wwPDB EM Validation Summary Report (i)

Aug 23, 2026 – 08:12 am BST

PDB ID	:	9SMI / pdb_00009smi
EMDB ID	:	EMD-55033
Title	:	Reduced bovine complex I in lipid nanodisc, NADH-deactive
Authors	:	Chung, I.; Hirst, J.
Deposited on	:	2025-09-08
Resolution	:	2.01 Å(reported)
Based on initial model	:	7QSM

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:

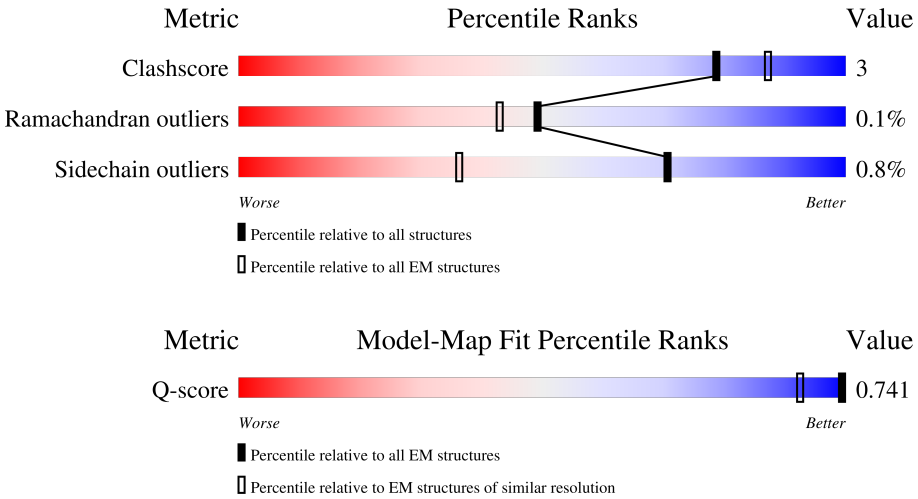
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.01 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.



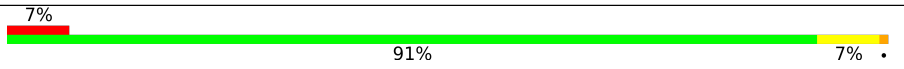
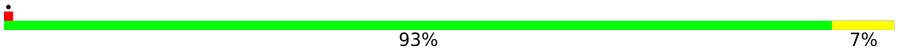
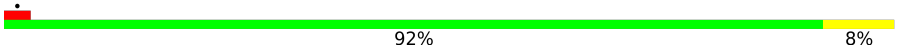
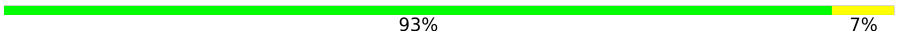
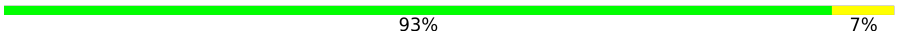
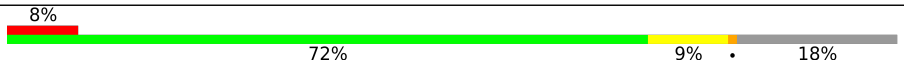
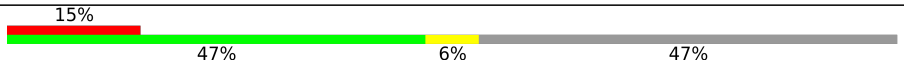
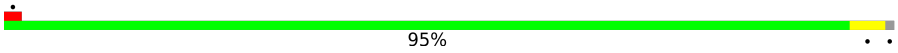
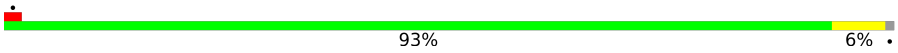
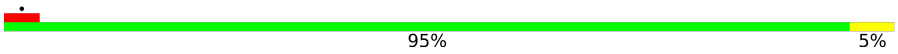
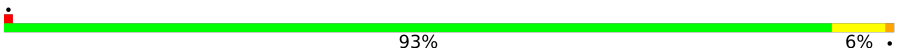
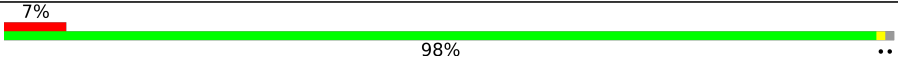
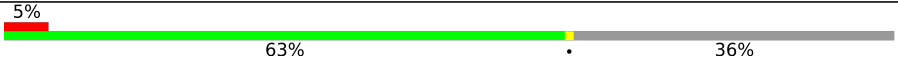
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1691 (1.52 - 2.51)

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	74% 14% 12%
2	B	216	64% 6% 28%
3	C	266	76% 22%
4	D	463	87% 6% 7%

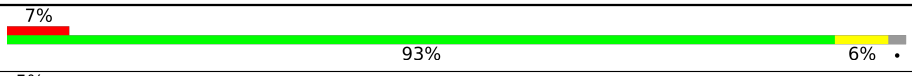
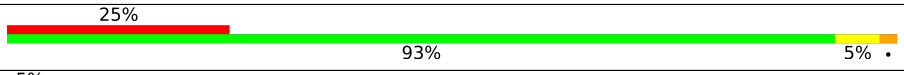
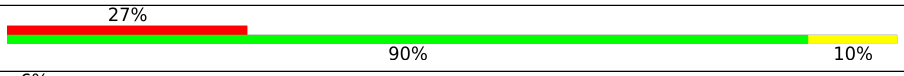
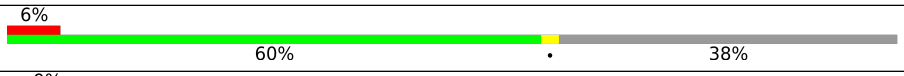
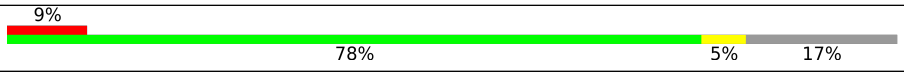
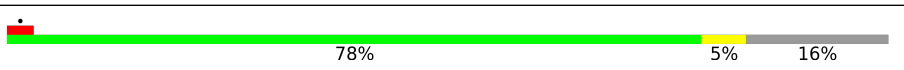
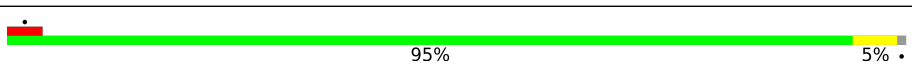
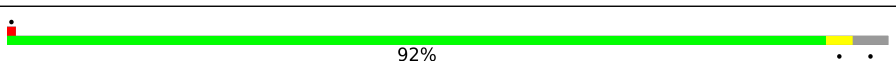
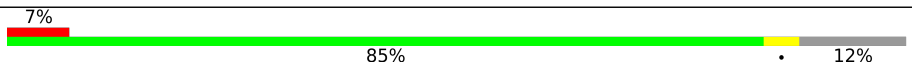
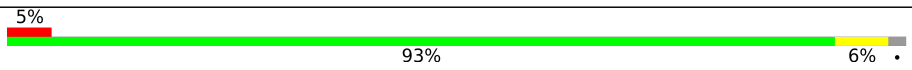
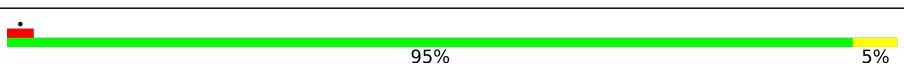
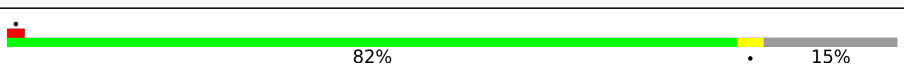
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	d	121	
30	e	106	
31	f	57	
32	g	154	
33	h	189	
34	i	128	
35	j	108	
36	k	98	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	109	

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 72093 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	101	821	560	119	137	5	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	155	1242	792	224	212	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	3459	2209	596	629	25	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	variant	UNP P17694

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1659	1059	278	312	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	432	Total	C	N	O	S	0	0
			3326	2096	594	616	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	689	Total	C	N	O	S	0	0
			5283	3309	921	1014	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	318	Total	C	N	O	S	0	0
			2509	1681	385	420	23		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	175	Total	C	N	O	S	0	0
			1345	906	191	236	12		

- 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
			745	486	112	131	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total 4802	C 3195	N 737	O 827	S 43	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total 3654	C 2436	N 570	O 609	S 39	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	347	Total 2733	C 1817	N 416	O 457	S 43	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	320	Total 2589	C 1662	N 429	O 488	S 10	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	255	LYS	ASN	variant	UNP P34942

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	311	Total 2475	C 1589	N 442	O 439	S 5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	125	Total 1016	C 641	N 181	O 191	S 3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	96	Total	C	N	O	S	0	0
			740	454	140	143	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	83	Total	C	N	O	S	0	0
			674	434	99	136	5		
20	U	86	Total	C	N	O	S	0	0
			693	447	102	139	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	115	Total	C	N	O	S	0	0
			928	600	157	168	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	115	Total	C	N	O	S	0	0
			977	625	181	167	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	171	Total	C	N	O	S	0	0
			1402	887	253	252	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	141	Total	C	N	O	S	0	0
			1030	657	176	191	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	1	ACE	-	acetylation	UNP Q8HXG6

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	142	Total	C	N	O	S	0	0
			1157	743	202	203	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	70	Total	C	N	O	S	0	0
			569	365	104	95	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	83	Total	C	N	O	S	0	0
			651	425	109	115	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	49	Total	C	N	O	0	0
			414	273	70	71		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	119	Total	C	N	O	S	0	0
			988	643	171	170	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	1	ACE	-	acetylation	UNP Q02827

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	98	Total	C	N	O	S	0	0
			825	521	157	141	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	57	Total	C	N	O	S	0	0
			492	322	86	82	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	100	Total	C	N	O	S	0	0
			837	539	139	155	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	138	Total	C	N	O	S	0	0
			1154	759	196	197	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	128	Total	C	N	O	S	0	0
			1097	722	191	183	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i	1	ACE	-	acetylation	UNP Q02367

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	67	Total	C	N	O	S	0	0
			580	381	95	103	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	81	Total	C	N	O	S	0	0
			653	427	110	114	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	156	Total	C	N	O	S	0	0
			1314	850	216	240	8		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
38	m	128	Total	C	N	O	0	0
			1067	684	188	195		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	171	Total	C	N	O	S	0	0
			1487	952	272	256	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	121	Total	C	N	O	S	0	0
			1040	649	200	182	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	173	Total	C	N	O	S	0	0
			1450	909	268	265	8		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	96	Total	C	N	O	S	0	0
			776	490	144	139	3		

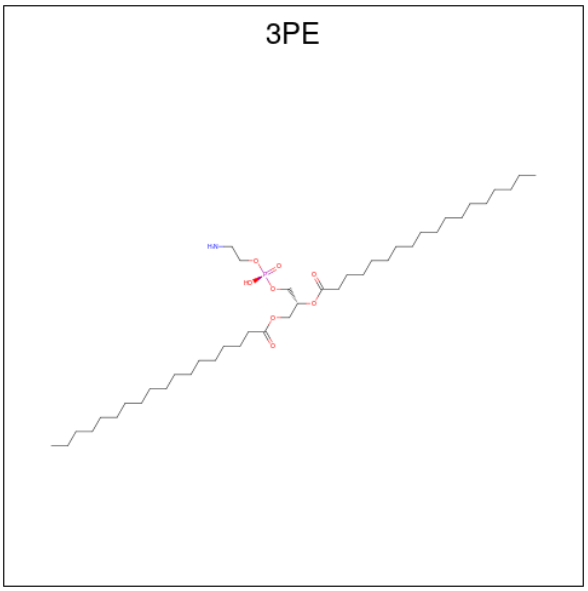
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	1	ACE	-	acetylation	UNP Q05752

