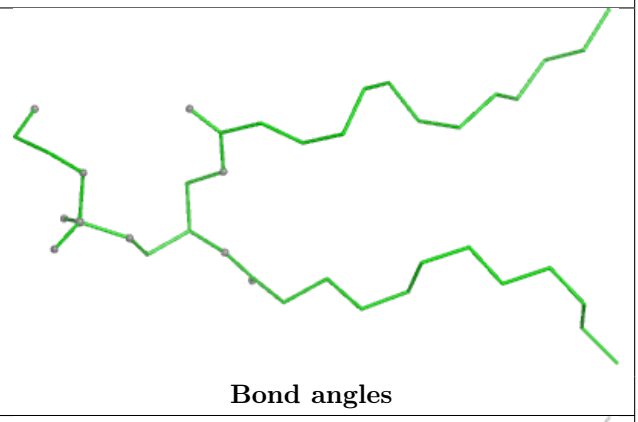


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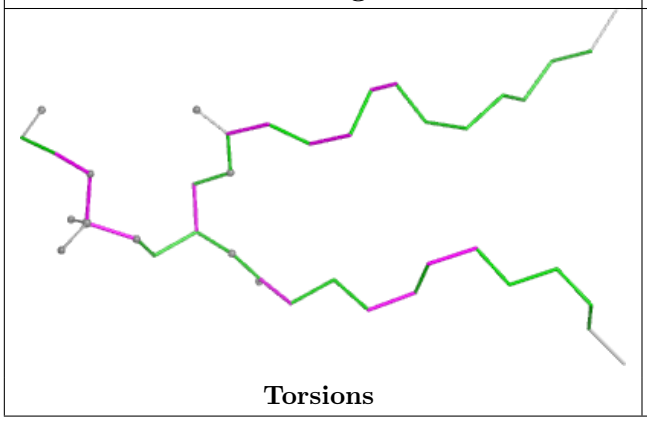
Ligand 3PE L 701



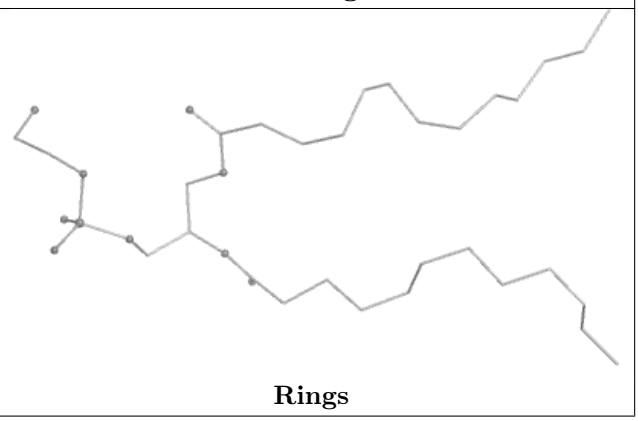
Bond lengths



Bond angles

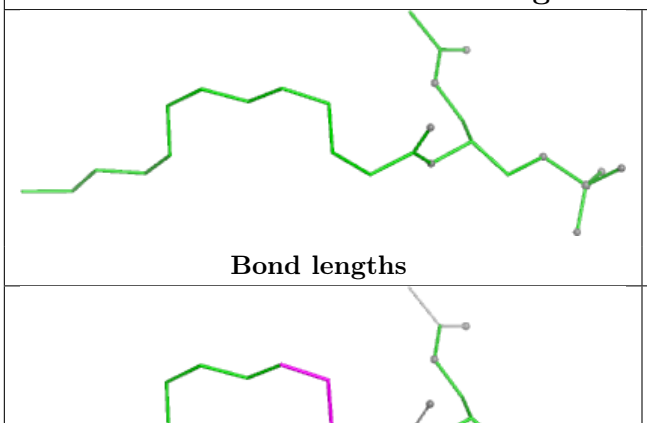


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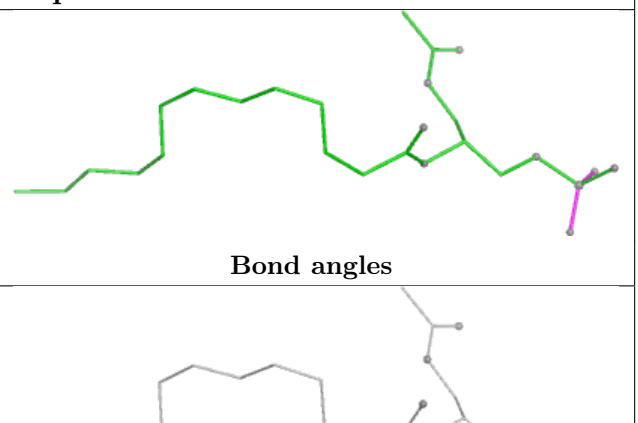