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

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

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



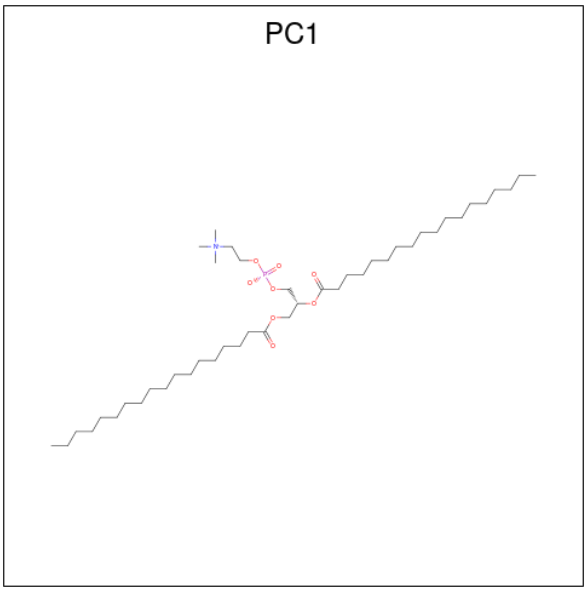
Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
45	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	D	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	H	1	Total	C	N	O	P	0
			38	28	1	8	1	
45	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	K	1	Total	C	N	O	P	0
			48	38	1	8	1	
45	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
45	L	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	M	1	Total	C	N	O	P	0
			45	35	1	8	1	
45	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	M	1	Total	C	N	O	P	0
			41	31	1	8	1	

Continued on next page...

Continued from previous page...

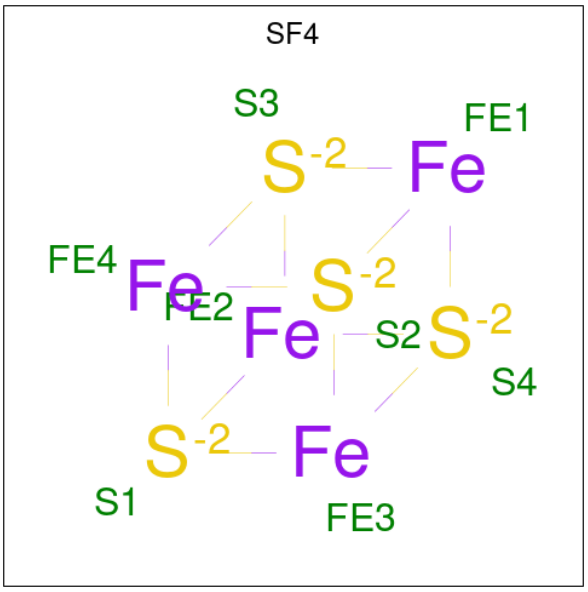
Mol	Chain	Residues	Atoms					AltConf
45	N	1	Total	C	N	O	P	0
			39	29	1	8	1	
45	X	1	Total	C	N	O	P	0
			38	28	1	8	1	
45	Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	Y	1	Total	C	N	O	P	0
			39	29	1	8	1	
45	Y	1	Total	C	N	O	P	0
			41	31	1	8	1	
45	Y	1	Total	C	N	O	P	0
			45	35	1	8	1	
45	Z	1	Total	C	N	O	P	0
			43	33	1	8	1	
45	Z	1	Total	C	N	O	P	0
			33	23	1	8	1	
45	d	1	Total	C	N	O	P	0
			49	39	1	8	1	
45	h	1	Total	C	N	O	P	0
			38	28	1	8	1	
45	h	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	m	1	Total	C	N	O	P	0
			41	31	1	8	1	

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



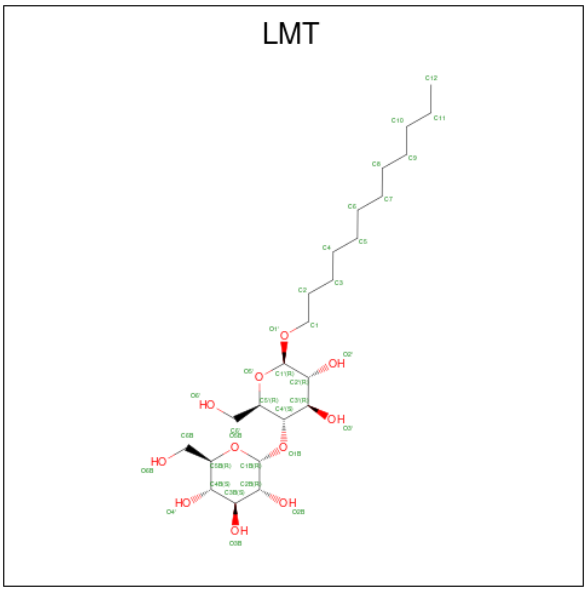
Mol	Chain	Residues	Atoms					AltConf
46	B	1	Total	C	N	O	P	0
			50	40	1	8	1	
46	B	1	Total	C	N	O	P	0
			47	37	1	8	1	
46	J	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	M	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	M	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	N	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	d	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



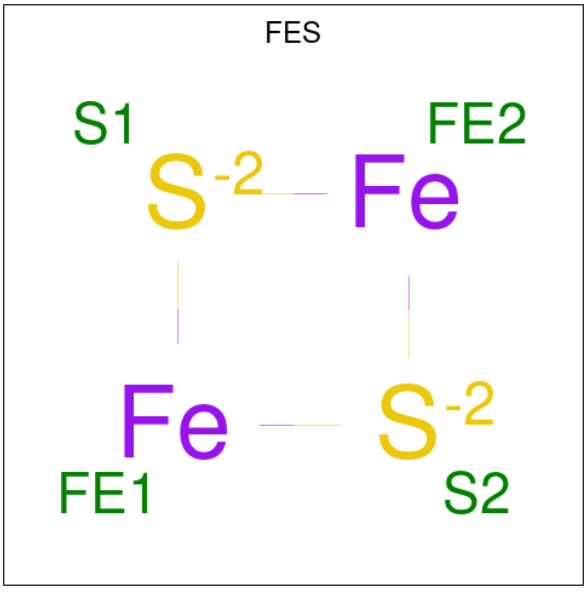
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 48 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



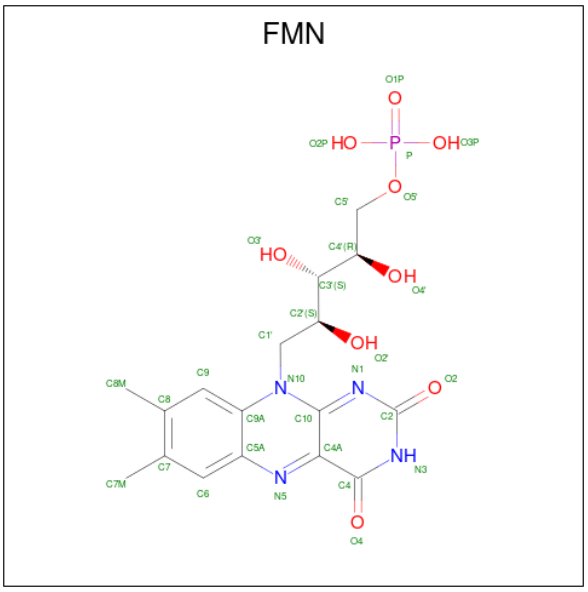
Mol	Chain	Residues	Atoms	AltConf
48	D	1	Total C O 35 24 11	0

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



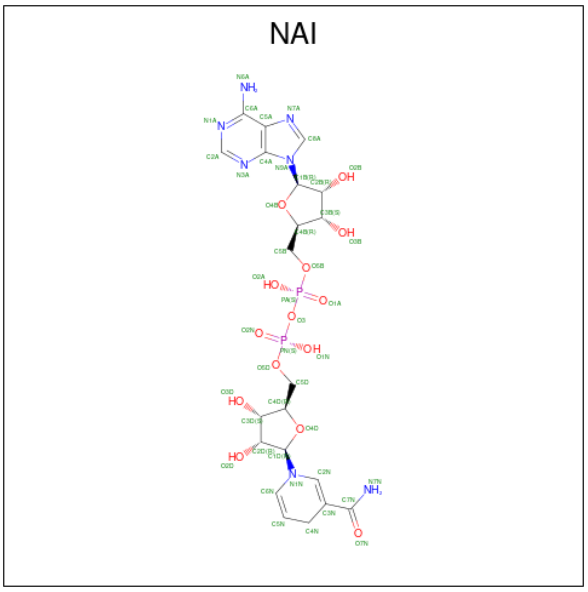
Mol	Chain	Residues	Atoms	AltConf
49	E	1	Total Fe S 4 2 2	0
49	G	1	Total Fe S 4 2 2	0

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



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

- Molecule 51 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).

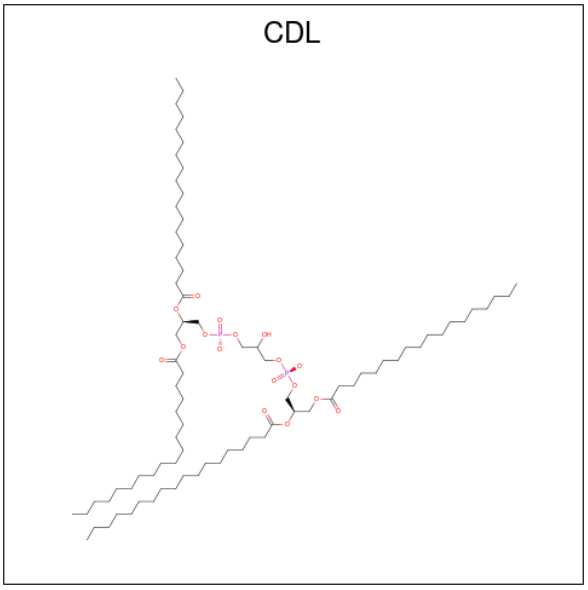


Mol	Chain	Residues	Atoms					AltConf
51	F	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 52 is POTASSIUM ION (CCD ID: K) (formula: K).