Rings

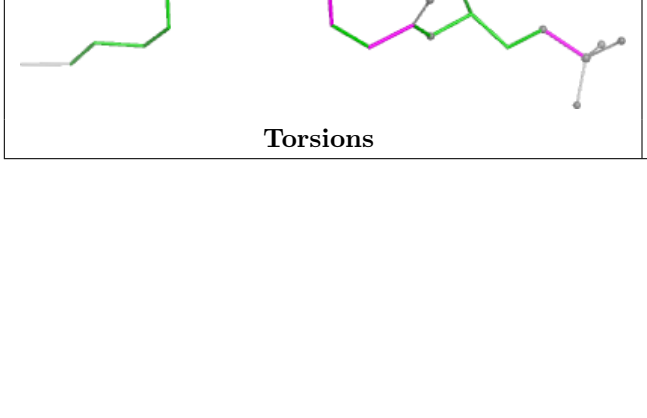
Ligand 3PE p 201



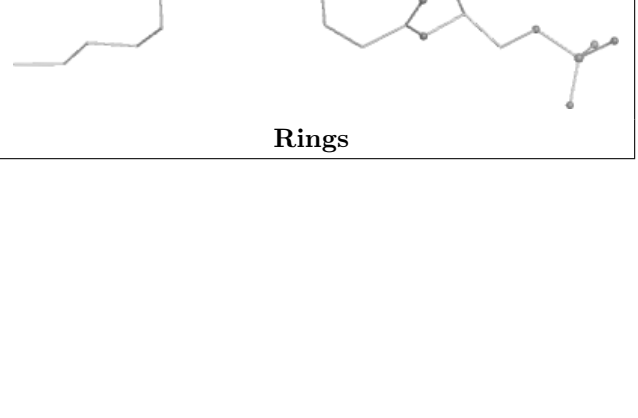
Bond lengths



Bond angles

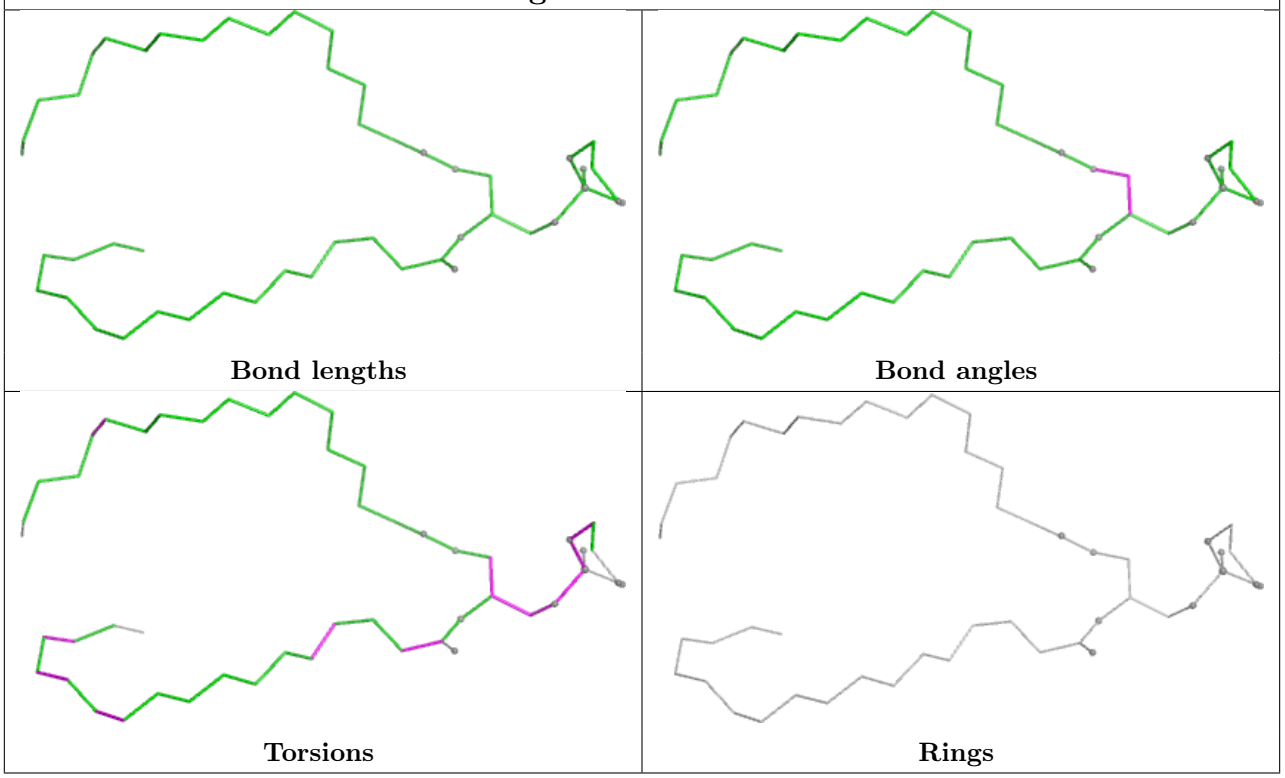


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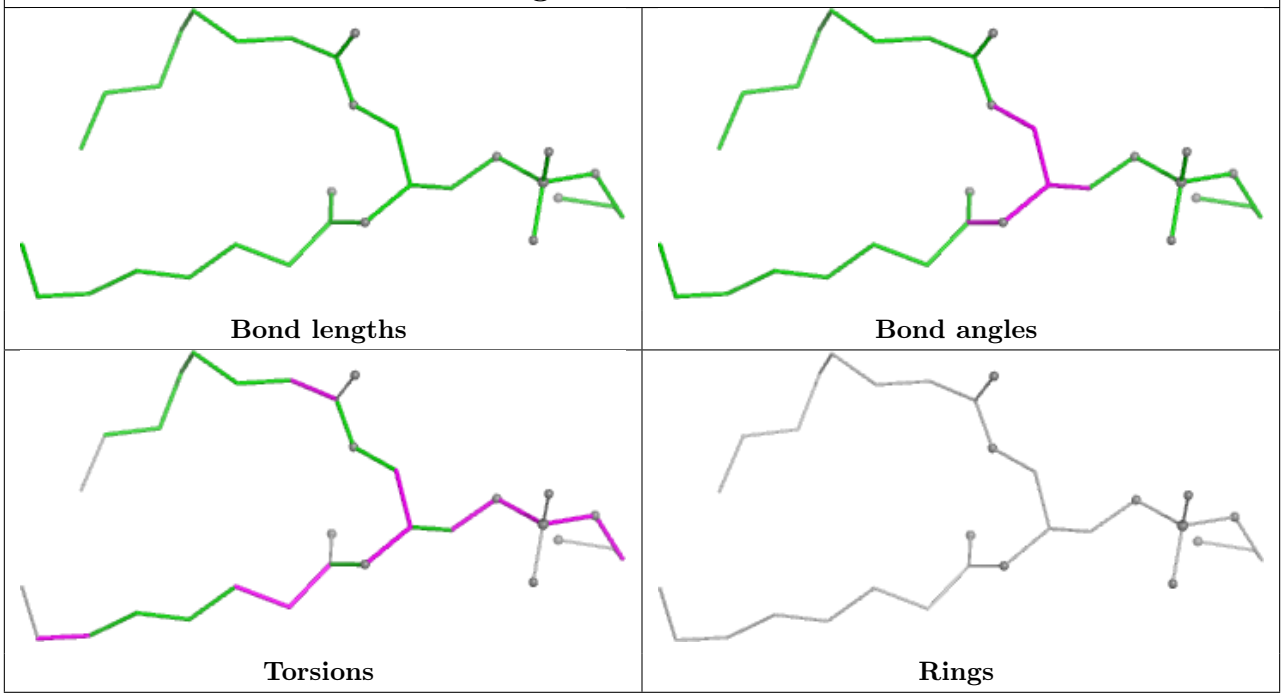