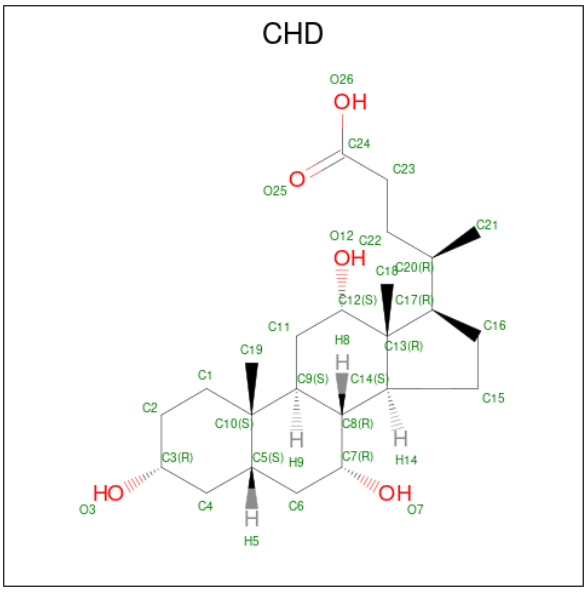
Mol	Chain	Residues	Atoms	AltConf
52	G	1	Total K 1 1	0

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



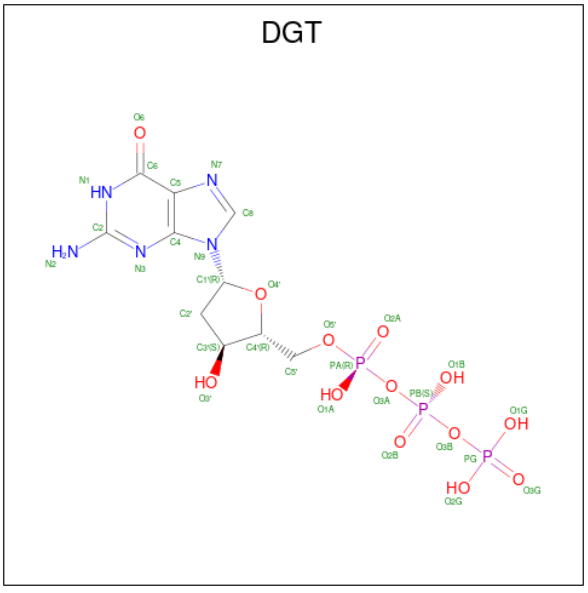
Mol	Chain	Residues	Atoms	AltConf
53	L	1	Total C O P 71 52 17 2	0
53	N	1	Total C O P 86 67 17 2	0
53	d	1	Total C O P 65 46 17 2	0
53	h	1	Total C O P 68 49 17 2	0
53	q	1	Total C O P 64 45 17 2	0

- Molecule 54 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
54	L	1	29	24	5	0

- Molecule 55 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

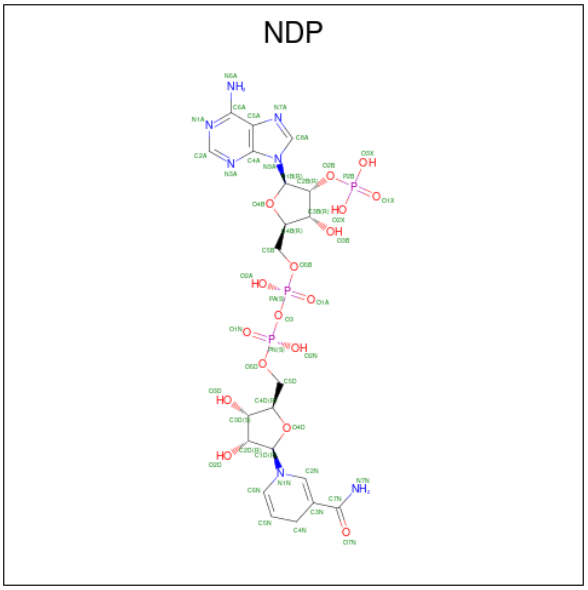


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
55	O	1	31	10	5	13	3	0

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	O	1	Total	Mg	0
			1	1	

- Molecule 57 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

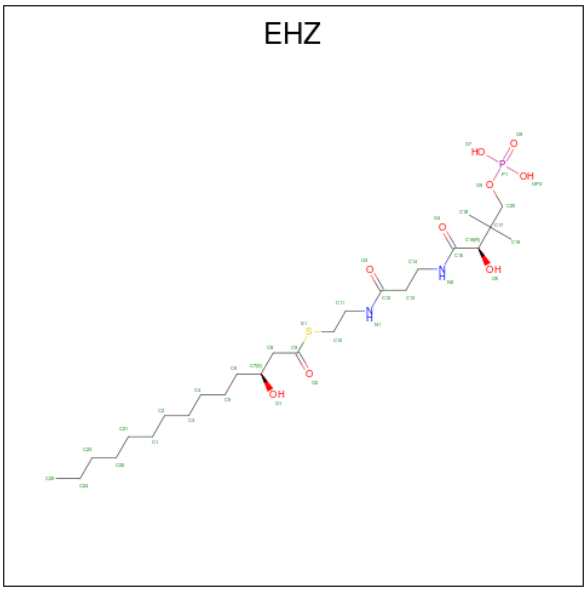


Mol	Chain	Residues	Atoms					AltConf
57	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

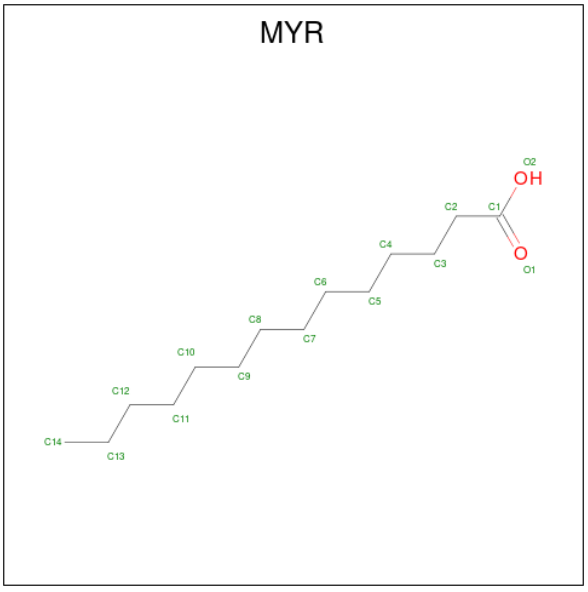
Mol	Chain	Residues	Atoms		AltConf
58	R	1	Total	Zn	0
			1	1	

- Molecule 59 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



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

- Molecule 60 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			AltConf
60	o	1	Total	C	O	0
			15	14	1	

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	AltConf
61	A	26	Total O 26 26	0
61	B	109	Total O 109 109	0
61	C	197	Total O 197 197	0
61	D	344	Total O 344 344	0
61	E	74	Total O 74 74	0
61	F	140	Total O 140 140	0
61	G	389	Total O 389 389	0
61	H	172	Total O 172 172	0
61	I	159	Total O 159 159	0
61	J	49	Total O 49 49	0
61	K	39	Total O 39 39	0
61	L	220	Total O 220 220	0
61	M	248	Total O 248 248	0
61	N	165	Total O 165 165	0
61	O	76	Total O 76 76	0
61	P	116	Total O 116 116	0
61	Q	153	Total O 153 153	0
61	R	68	Total O 68 68	0
61	S	8	Total O 8 8	0
61	U	23	Total O 23 23	0
61	V	43	Total O 43 43	0
61	W	56	Total O 56 56	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
61	X	61	Total O 61 61	0
61	Y	12	Total O 12 12	0
61	Z	75	Total O 75 75	0
61	a	48	Total O 48 48	0
61	b	28	Total O 28 28	0
61	c	3	Total O 3 3	0
61	d	49	Total O 49 49	0
61	e	63	Total O 63 63	0
61	f	9	Total O 9 9	0
61	g	40	Total O 40 40	0
61	h	68	Total O 68 68	0
61	i	17	Total O 17 17	0
61	j	5	Total O 5 5	0
61	k	6	Total O 6 6	0
61	l	57	Total O 57 57	0
61	m	52	Total O 52 52	0
61	n	80	Total O 80 80	0
61	o	14	Total O 14 14	0
61	p	73	Total O 73 73	0
61	q	86	Total O 86 86	0
61	r	55	Total O 55 55	0

Continued on next page...

Continued from previous page...

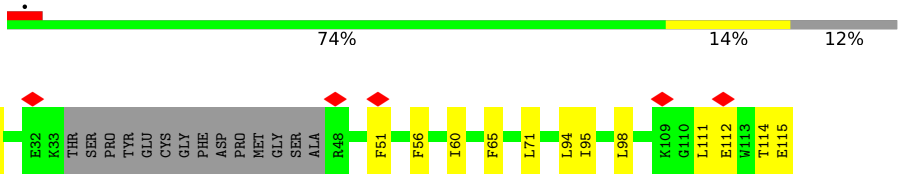
Mol	Chain	Residues	Atoms		AltConf
61	s	22	Total	O	0
			22	22	

3 Residue-property plots (i)

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

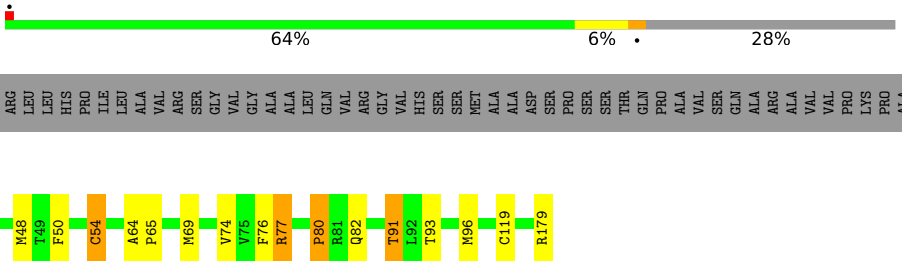
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:



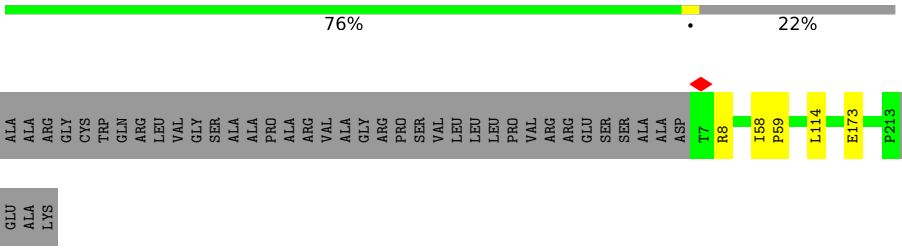
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B:



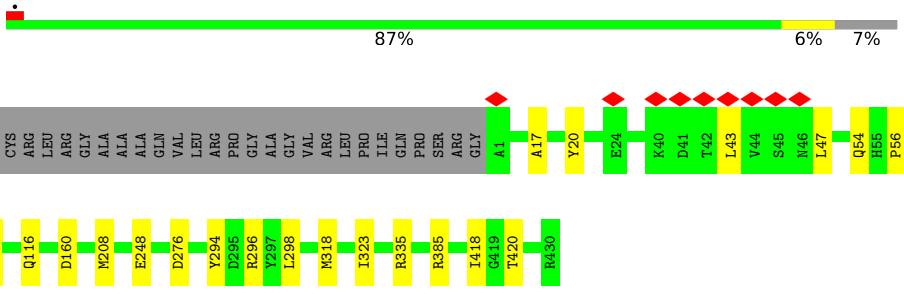
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:



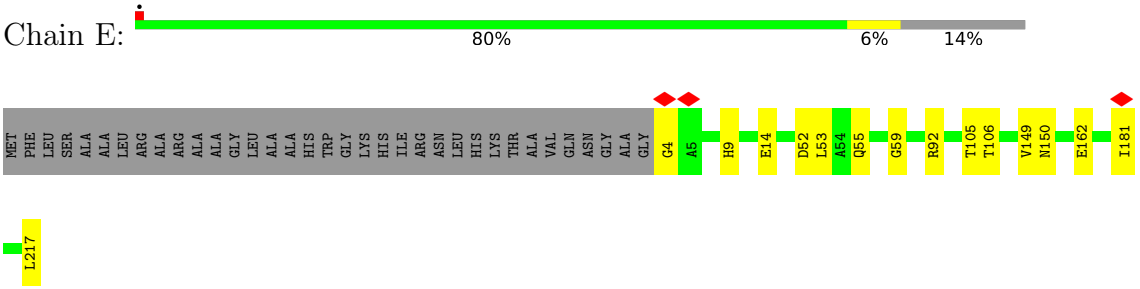
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D:



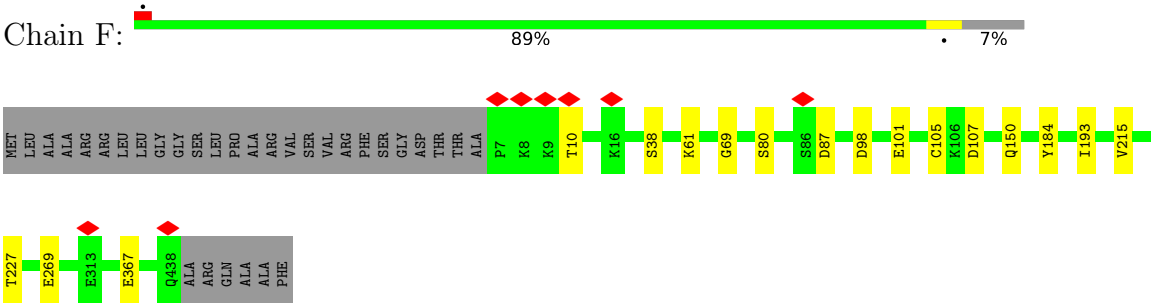
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:



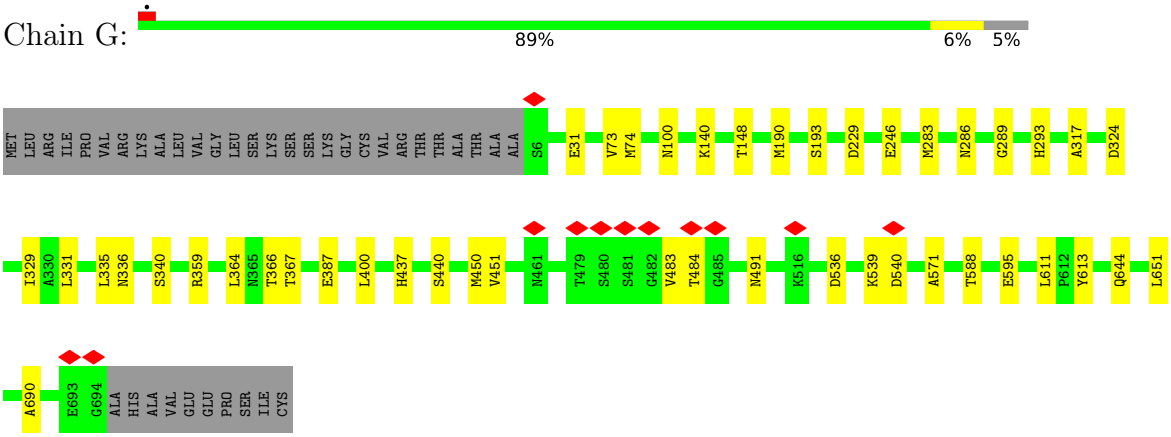
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:



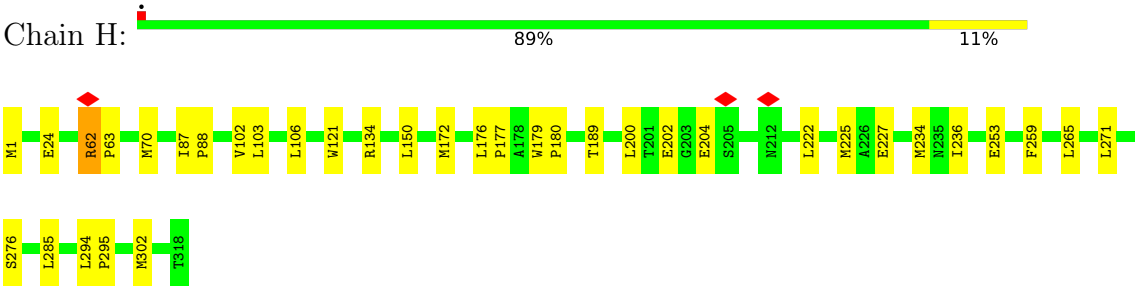
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:



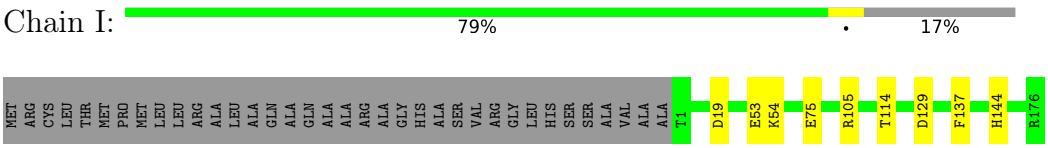
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:



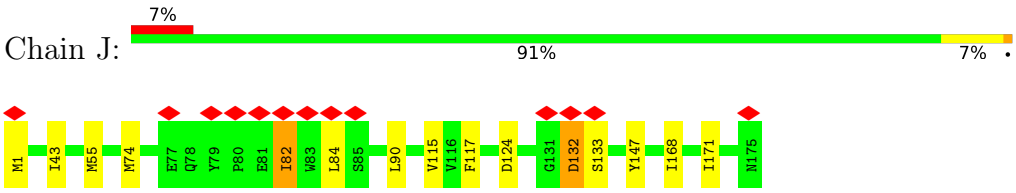
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:



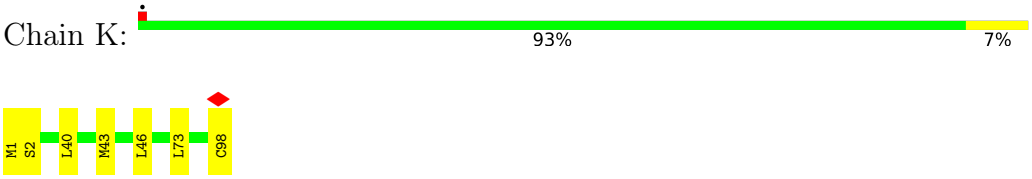
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:



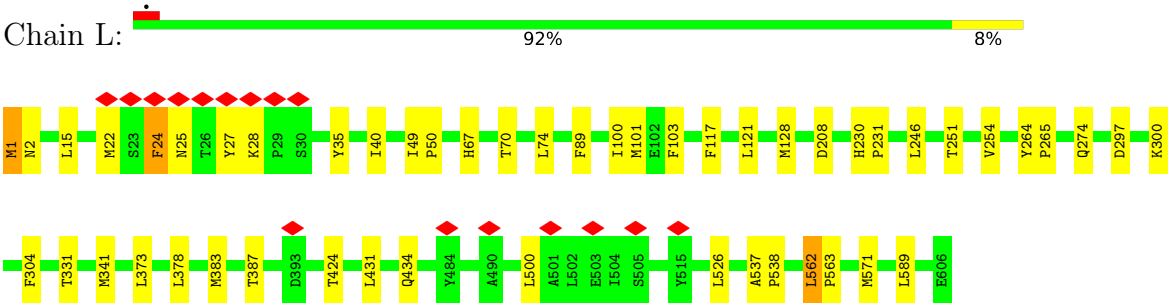
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:



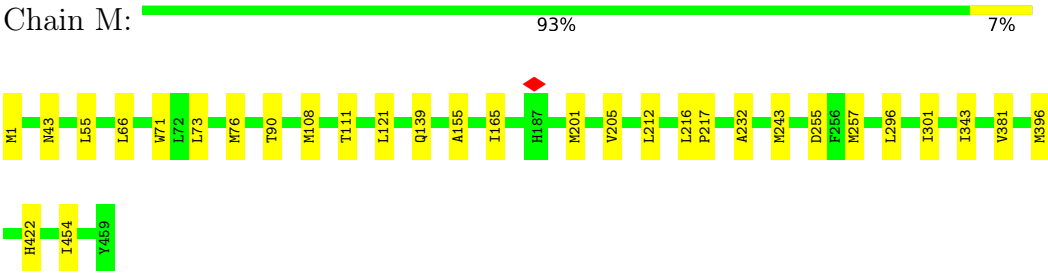
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:



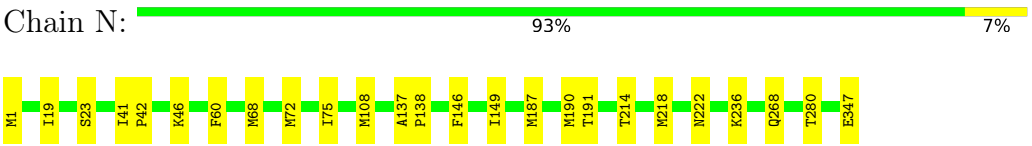
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:



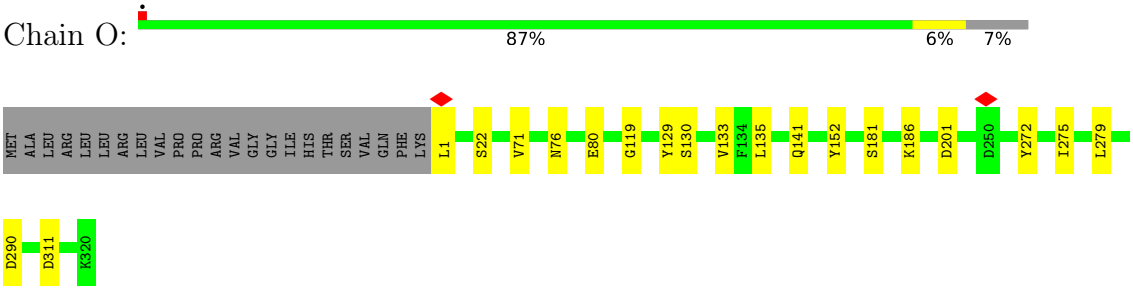
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:



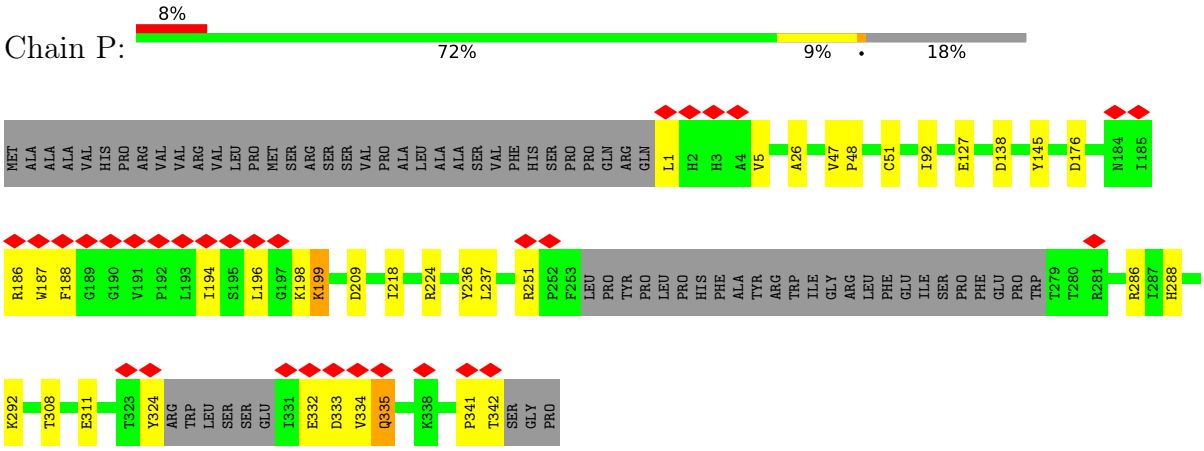
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:



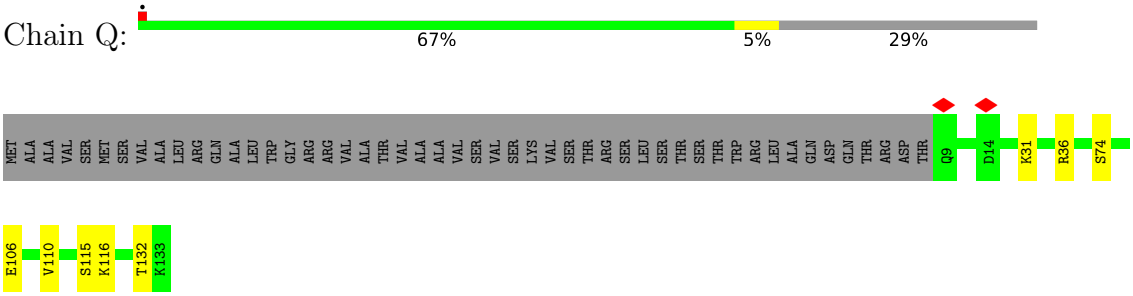
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:



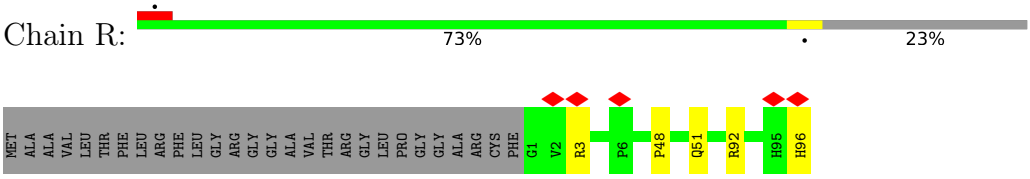
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:



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

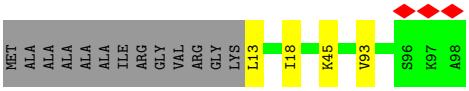
Chain R:



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

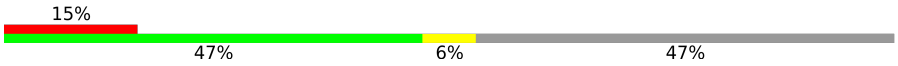
Chain S:

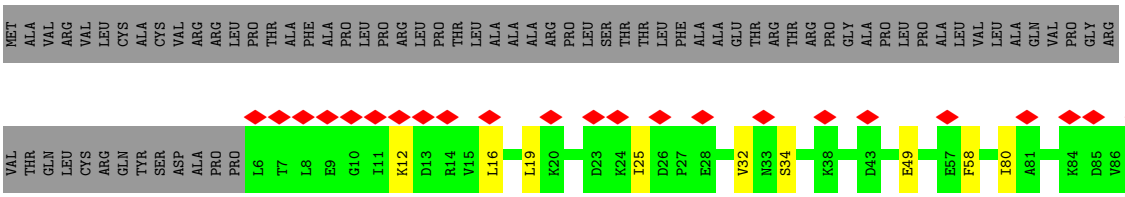




• Molecule 20: Acyl carrier protein, mitochondrial

Chain T:

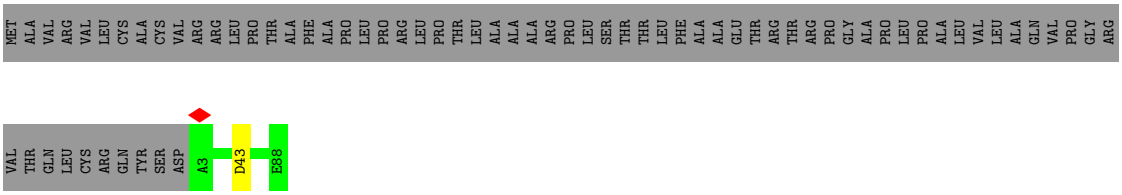




• Molecule 20: Acyl carrier protein, mitochondrial

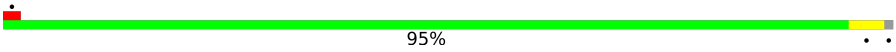
Chain U:

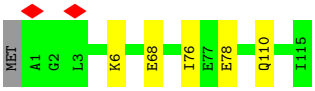




• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:

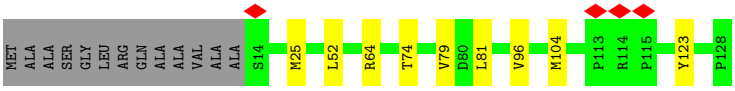




• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

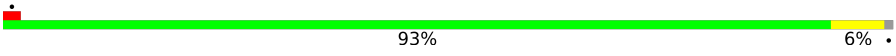
Chain W:

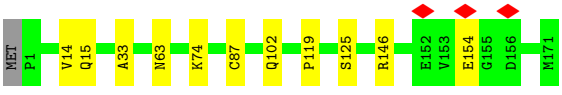




• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

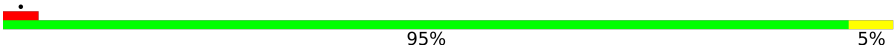
Chain X:

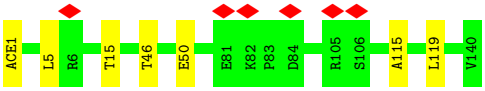




• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:

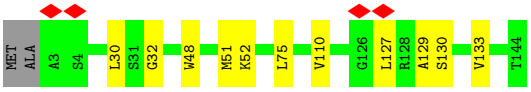




• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

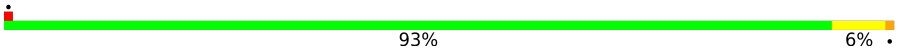
Chain Z:

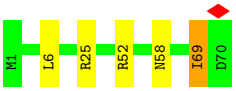




• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

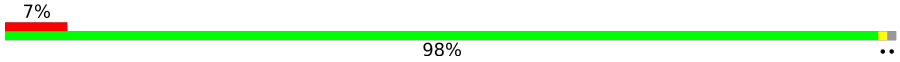
Chain a:

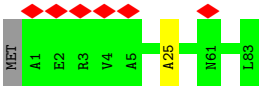




• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:

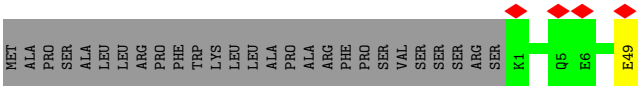




• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

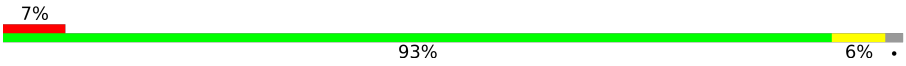
Chain c:

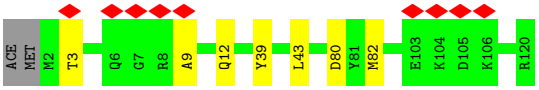




• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:

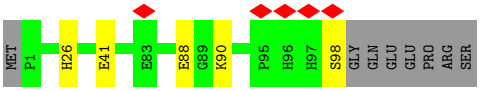




• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

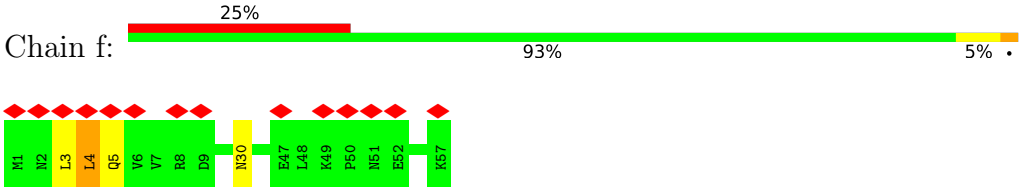
Chain e:





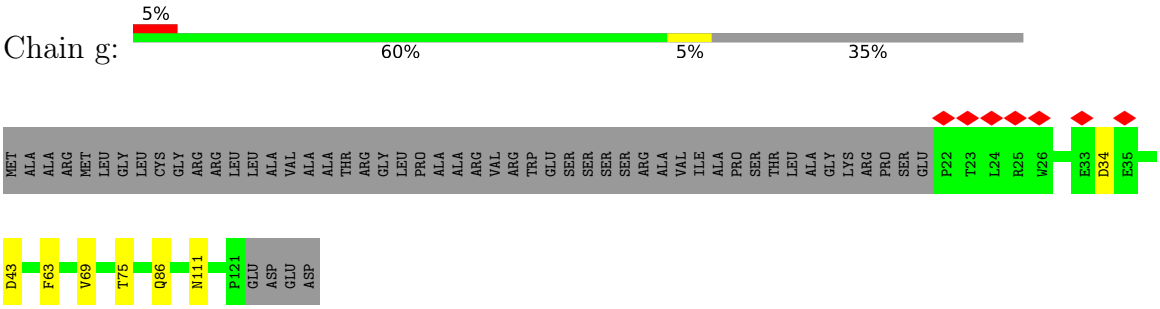
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:



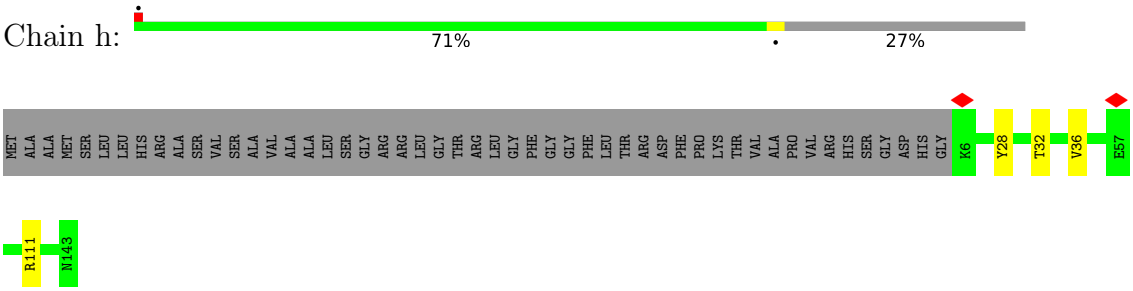
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:



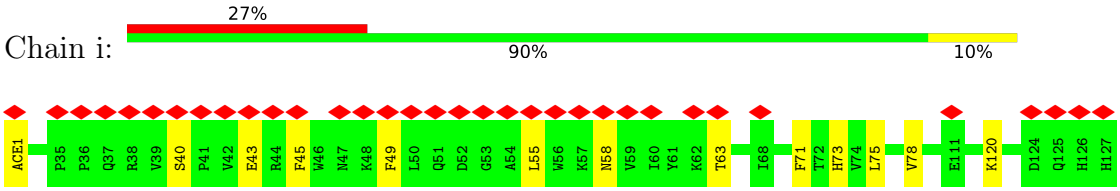
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:



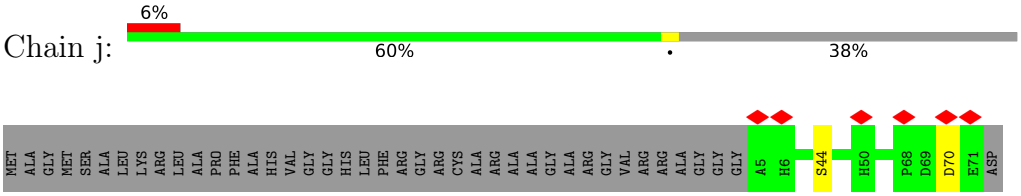
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



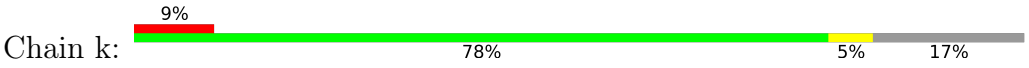
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