Rings

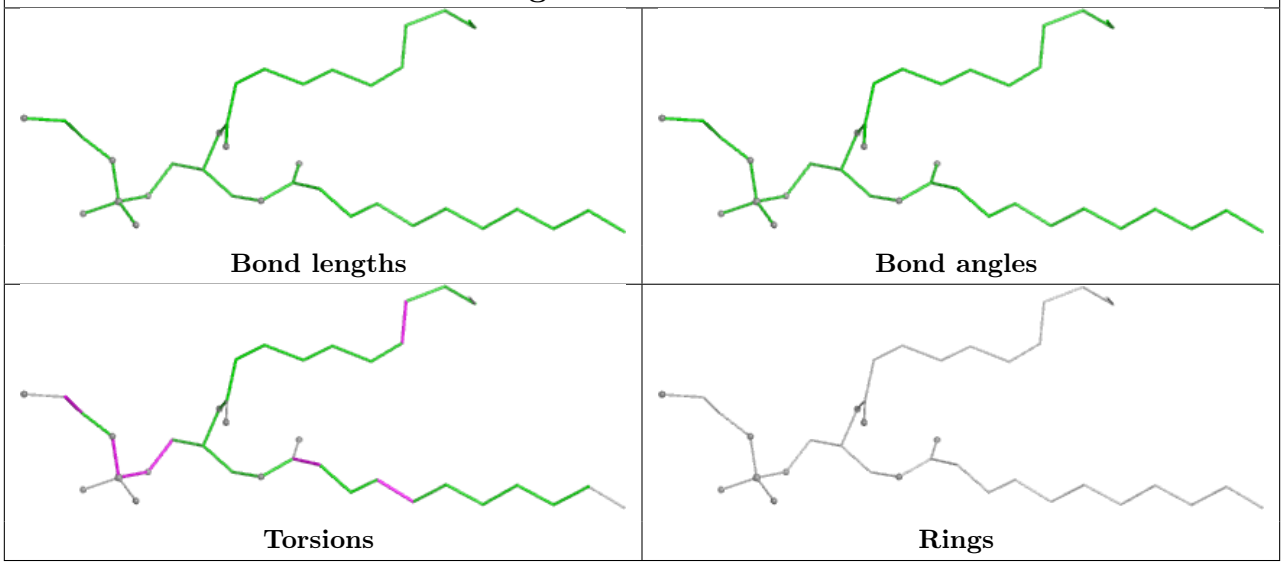
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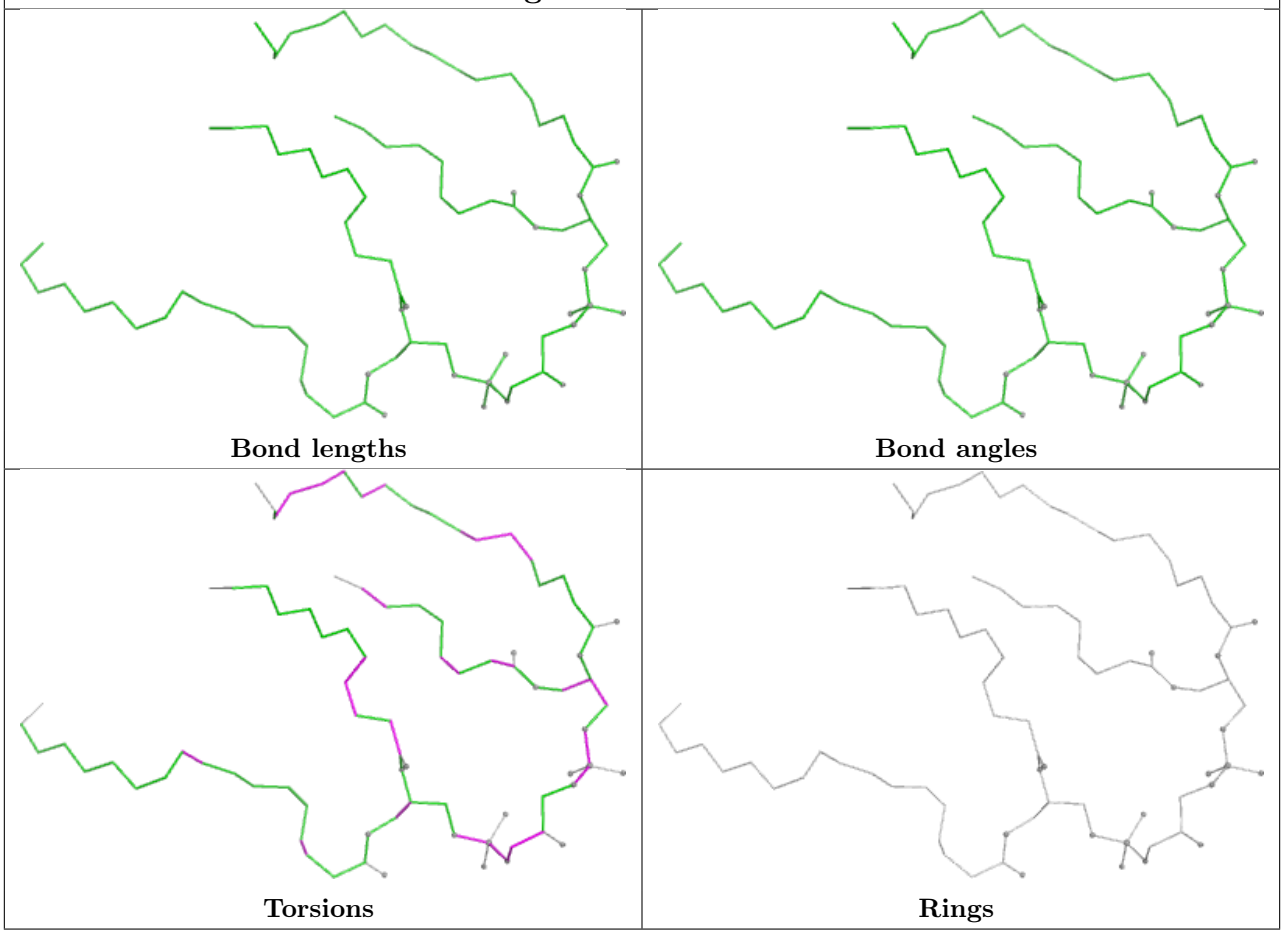
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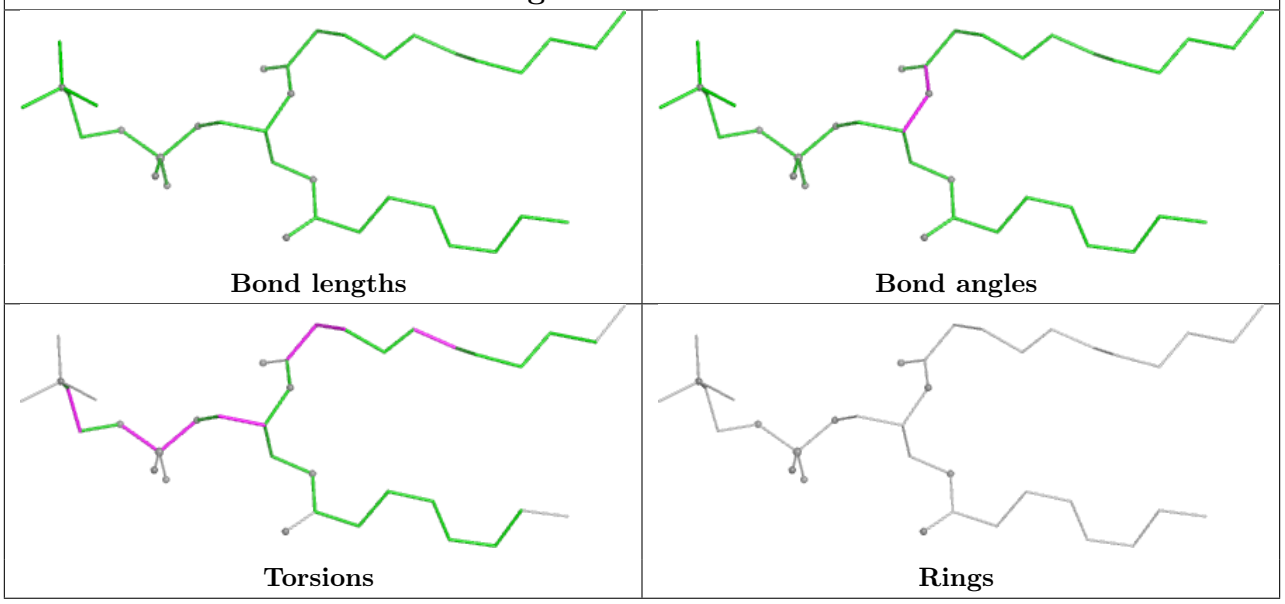
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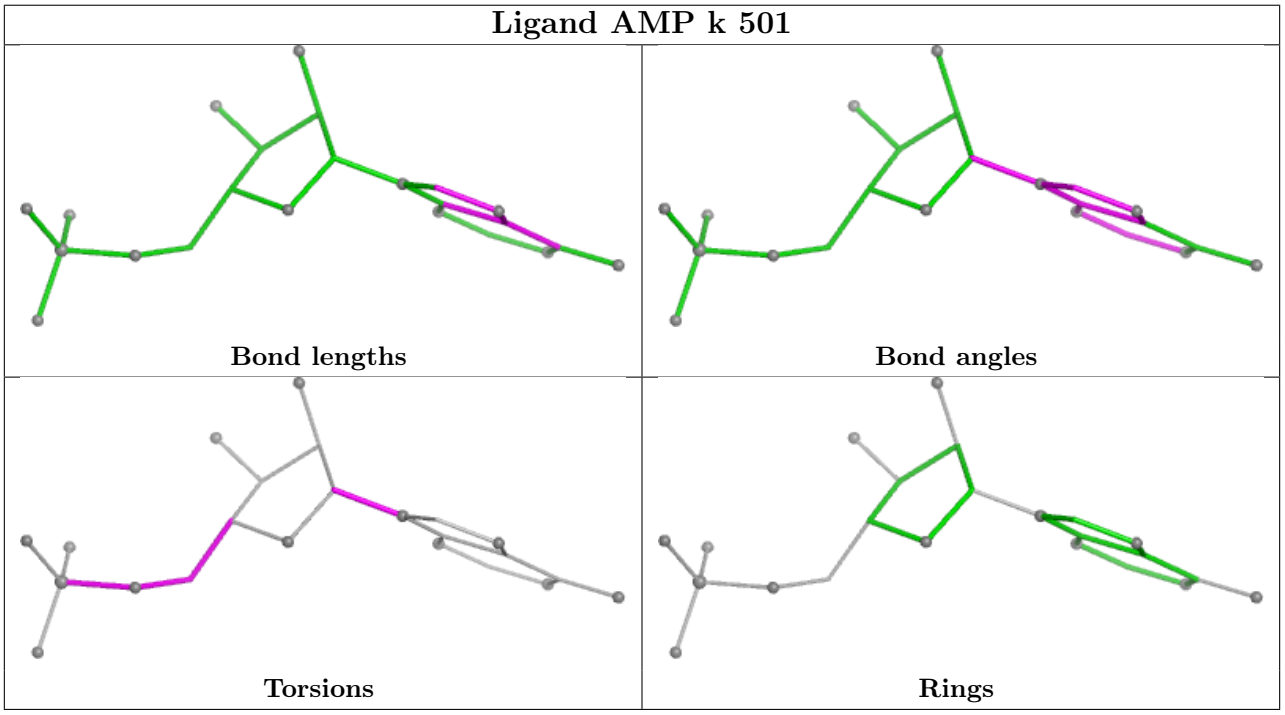
Ligand CDL V 204



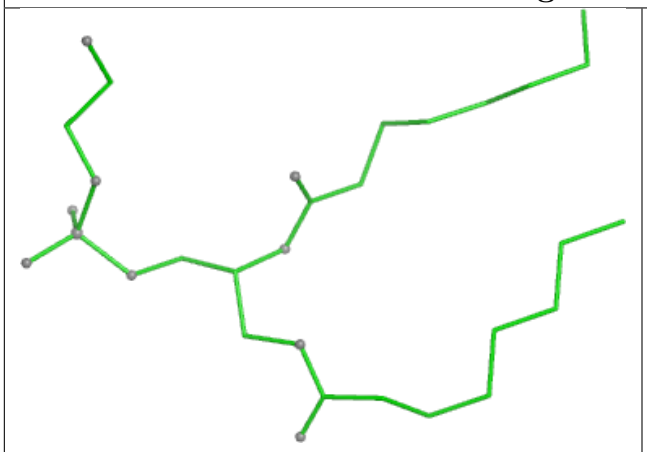
Ligand PC1 A 402



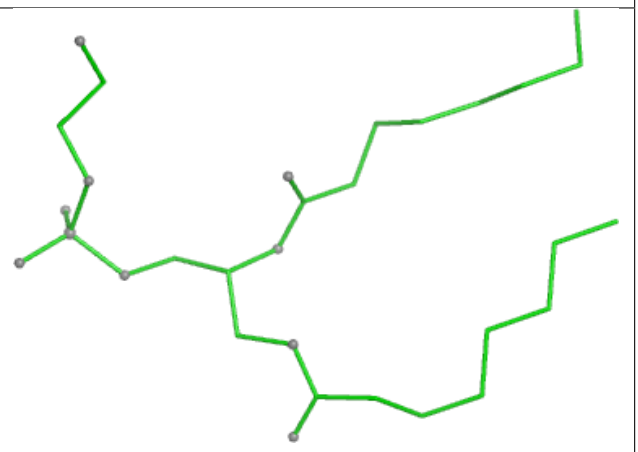
Ligand AMP k 501



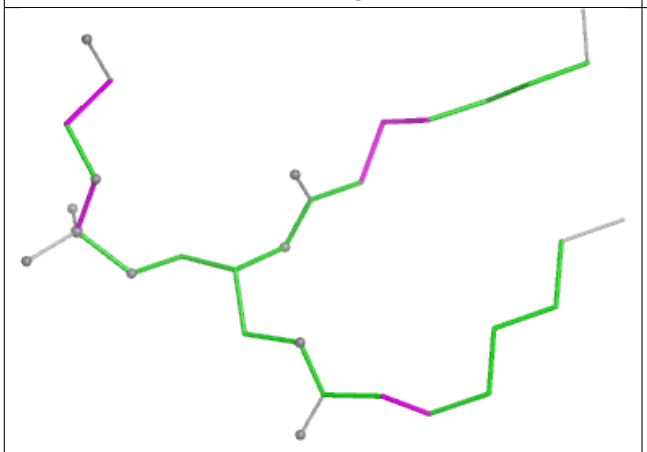
Ligand 3PE l 501



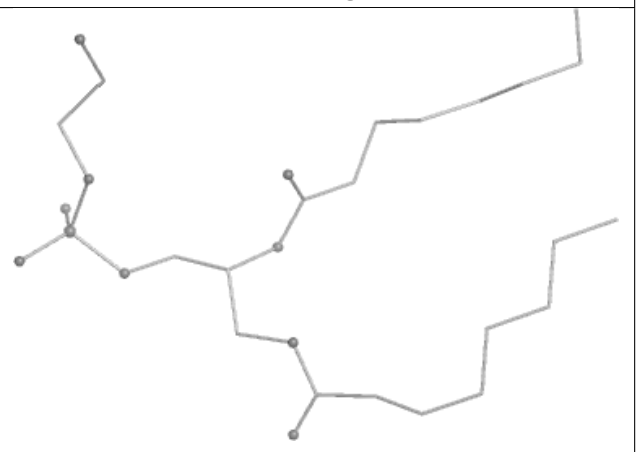
Bond lengths



Bond angles

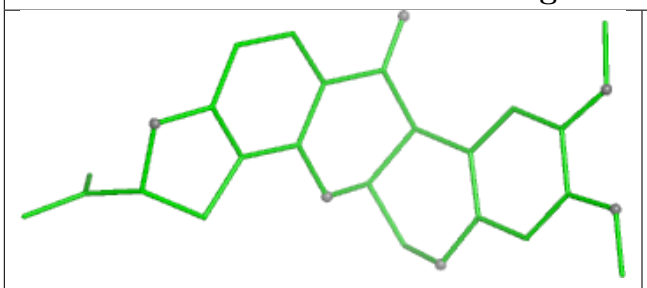


Torsions

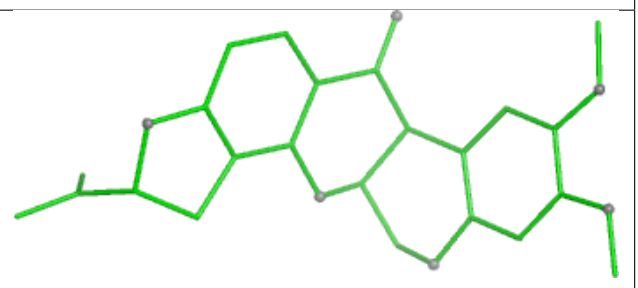


Rings

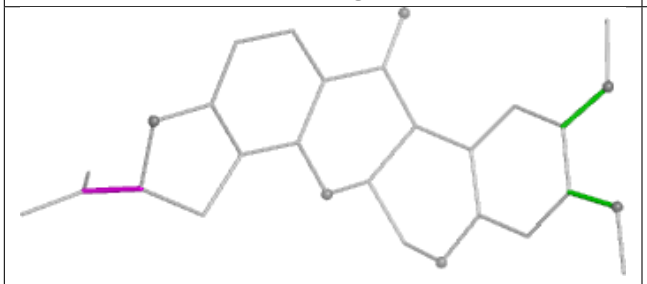
Ligand 970 6 501



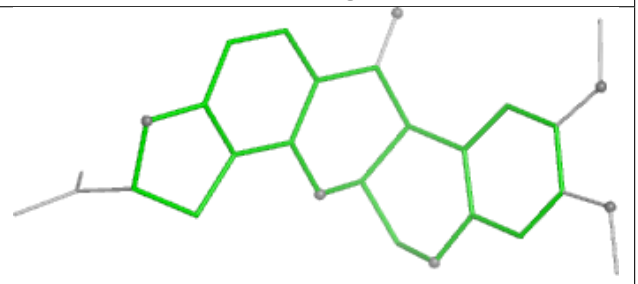
Bond lengths



Bond angles

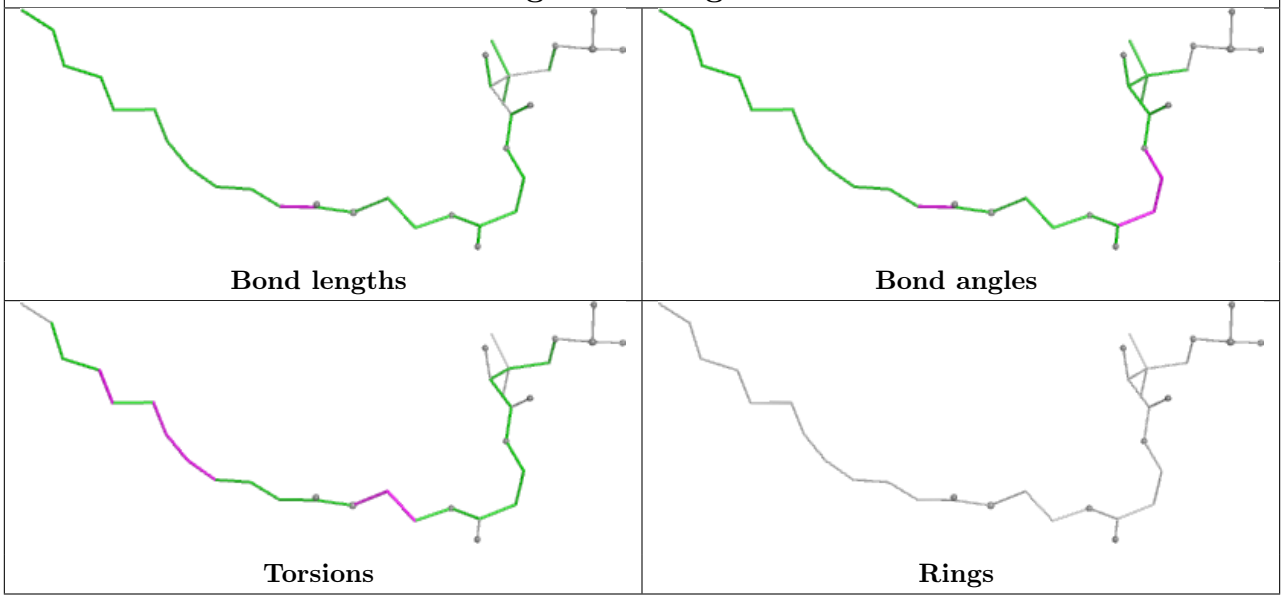


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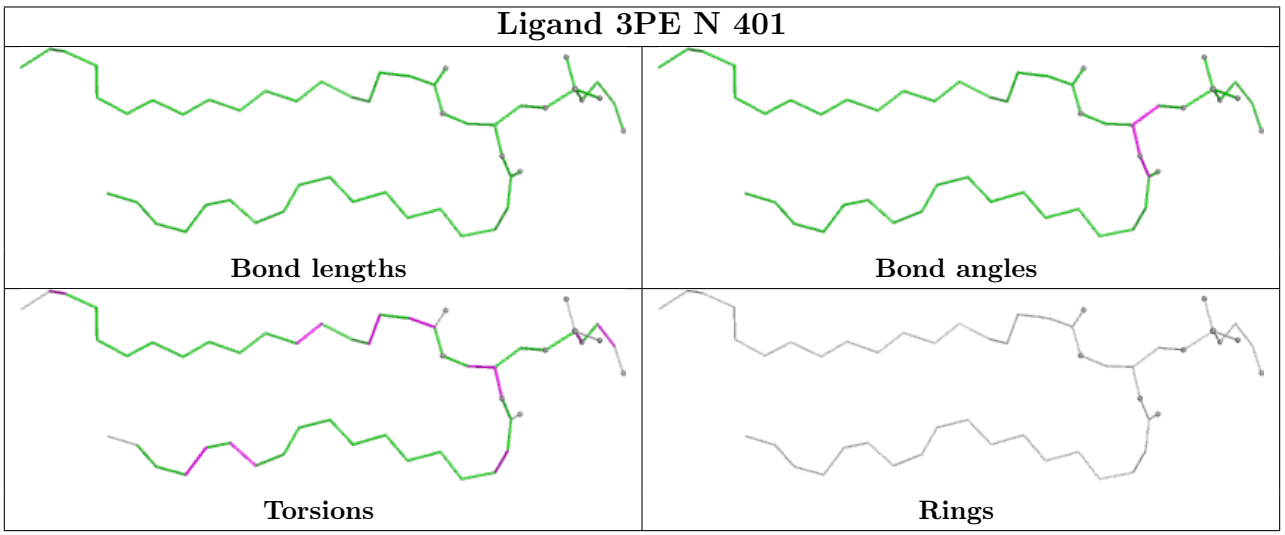