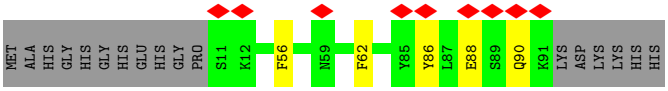
Chain j:



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

Chain k:

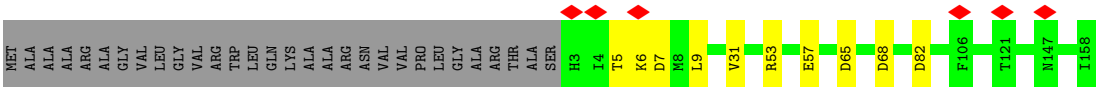




• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

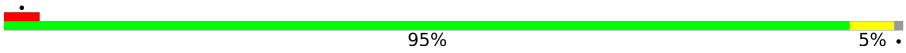
Chain l:

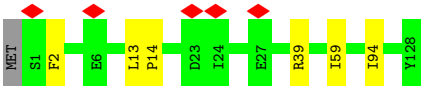




• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

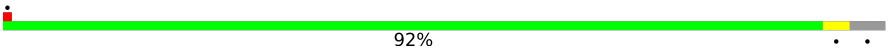
Chain m:

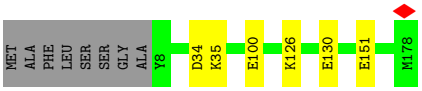




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n:

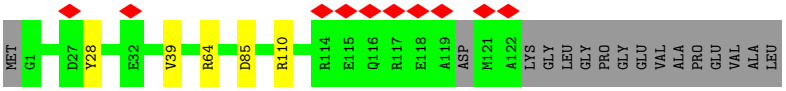




• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

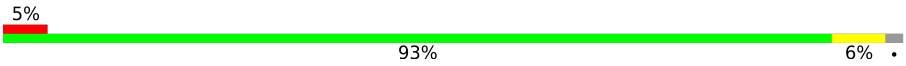
Chain o:

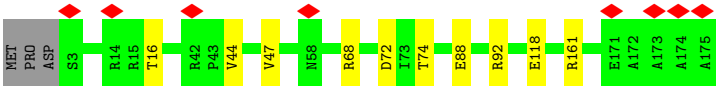




• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

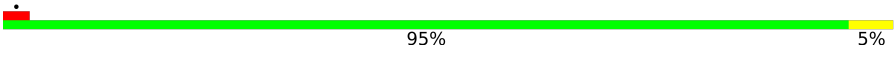
Chain p:

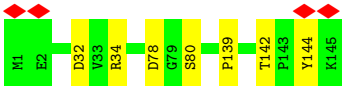




• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:

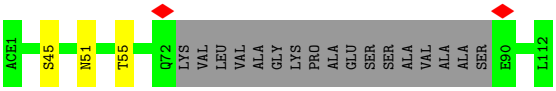




• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:



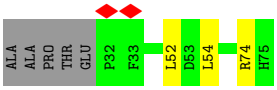


• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	521652	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.29	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	57.967	Depositor
Minimum map value	-27.452	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.777	Depositor
Recommended contour level	3	Depositor
Map size (Å)	482.40002, 482.40002, 482.40002	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.75375, 0.75375, 0.75375	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 3PE, NDP, PC1, K, NAI, MG, SF4, EHZ, ACE, LMT, CHD, FES, MYR, CDL, ARO, FME, 2MR, FMN, DGT

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	0.10	0/831	0.26	0/1136
2	B	0.14	0/1260	0.32	1/1703 (0.1%)
3	C	0.10	0/1772	0.27	0/2413
4	D	0.10	0/3537	0.25	0/4794
5	E	0.09	0/1699	0.26	0/2312
6	F	0.09	0/3401	0.25	0/4595
7	G	0.09	0/5371	0.27	0/7279
8	H	0.11	0/2571	0.28	0/3513
9	I	0.12	0/1445	0.28	0/1956
10	J	0.09	0/1370	0.24	0/1859
11	K	0.09	0/745	0.23	0/1008
12	L	0.09	0/4920	0.25	0/6694
13	M	0.09	0/3738	0.25	0/5097
14	N	0.10	0/2792	0.25	0/3800
15	O	0.09	0/2651	0.23	0/3587
16	P	0.11	0/2533	0.28	0/3427
17	Q	0.09	0/1039	0.25	0/1404
18	R	0.13	0/753	0.25	0/1014
19	S	0.09	0/702	0.25	0/945
20	T	0.08	0/684	0.23	0/921
20	U	0.08	0/705	0.22	0/952
21	V	0.09	0/948	0.21	0/1284
22	W	0.09	0/1001	0.23	0/1345
23	X	0.09	0/1439	0.24	0/1942
24	Y	0.18	1/1048 (0.1%)	0.20	0/1423
25	Z	0.09	0/1186	0.23	0/1599
26	a	0.12	0/584	0.22	0/786
27	b	0.12	0/672	0.23	0/923
28	c	0.12	0/427	0.20	0/579
29	d	0.08	0/1018	0.24	0/1375
30	e	0.09	0/846	0.24	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	f	0.11	0/505	0.27	0/681
32	g	0.09	0/864	0.26	0/1174
33	h	0.09	0/1188	0.23	0/1607
34	i	0.18	1/1134 (0.1%)	0.25	0/1544
35	j	0.08	0/607	0.22	0/833
36	k	0.08	0/672	0.21	0/906
37	l	0.09	0/1369	0.24	0/1873
38	m	0.10	0/1094	0.21	0/1480
39	n	0.08	0/1540	0.22	0/2085
40	o	0.08	0/1064	0.22	0/1423
41	p	0.08	0/1483	0.23	0/2000
42	q	0.10	0/1250	0.25	0/1698
43	r	0.21	0/795	0.28	0/1077
44	s	0.08	0/383	0.25	0/518
All	All	0.10	2/67636 (0.0%)	0.25	1/91695 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	i	1	ACE	C-N	5.14	1.45	1.34
24	Y	1	ACE	C-N	5.01	1.45	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	80	PRO	CB-CG-CD	-5.09	89.81	106.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	821	0	867	15	0
2	B	1242	0	1250	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1721	0	1675	4	0
4	D	3459	0	3404	21	0
5	E	1659	0	1664	13	0
6	F	3326	0	3282	13	0
7	G	5283	0	5304	32	0
8	H	2509	0	2621	30	0
9	I	1414	0	1370	7	0
10	J	1345	0	1352	17	0
11	K	745	0	785	10	0
12	L	4802	0	4960	33	0
13	M	3654	0	3852	26	0
14	N	2733	0	2912	22	0
15	O	2589	0	2566	11	0
16	P	2475	0	2508	22	0
17	Q	1016	0	1014	4	0
18	R	740	0	714	2	0
19	S	691	0	706	5	0
20	T	674	0	669	4	0
20	U	693	0	688	1	0
21	V	928	0	972	3	0
22	W	977	0	994	7	0
23	X	1402	0	1383	7	0
24	Y	1030	0	1039	3	0
25	Z	1157	0	1156	11	0
26	a	569	0	568	6	0
27	b	651	0	662	1	0
28	c	414	0	415	0	0
29	d	988	0	975	4	0
30	e	825	0	826	3	0
31	f	492	0	501	2	0
32	g	837	0	792	8	0
33	h	1154	0	1168	3	0
34	i	1097	0	1108	7	0
35	j	580	0	519	0	0
36	k	653	0	639	2	0
37	l	1314	0	1210	6	0
38	m	1067	0	1067	4	0
39	n	1487	0	1433	4	0
40	o	1040	0	1011	3	0
41	p	1450	0	1426	7	0
42	q	1209	0	1182	4	0
43	r	776	0	782	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	s	371	0	344	4	0
45	A	82	0	115	1	0
45	D	51	0	82	2	0
45	H	89	0	135	3	0
45	I	51	0	82	2	0
45	K	48	0	73	0	0
45	L	131	0	190	0	0
45	M	188	0	284	8	0
45	N	39	0	55	1	0
45	X	38	0	50	2	0
45	Y	227	0	342	6	0
45	Z	76	0	103	4	0
45	d	49	0	75	0	0
45	h	89	0	132	5	0
45	m	41	0	59	1	0
46	B	97	0	148	4	0
46	J	48	0	73	0	0
46	M	92	0	135	2	0
46	N	35	0	44	2	0
46	d	46	0	69	1	0
47	B	8	0	0	1	0
47	F	8	0	0	0	0
47	G	16	0	0	0	0
47	I	16	0	0	0	0
48	D	35	0	46	2	0
49	E	4	0	0	0	0
49	G	4	0	0	0	0
50	F	31	0	19	0	0
51	F	44	0	25	3	0
52	G	1	0	0	0	0
53	L	71	0	86	0	0
53	N	86	0	119	1	0
53	d	65	0	77	0	0
53	h	68	0	80	1	0
53	q	64	0	72	6	0
54	L	29	0	38	1	0
55	O	31	0	12	0	0
56	O	1	0	0	0	0
57	P	48	0	26	0	0
58	R	1	0	0	0	0
59	T	37	0	0	0	0
59	U	37	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	o	15	0	27	0	0
61	A	26	0	0	0	0
61	B	109	0	0	7	0
61	C	197	0	0	1	0
61	D	344	0	0	6	0
61	E	74	0	0	4	0
61	F	140	0	0	5	0
61	G	389	0	0	11	0
61	H	172	0	0	4	0
61	I	159	0	0	2	0
61	J	49	0	0	1	0
61	K	39	0	0	1	0
61	L	220	0	0	3	0
61	M	248	0	0	6	0
61	N	165	0	0	2	0
61	O	76	0	0	3	0
61	P	116	0	0	2	0
61	Q	153	0	0	3	0
61	R	68	0	0	1	0
61	S	8	0	0	0	0
61	U	23	0	0	0	0
61	V	43	0	0	2	0
61	W	56	0	0	1	0
61	X	61	0	0	1	0
61	Y	12	0	0	0	0
61	Z	75	0	0	2	0
61	a	48	0	0	0	0
61	b	28	0	0	0	0
61	c	3	0	0	0	0
61	d	49	0	0	2	0
61	e	63	0	0	1	0
61	f	9	0	0	0	0
61	g	40	0	0	3	0
61	h	68	0	0	1	0
61	i	17	0	0	0	0
61	j	5	0	0	0	0
61	k	6	0	0	0	0
61	l	57	0	0	1	0
61	m	52	0	0	0	0
61	n	80	0	0	1	0
61	o	14	0	0	0	0
61	p	73	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	q	86	0	0	1	0
61	r	55	0	0	0	0
61	s	22	0	0	2	0
All	All	72093	0	69208	381	0

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

The worst 5 of 381 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)
13:M:139:GLN:NE2	61:M:703:HOH:O	2.09	0.84
45:M:602:3PE:O14	61:M:701:HOH:O	1.97	0.82
29:d:80:ASP:OD2	61:d:302:HOH:O	1.97	0.82
24:Y:46:THR:OG1	24:Y:50:GLU:OE1	1.97	0.82
10:J:132:ASP:O	61:J:301:HOH:O	2.03	0.76

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	A	97/115 (84%)	94 (97%)	3 (3%)	0	100	100
2	B	152/216 (70%)	148 (97%)	4 (3%)	0	100	100
3	C	205/266 (77%)	201 (98%)	4 (2%)	0	100	100
4	D	427/463 (92%)	416 (97%)	11 (3%)	0	100	100
5	E	212/249 (85%)	208 (98%)	4 (2%)	0	100	100
6	F	430/464 (93%)	424 (99%)	6 (1%)	0	100	100
7	G	687/727 (94%)	674 (98%)	13 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	316/318 (99%)	311 (98%)	5 (2%)	0	100	100
9	I	174/212 (82%)	170 (98%)	4 (2%)	0	100	100
10	J	173/175 (99%)	166 (96%)	6 (4%)	1 (1%)	21	17
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	604/606 (100%)	584 (97%)	19 (3%)	1 (0%)	43	42
13	M	457/459 (100%)	455 (100%)	2 (0%)	0	100	100
14	N	345/347 (99%)	342 (99%)	3 (1%)	0	100	100
15	O	318/343 (93%)	315 (99%)	3 (1%)	0	100	100
16	P	305/380 (80%)	293 (96%)	10 (3%)	2 (1%)	18	14
17	Q	123/175 (70%)	123 (100%)	0	0	100	100
18	R	94/124 (76%)	93 (99%)	1 (1%)	0	100	100
19	S	84/99 (85%)	84 (100%)	0	0	100	100
20	T	81/156 (52%)	79 (98%)	2 (2%)	0	100	100
20	U	84/156 (54%)	84 (100%)	0	0	100	100
21	V	113/116 (97%)	113 (100%)	0	0	100	100
22	W	113/128 (88%)	111 (98%)	2 (2%)	0	100	100
23	X	169/172 (98%)	167 (99%)	2 (1%)	0	100	100
24	Y	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
25	Z	140/144 (97%)	139 (99%)	1 (1%)	0	100	100
26	a	68/70 (97%)	68 (100%)	0	0	100	100
27	b	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
28	c	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
29	d	117/121 (97%)	116 (99%)	1 (1%)	0	100	100
30	e	96/106 (91%)	96 (100%)	0	0	100	100
31	f	55/57 (96%)	53 (96%)	2 (4%)	0	100	100
32	g	98/154 (64%)	92 (94%)	6 (6%)	0	100	100
33	h	136/189 (72%)	135 (99%)	1 (1%)	0	100	100
34	i	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
35	j	65/108 (60%)	64 (98%)	1 (2%)	0	100	100
36	k	79/98 (81%)	79 (100%)	0	0	100	100
37	l	154/186 (83%)	148 (96%)	6 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
38	m	126/129 (98%)	125 (99%)	0	1 (1%)	16 11
39	n	169/179 (94%)	164 (97%)	5 (3%)	0	100 100
40	o	117/137 (85%)	115 (98%)	2 (2%)	0	100 100
41	p	171/176 (97%)	171 (100%)	0	0	100 100
42	q	143/145 (99%)	142 (99%)	1 (1%)	0	100 100
43	r	92/113 (81%)	90 (98%)	2 (2%)	0	100 100
44	s	42/109 (38%)	41 (98%)	1 (2%)	0	100 100
All	All	8120/9214 (88%)	7969 (98%)	146 (2%)	5 (0%)	49 46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	562	LEU
16	P	199	LYS
16	P	335	GLN
10	J	82	ILE
38	m	2	PHE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	89/100 (89%)	87 (98%)	2 (2%)	45 50
2	B	130/174 (75%)	126 (97%)	4 (3%)	35 37
3	C	188/228 (82%)	188 (100%)	0	100 100
4	D	370/392 (94%)	369 (100%)	1 (0%)	86 91
5	E	183/205 (89%)	182 (100%)	1 (0%)	81 87
6	F	346/368 (94%)	344 (99%)	2 (1%)	78 85
7	G	578/608 (95%)	573 (99%)	5 (1%)	70 78
8	H	274/274 (100%)	273 (100%)	1 (0%)	84 89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	151/175 (86%)	151 (100%)	0	100	100
10	J	141/141 (100%)	140 (99%)	1 (1%)	76	82
11	K	85/85 (100%)	85 (100%)	0	100	100
12	L	533/533 (100%)	531 (100%)	2 (0%)	84	89
13	M	412/412 (100%)	412 (100%)	0	100	100
14	N	315/315 (100%)	315 (100%)	0	100	100
15	O	283/303 (93%)	280 (99%)	3 (1%)	65	73
16	P	267/327 (82%)	262 (98%)	5 (2%)	50	56
17	Q	112/153 (73%)	109 (97%)	3 (3%)	39	42
18	R	79/97 (81%)	77 (98%)	2 (2%)	42	45
19	S	76/82 (93%)	76 (100%)	0	100	100
20	T	77/135 (57%)	75 (97%)	2 (3%)	40	44
20	U	79/135 (58%)	79 (100%)	0	100	100
21	V	101/102 (99%)	100 (99%)	1 (1%)	68	75
22	W	108/114 (95%)	108 (100%)	0	100	100
23	X	154/155 (99%)	153 (99%)	1 (1%)	78	85
24	Y	101/101 (100%)	100 (99%)	1 (1%)	68	75
25	Z	120/121 (99%)	119 (99%)	1 (1%)	73	80
26	a	59/59 (100%)	58 (98%)	1 (2%)	53	60
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	45/68 (66%)	44 (98%)	1 (2%)	45	50
29	d	105/106 (99%)	104 (99%)	1 (1%)	68	75
30	e	89/96 (93%)	88 (99%)	1 (1%)	65	73
31	f	54/54 (100%)	52 (96%)	2 (4%)	30	30
32	g	91/131 (70%)	91 (100%)	0	100	100
33	h	121/158 (77%)	121 (100%)	0	100	100
34	i	121/121 (100%)	117 (97%)	4 (3%)	33	34
35	j	61/84 (73%)	59 (97%)	2 (3%)	33	34
36	k	63/76 (83%)	60 (95%)	3 (5%)	23	21
37	l	140/159 (88%)	139 (99%)	1 (1%)	76	82
38	m	114/115 (99%)	114 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
39	n	156/161 (97%)	156 (100%)	0	100 100
40	o	109/120 (91%)	109 (100%)	0	100 100
41	p	154/157 (98%)	152 (99%)	2 (1%)	61 68
42	q	131/131 (100%)	129 (98%)	2 (2%)	57 64
43	r	85/96 (88%)	85 (100%)	0	100 100
44	s	43/92 (47%)	43 (100%)	0	100 100
All	All	7164/7891 (91%)	7106 (99%)	58 (1%)	70 80

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Q	74	SER
41	p	68	ARG
23	X	63	ASN
41	p	44	VAL
35	j	70	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
20	T	74	GLN
34	i	37	GLN
44	s	75	HIS
21	V	85	ASN
30	e	6	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)

9 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	2.45	2 (20%)	5,13,15	1.23	1 (20%)
12	FME	L	1	12	8,9,10	1.51	1 (12%)	7,9,11	1.69	3 (42%)
1	FME	A	1	1	8,9,10	1.51	1 (12%)	7,9,11	1.84	1 (14%)
14	FME	N	1	14	8,9,10	1.53	1 (12%)	7,9,11	1.51	1 (14%)
11	FME	K	1	11	8,9,10	1.51	1 (12%)	7,9,11	1.59	2 (28%)
13	FME	M	1	13	8,9,10	1.52	1 (12%)	7,9,11	1.65	1 (14%)
2	ARO	B	77	2	9,11,12	2.53	2 (22%)	7,13,15	0.49	0
8	FME	H	1	8	8,9,10	1.50	1 (12%)	7,9,11	1.64	2 (28%)
10	FME	J	1	10	8,9,10	1.51	1 (12%)	7,9,11	1.64	2 (28%)

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	-	0/10/13/15	-
12	FME	L	1	12	-	3/7/9/11	-
1	FME	A	1	1	-	4/7/9/11	-
14	FME	N	1	14	-	3/7/9/11	-
11	FME	K	1	11	-	1/7/9/11	-
13	FME	M	1	13	-	2/7/9/11	-
2	ARO	B	77	2	-	4/10/11/13	-
8	FME	H	1	8	-	3/7/9/11	-
10	FME	J	1	10	-	4/7/9/11	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	77	ARO	CZ-NE	6.70	1.46	1.33
4	D	85	2MR	CZ-NH2	5.44	1.45	1.33
4	D	85	2MR	CZ-NE	5.20	1.45	1.34
14	N	1	FME	CN-N	3.73	1.45	1.33
11	K	1	FME	CN-N	3.69	1.45	1.33

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	FME	CE-SD-CG	3.47	112.33	100.40
14	N	1	FME	CE-SD-CG	2.98	110.64	100.40
13	M	1	FME	CE-SD-CG	2.69	109.65	100.40
10	J	1	FME	CE-SD-CG	2.60	109.34	100.40
12	L	1	FME	CE-SD-CG	2.59	109.28	100.40