Rings

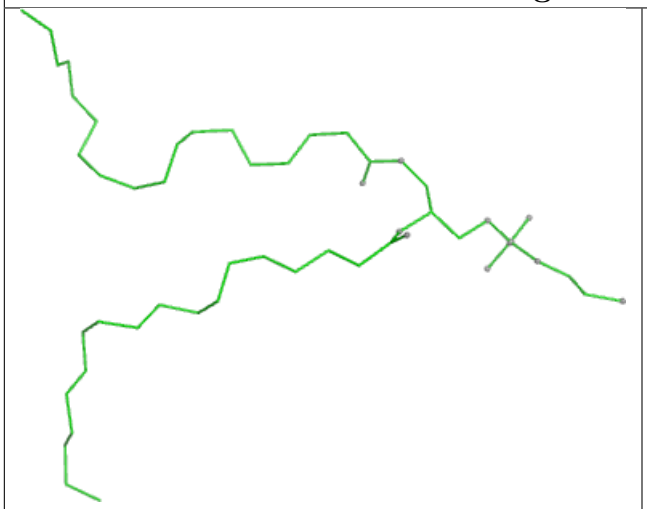
Ligand ZMP g 201



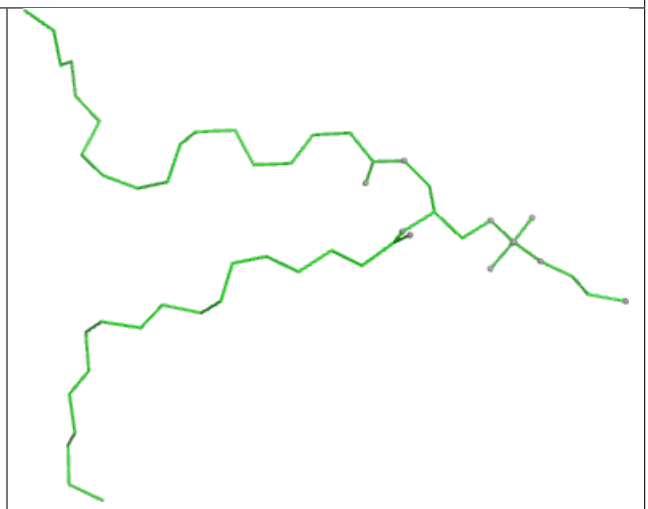
Ligand 3PE N 401



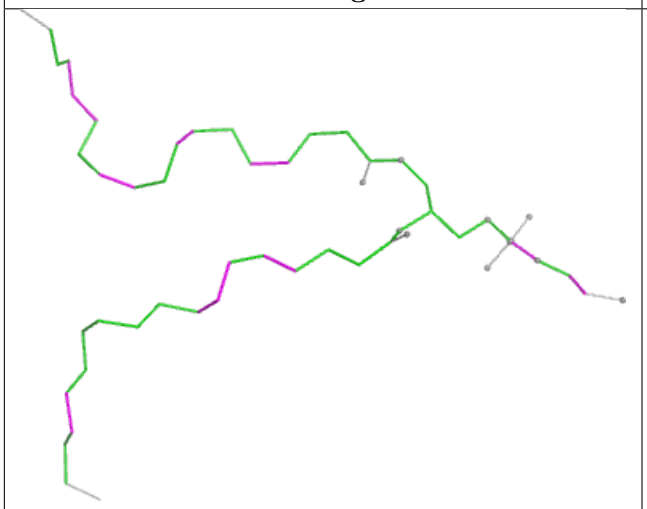
Ligand 3PE 6 503



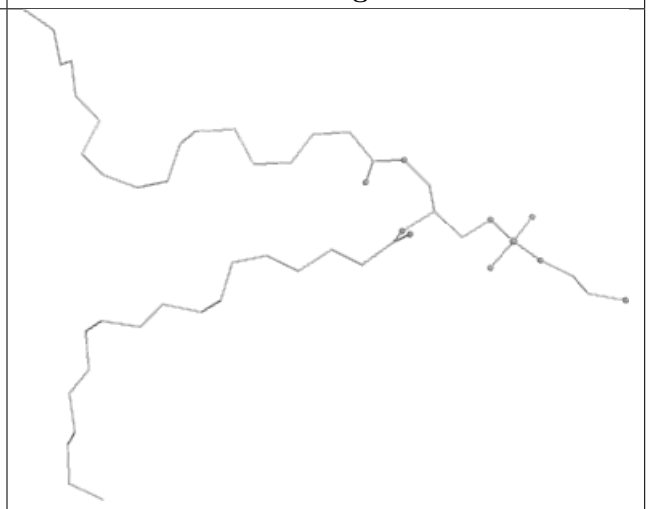
Bond lengths



Bond angles

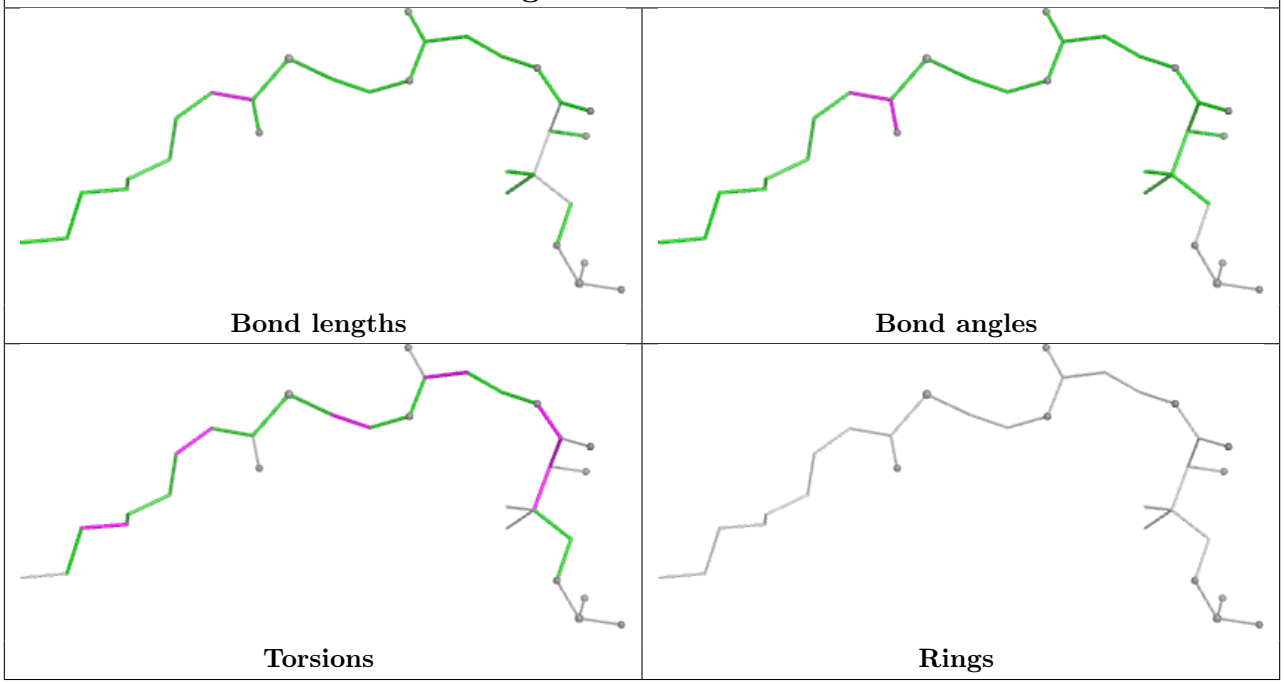


Torsions



Rings

Ligand ZMP X 101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

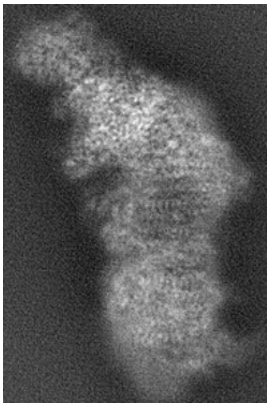
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11253. These allow visual inspection of the internal detail of the map and identification of artifacts.

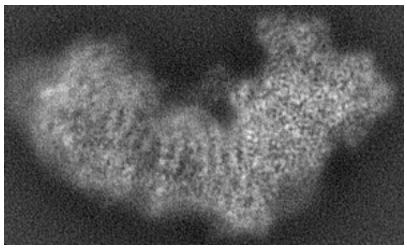
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

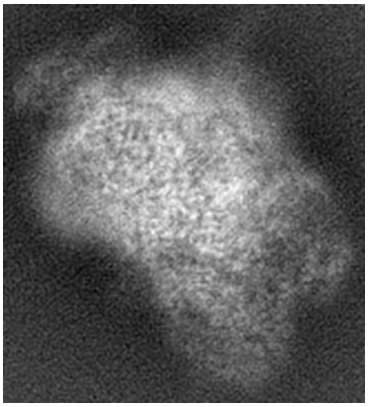
6.1.1 Primary map



X



Y

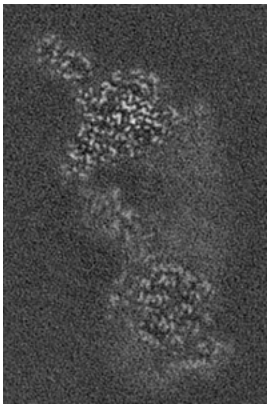


Z

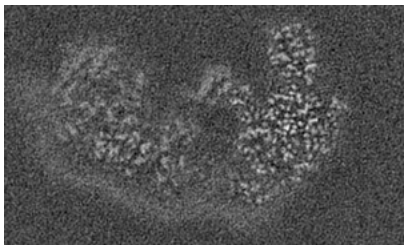
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 81



Y Index: 90

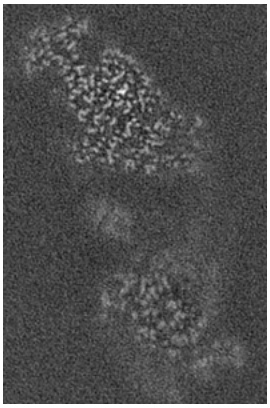


Z Index: 136

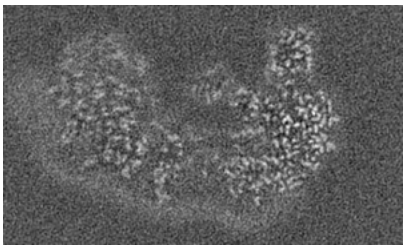
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

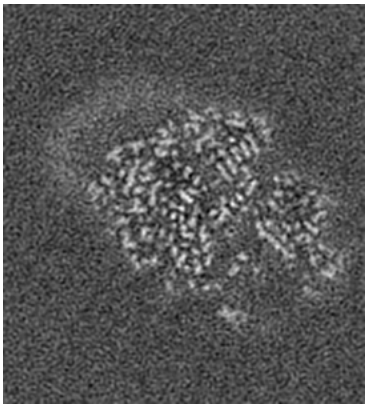
6.3.1 Primary map



X Index: 92



Y Index: 95

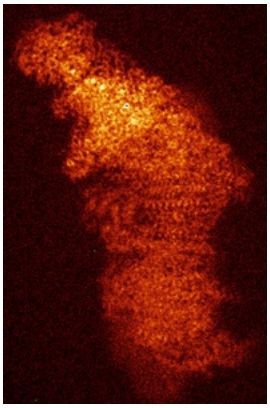


Z Index: 195

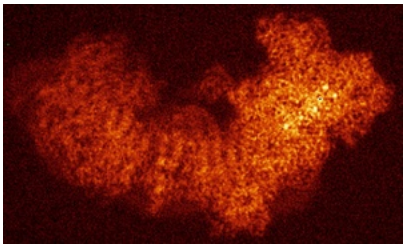
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

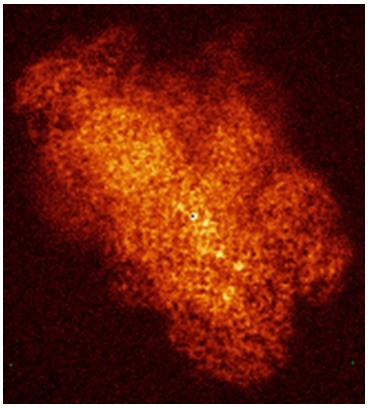
6.4.1 Primary map



X



Y



Z

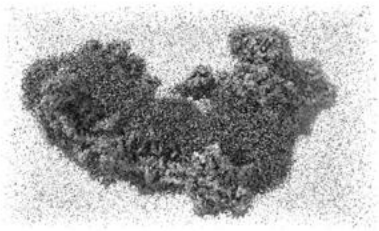
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

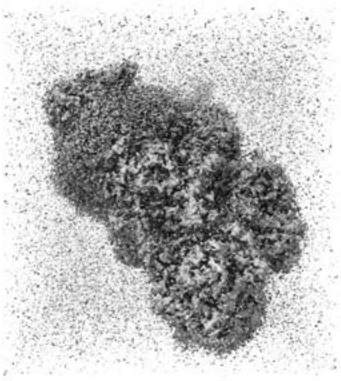
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

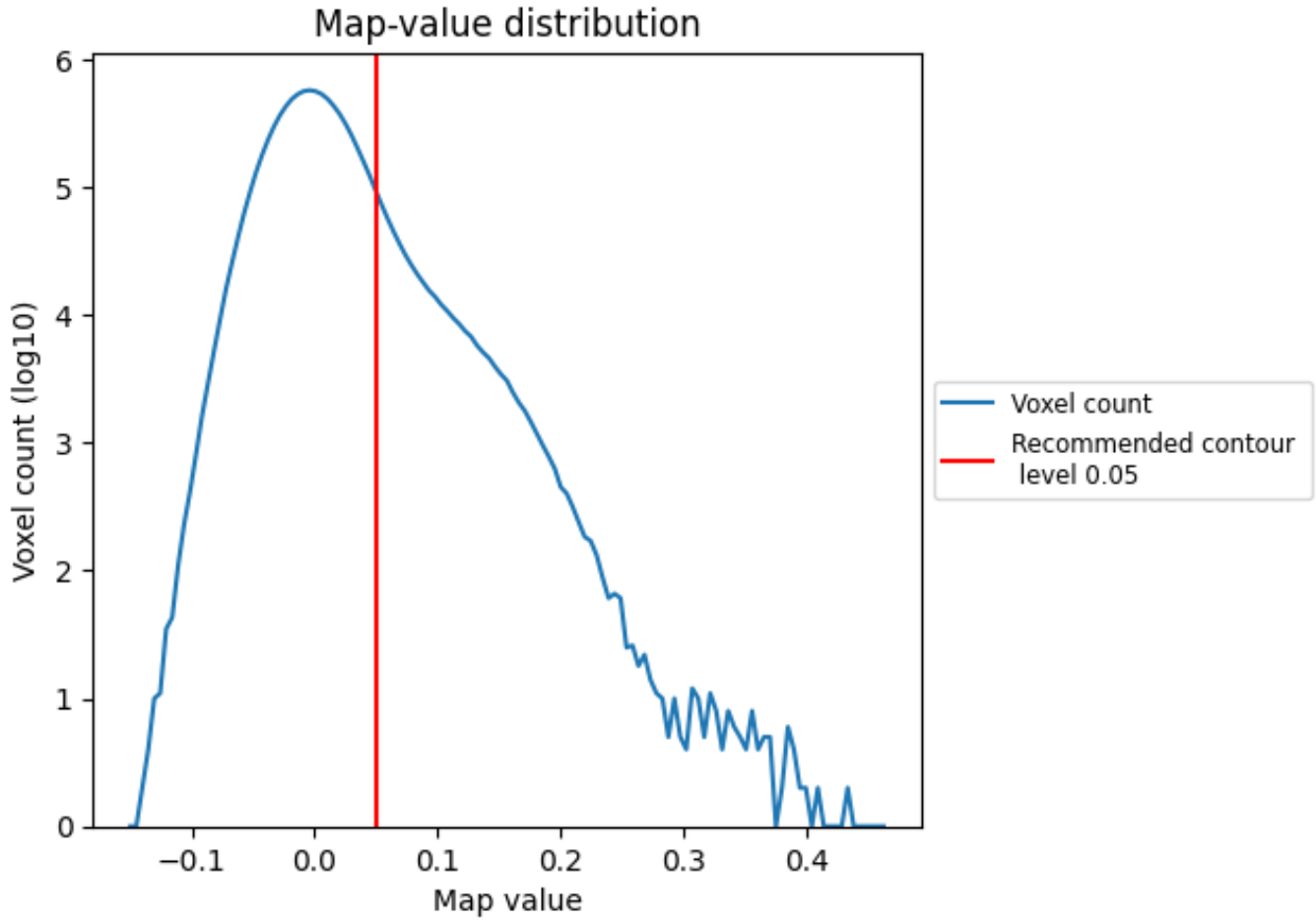
6.6 Mask visualisation (i)

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

7 Map analysis

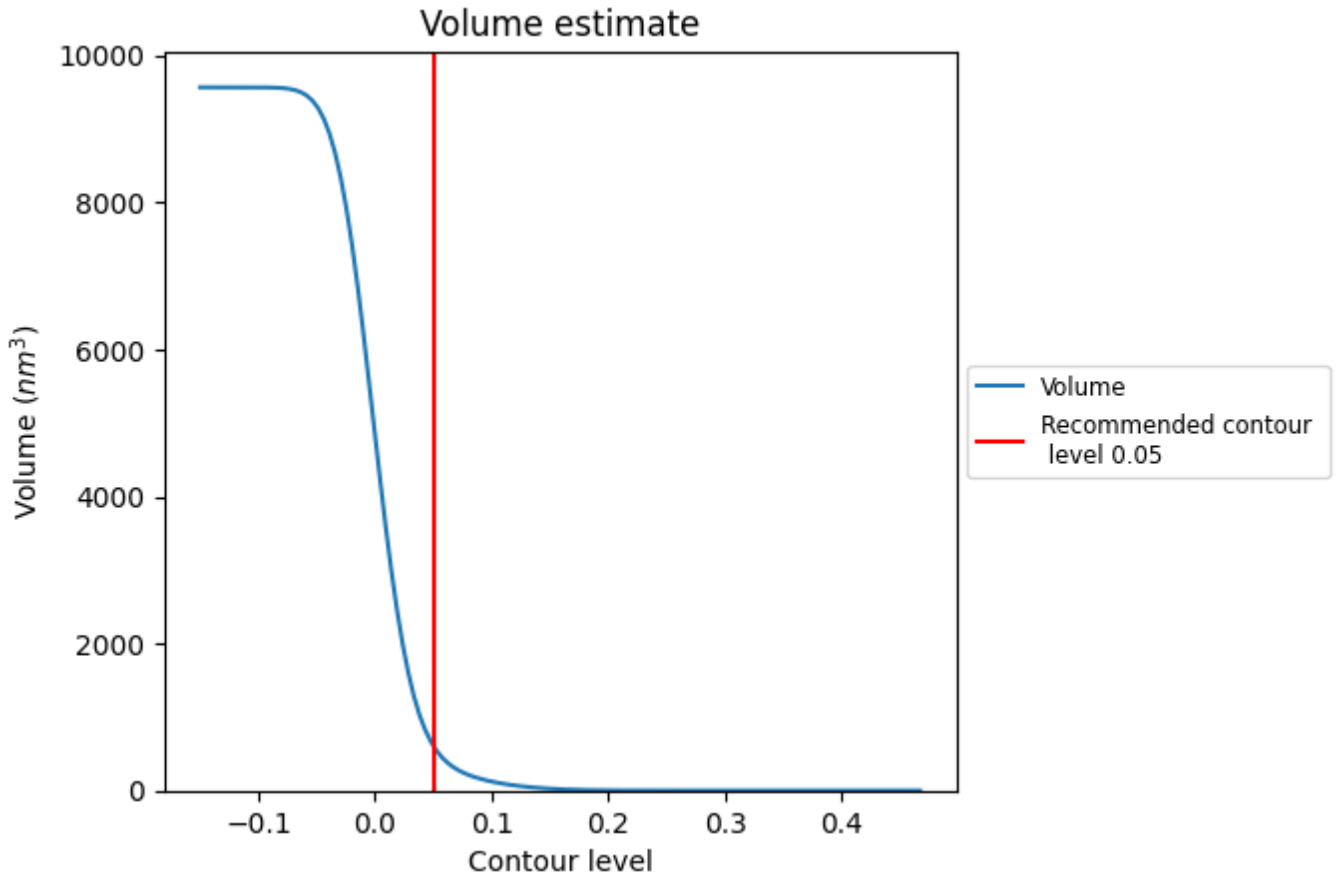
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate (i)



The volume at the recommended contour level is 614 nm^3; this corresponds to an approximate mass of 555 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

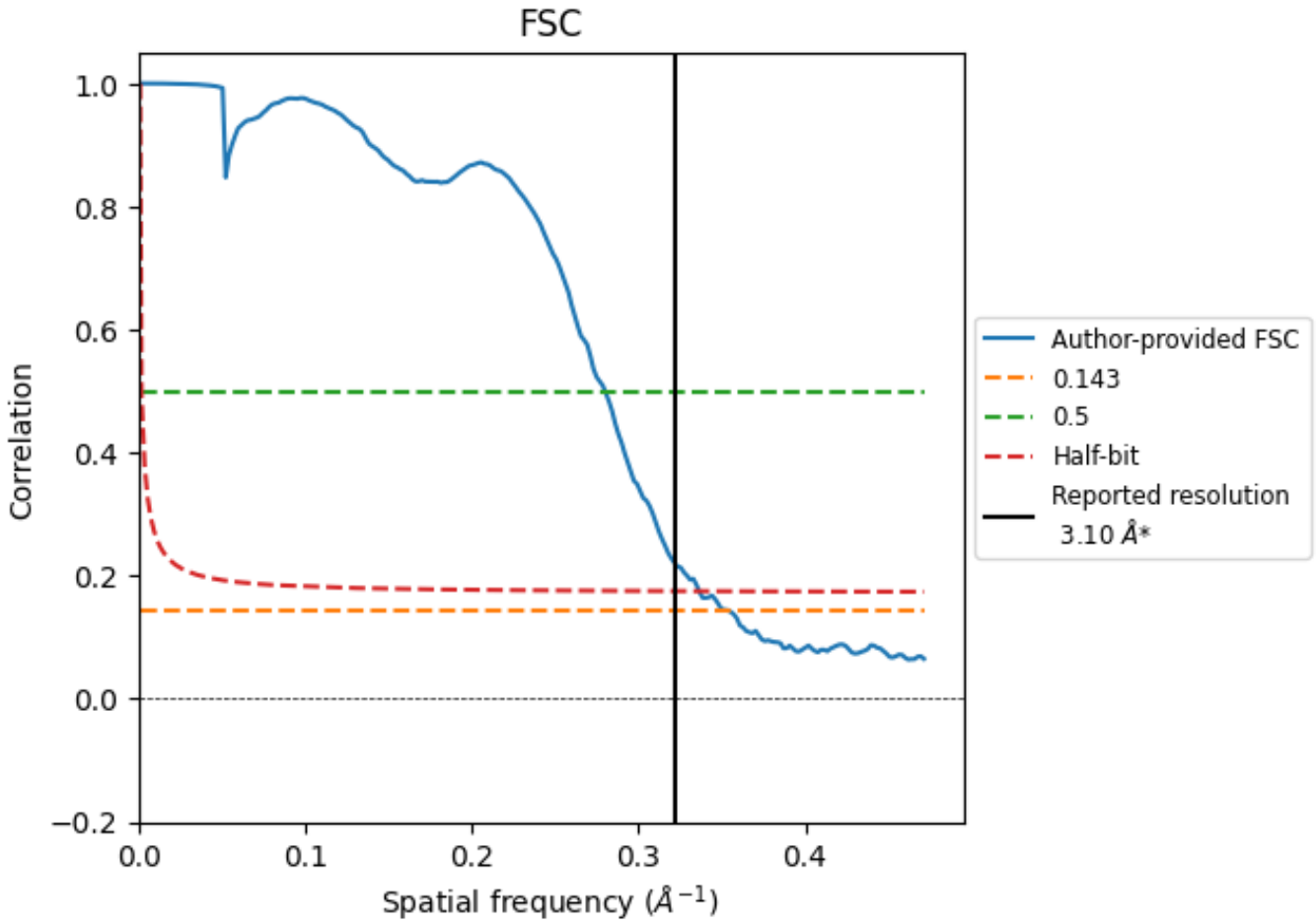
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

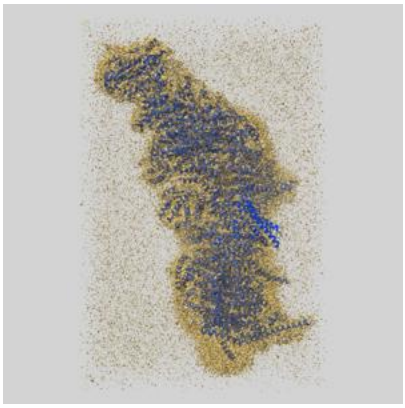
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	2.82	3.57	2.97
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

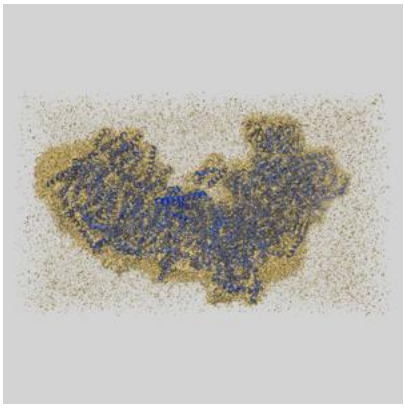
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11253 and PDB model 6ZKL. Per-residue inclusion information can be found in section 3 on page 21.

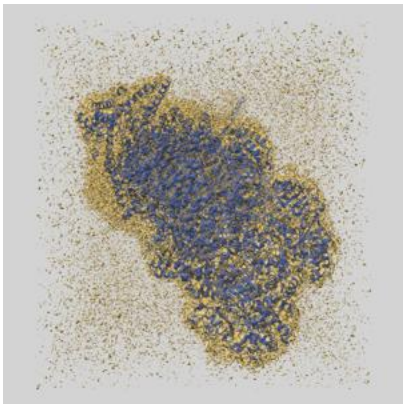
9.1 Map-model overlay



X



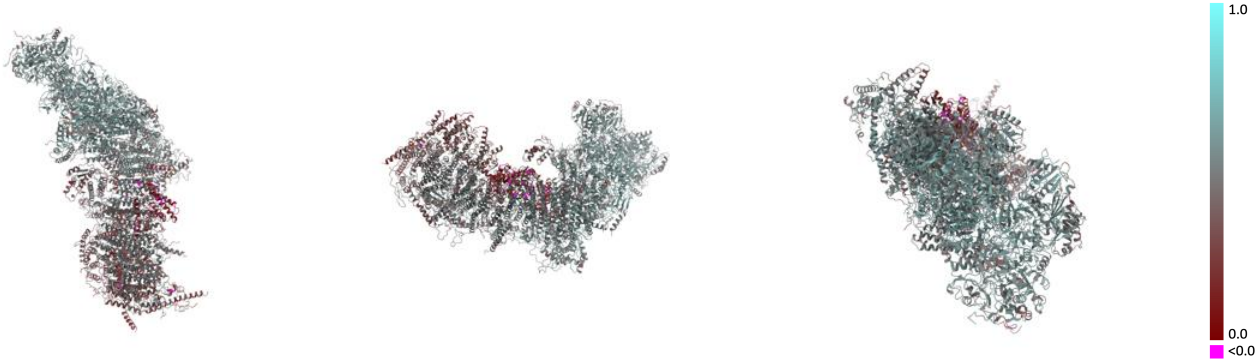
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

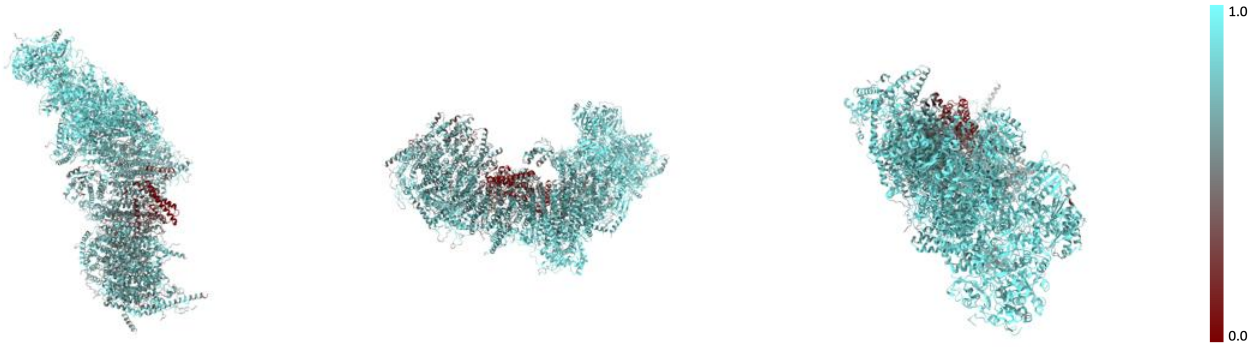
9.2 Q-score mapped to coordinate model (i)



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.

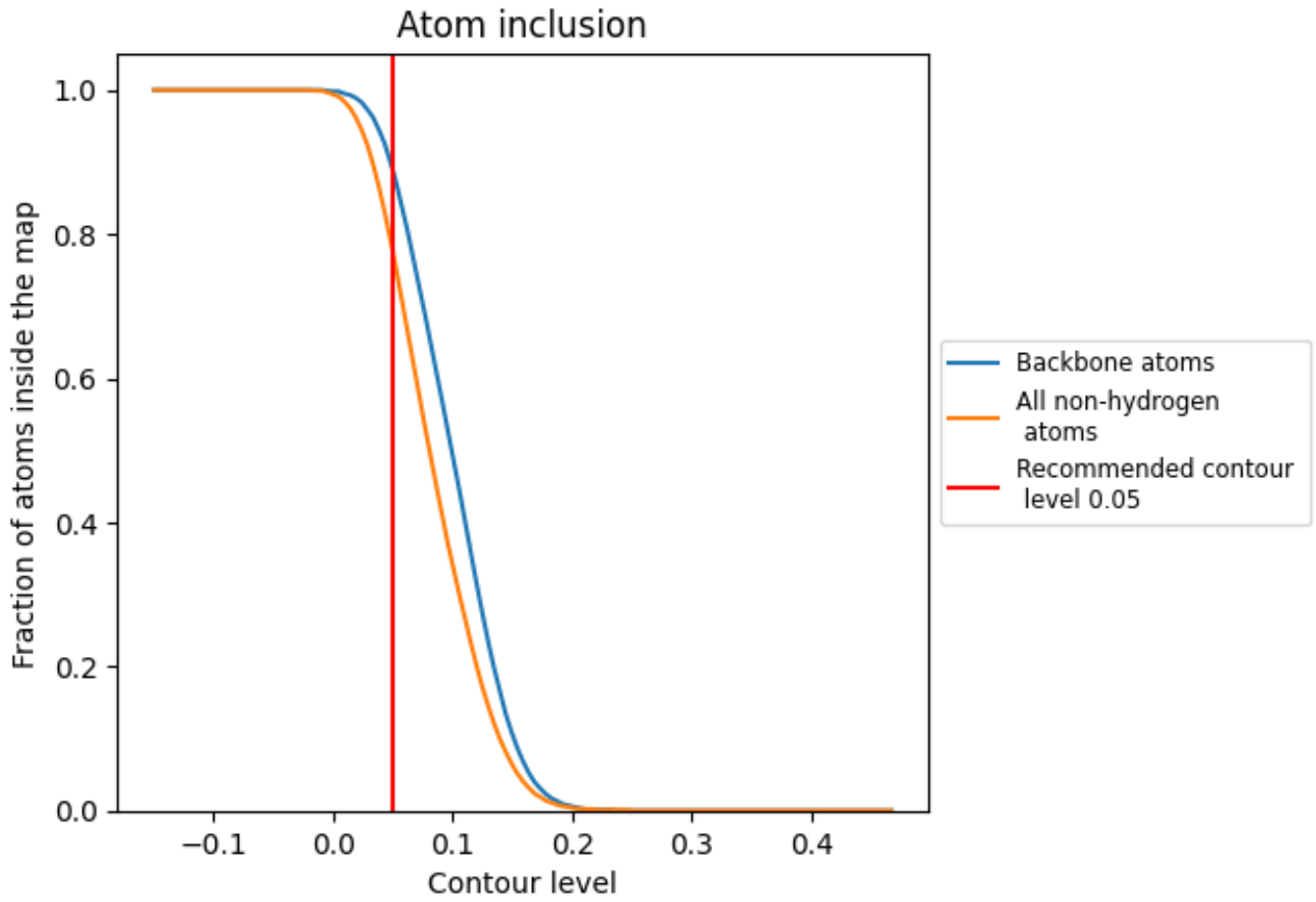
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7750	0.4880
1	0.8900	0.5390
2	0.8560	0.5240
3	0.8780	0.5570
4	0.8430	0.5620
5	0.8990	0.5880
6	0.8970	0.5780
9	0.9080	0.5870
A	0.6490	0.4650
H	0.8170	0.5430
J	0.6460	0.4430
K	0.7330	0.5090
L	0.6690	0.4240
M	0.7710	0.5050
N	0.7880	0.5230
V	0.1710	0.2130
W	0.7730	0.4880
X	0.6010	0.3480
Y	0.8150	0.5000
Z	0.7570	0.4360
a	0.8650	0.5030
b	0.8890	0.5750
c	0.8650	0.5750
d	0.8480	0.5270
e	0.8420	0.4910
f	0.8290	0.5250
g	0.8060	0.5350
h	0.8560	0.5600
i	0.8670	0.5570
j	0.6660	0.3920
k	0.7130	0.4250
l	0.7950	0.4910
m	0.8370	0.5110
n	0.6070	0.3080
o	0.7110	0.4620



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Chain	Atom inclusion	Q-score
p	0.5950	0.3620
q	0.8460	0.5200
r	0.7190	0.3900
s	0.6910	0.3490
t	0.6710	0.3550
u	0.7120	0.3640
v	0.6700	0.3860
w	0.7230	0.4650
x	0.7300	0.4000
y	0.7190	0.4380
z	0.8700	0.5400