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
2	B	77	ARO	CA-CB-CG-OH
8	H	1	FME	O1-CN-N-CA
10	J	1	FME	O1-CN-N-CA
10	J	1	FME	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	L	1	FME	1	0
2	B	77	ARO	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 59 ligands modelled in this entry, 3 are monoatomic - leaving 56 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	$\#\|Z\|>2$
45	3PE	M	604	-	50,50,50	0.85	4 (8%)	53,55,55	1.06	3 (5%)
45	3PE	Y	203	-	38,38,50	0.98	4 (10%)	41,43,55	1.06	2 (4%)
46	PC1	B	201	-	49,49,53	1.34	6 (12%)	55,57,61	0.98	2 (3%)
45	3PE	Z	201	-	42,42,50	0.94	4 (9%)	45,47,55	1.15	2 (4%)
45	3PE	Y	201	-	50,50,50	0.86	3 (6%)	53,55,55	1.04	2 (3%)
55	DGT	O	401	56	29,33,33	3.21	14 (48%)	44,52,52	1.98	12 (27%)
53	CDL	h	201	-	67,67,99	1.10	7 (10%)	73,79,111	1.17	4 (5%)
45	3PE	m	201	-	40,40,50	0.96	4 (10%)	43,45,55	1.10	2 (4%)
45	3PE	M	602	-	50,50,50	0.86	4 (8%)	53,55,55	1.04	2 (3%)
46	PC1	M	605	-	45,45,53	1.40	6 (13%)	51,53,61	0.97	2 (3%)
54	CHD	L	704	-	32,32,32	3.21	10 (31%)	51,51,51	1.78	14 (27%)
53	CDL	N	401	-	85,85,99	0.98	7 (8%)	91,97,111	1.01	4 (4%)
45	3PE	Y	204	-	40,40,50	0.95	4 (10%)	43,45,55	1.09	2 (4%)
46	PC1	J	201	-	47,47,53	1.34	6 (12%)	53,55,61	1.01	2 (3%)
59	EHZ	U	101	20	29,36,37	1.68	5 (17%)	35,44,47	1.60	5 (14%)
45	3PE	X	201	-	37,37,50	0.99	4 (10%)	40,42,55	1.14	3 (7%)
53	CDL	d	203	-	64,64,99	1.09	7 (10%)	70,76,111	1.12	4 (5%)
51	NAI	F	503	-	45,48,48	3.72	19 (42%)	60,73,73	1.78	13 (21%)
45	3PE	D	502	-	50,50,50	0.87	4 (8%)	53,55,55	0.96	1 (1%)
45	3PE	L	701	-	41,41,50	0.95	4 (9%)	44,46,55	1.04	2 (4%)
46	PC1	d	202	-	45,45,53	1.39	6 (13%)	51,53,61	1.04	2 (3%)
46	PC1	B	203	-	46,46,53	1.35	6 (13%)	52,54,61	1.02	2 (3%)
45	3PE	d	201	-	48,48,50	0.89	4 (8%)	51,53,55	1.01	2 (3%)
45	3PE	H	401	-	37,37,50	1.00	3 (8%)	40,42,55	1.16	2 (5%)
47	SF4	G	801	7	0,12,12	-	-	-		
46	PC1	N	402	-	34,34,53	1.53	6 (17%)	40,42,61	1.08	2 (5%)
59	EHZ	T	101	20	29,36,37	1.71	5 (17%)	35,44,47	1.46	4 (11%)
45	3PE	L	705	-	43,43,50	0.94	4 (9%)	46,48,55	1.07	2 (4%)
45	3PE	K	101	-	47,47,50	0.88	4 (8%)	50,52,55	1.10	2 (4%)
45	3PE	Y	202	-	50,50,50	0.88	4 (8%)	53,55,55	0.98	2 (3%)
45	3PE	A	201	-	46,46,50	0.89	3 (6%)	49,51,55	1.02	2 (4%)
45	3PE	h	202	-	37,37,50	0.99	4 (10%)	40,42,55	1.05	2 (5%)
48	LMT	D	501	-	36,36,36	1.14	2 (5%)	47,47,47	0.99	2 (4%)
50	FMN	F	501	-	33,33,33	2.78	10 (30%)	48,50,50	1.76	13 (27%)
45	3PE	Y	205	-	44,44,50	0.91	3 (6%)	47,49,55	1.11	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	3PE	H	402	-	50,50,50	0.87	4 (8%)	53,55,55	0.95	2 (3%)
60	MYR	o	201	40	14,14,15	0.45	0	13,13,15	0.87	0
46	PC1	M	603	-	45,45,53	1.37	6 (13%)	51,53,61	0.96	2 (3%)
57	NDP	P	501	-	49,52,52	3.97	25 (51%)	66,80,80	2.00	14 (21%)
47	SF4	F	502	6	0,12,12	-	-	-		
49	FES	G	803	7	0,4,4	-	-	-		
47	SF4	B	202	2	0,12,12	-	-	-		
47	SF4	G	802	7	0,12,12	-	-	-		
53	CDL	q	201	-	63,63,99	1.11	6 (9%)	69,75,111	1.09	4 (5%)
53	CDL	L	702	-	70,70,99	1.06	7 (10%)	76,82,111	1.07	4 (5%)
45	3PE	L	703	-	44,44,50	0.92	4 (9%)	47,49,55	1.04	2 (4%)
47	SF4	I	202	9	0,12,12	-	-	-		
45	3PE	A	202	-	34,34,50	1.02	4 (11%)	37,39,55	1.12	2 (5%)
45	3PE	N	403	-	38,38,50	0.99	4 (10%)	41,43,55	1.10	2 (4%)
45	3PE	I	203	-	50,50,50	0.86	3 (6%)	53,55,55	0.99	2 (3%)
45	3PE	h	203	-	50,50,50	0.87	4 (8%)	53,55,55	0.95	2 (3%)
45	3PE	M	601	-	44,44,50	0.91	3 (6%)	47,49,55	1.08	2 (4%)
47	SF4	I	201	9	0,12,12	-	-	-		
49	FES	E	301	5	0,4,4	-	-	-		
45	3PE	Z	202	-	32,32,50	1.04	4 (12%)	35,37,55	1.12	2 (5%)
45	3PE	M	606	-	40,40,50	0.95	3 (7%)	43,45,55	1.07	2 (4%)

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
45	3PE	M	604	-	-	18/54/54/54	-
45	3PE	Y	203	-	-	17/42/42/54	-
46	PC1	B	201	-	-	19/53/53/57	-
45	3PE	Z	201	-	-	21/46/46/54	-
45	3PE	Y	201	-	-	28/54/54/54	-
55	DGT	O	401	56	-	4/22/34/34	0/3/3/3
53	CDL	h	201	-	-	40/78/78/110	-
45	3PE	m	201	-	-	25/44/44/54	-
45	3PE	M	602	-	-	23/54/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PC1	M	605	-	-	21/49/49/57	-
54	CHD	L	704	-	-	8/9/74/74	0/4/4/4
53	CDL	N	401	-	-	34/96/96/110	-
45	3PE	Y	204	-	-	18/44/44/54	-
46	PC1	J	201	-	-	15/51/51/57	-
59	EHZ	U	101	20	-	14/42/44/45	-
45	3PE	X	201	-	-	17/41/41/54	-
53	CDL	d	203	-	-	39/75/75/110	-
51	NAI	F	503	-	-	3/29/72/72	0/5/5/5
45	3PE	D	502	-	-	24/54/54/54	-
45	3PE	L	701	-	-	19/45/45/54	-
46	PC1	d	202	-	-	24/49/49/57	-
46	PC1	B	203	-	-	22/50/50/57	-
45	3PE	d	201	-	-	24/52/52/54	-
45	3PE	H	401	-	-	18/41/41/54	-
47	SF4	G	801	7	-	-	0/6/5/5
46	PC1	N	402	-	-	14/38/38/57	-
59	EHZ	T	101	20	-	6/42/44/45	-
45	3PE	L	705	-	-	26/47/47/54	-
45	3PE	K	101	-	-	11/51/51/54	-
45	3PE	Y	202	-	-	23/54/54/54	-
45	3PE	A	201	-	-	19/50/50/54	-
45	3PE	h	202	-	-	14/41/41/54	-
48	LMT	D	501	-	-	2/21/61/61	0/2/2/2
50	FMN	F	501	-	-	1/18/18/18	0/3/3/3
45	3PE	Y	205	-	-	21/48/48/54	-
45	3PE	H	402	-	-	20/54/54/54	-
60	MYR	o	201	40	-	3/11/12/13	-
46	PC1	M	603	-	-	14/49/49/57	-
57	NDP	P	501	-	-	6/34/77/77	0/5/5/5
47	SF4	F	502	6	-	-	0/6/5/5
49	FES	G	803	7	-	-	0/1/1/1
47	SF4	B	202	2	-	-	0/6/5/5
47	SF4	G	802	7	-	-	0/6/5/5
53	CDL	q	201	-	-	39/74/74/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	CDL	L	702	-	-	39/81/81/110	-
45	3PE	L	703	-	-	24/48/48/54	-
47	SF4	I	202	9	-	-	0/6/5/5
45	3PE	A	202	-	-	12/38/38/54	-
45	3PE	N	403	-	-	21/42/42/54	-
45	3PE	I	203	-	-	26/54/54/54	-
45	3PE	h	203	-	-	26/54/54/54	-
45	3PE	M	601	-	-	26/48/48/54	-
47	SF4	I	201	9	-	-	0/6/5/5
49	FES	E	301	5	-	-	0/1/1/1
45	3PE	Z	202	-	-	16/36/36/54	-
45	3PE	M	606	-	-	23/44/44/54	-

The worst 5 of 267 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	P	501	NDP	C6N-C5N	12.19	1.55	1.33
51	F	503	NAI	C6N-C5N	11.11	1.53	1.33
54	L	704	CHD	C11-C12	8.81	1.68	1.53
51	F	503	NAI	O4B-C1B	8.52	1.62	1.42
57	P	501	NDP	C2B-C1B	-8.50	1.31	1.53

The worst 5 of 166 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	U	101	EHZ	C8-C9-S1	5.71	120.69	113.63
57	P	501	NDP	N6A-C6A-N1A	-5.61	106.06	118.35
57	P	501	NDP	C5A-C4A-N3A	-5.51	119.56	126.75
51	F	503	NAI	N3A-C2A-N1A	-5.42	120.12	128.60
57	P	501	NDP	N3A-C2A-N1A	-5.40	120.16	128.60

There are no chirality outliers.

5 of 927 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	202	3PE	C22-C21-O21-C2
45	D	502	3PE	C1-O11-P-O12
45	D	502	3PE	C1-O11-P-O13
45	D	502	3PE	C1-O11-P-O14
45	H	401	3PE	C1-O11-P-O12

There are no ring outliers.

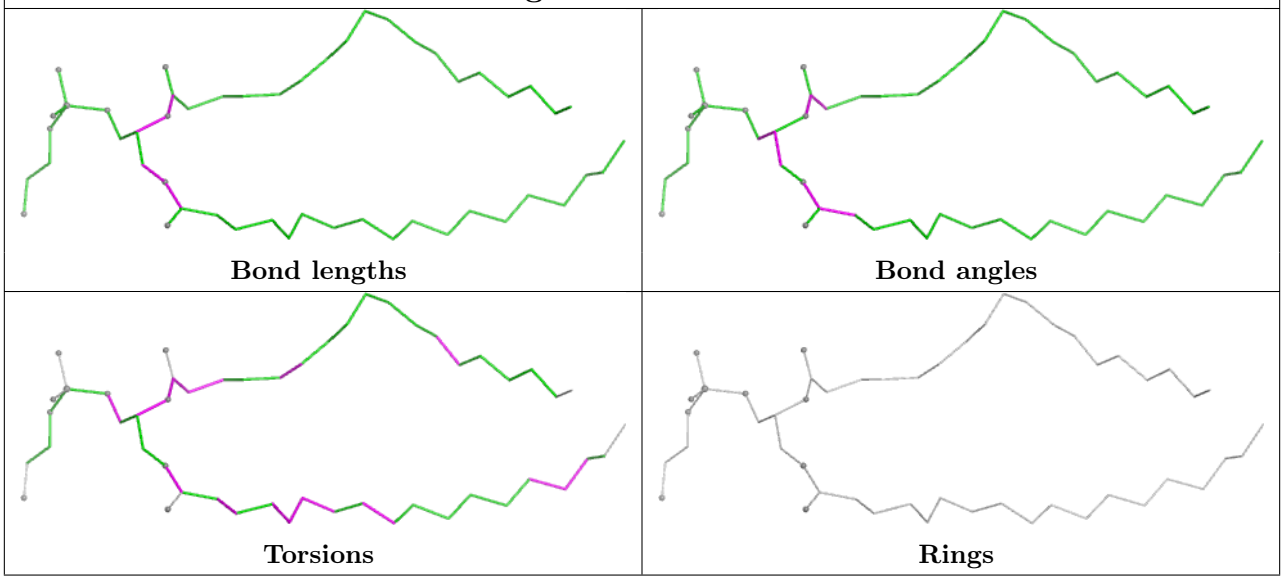
32 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	M	604	3PE	1	0
45	Y	203	3PE	2	0
46	B	201	PC1	2	0
45	Z	201	3PE	1	0
45	Y	201	3PE	1	0
53	h	201	CDL	1	0
45	m	201	3PE	1	0
45	M	602	3PE	3	0
46	M	605	PC1	2	0
54	L	704	CHD	1	0
53	N	401	CDL	1	0
45	Y	204	3PE	2	0
59	U	101	EHZ	1	0
45	X	201	3PE	2	0
51	F	503	NAI	3	0
45	D	502	3PE	2	0
46	d	202	PC1	1	0
46	B	203	PC1	2	0
45	H	401	3PE	3	0
46	N	402	PC1	2	0
45	A	201	3PE	1	0
45	h	202	3PE	4	0
48	D	501	LMT	2	0
45	Y	205	3PE	1	0
47	B	202	SF4	1	0
53	q	201	CDL	6	0
45	N	403	3PE	1	0
45	I	203	3PE	2	0
45	h	203	3PE	1	0
45	M	601	3PE	3	0
45	Z	202	3PE	3	0
45	M	606	3PE	2	0

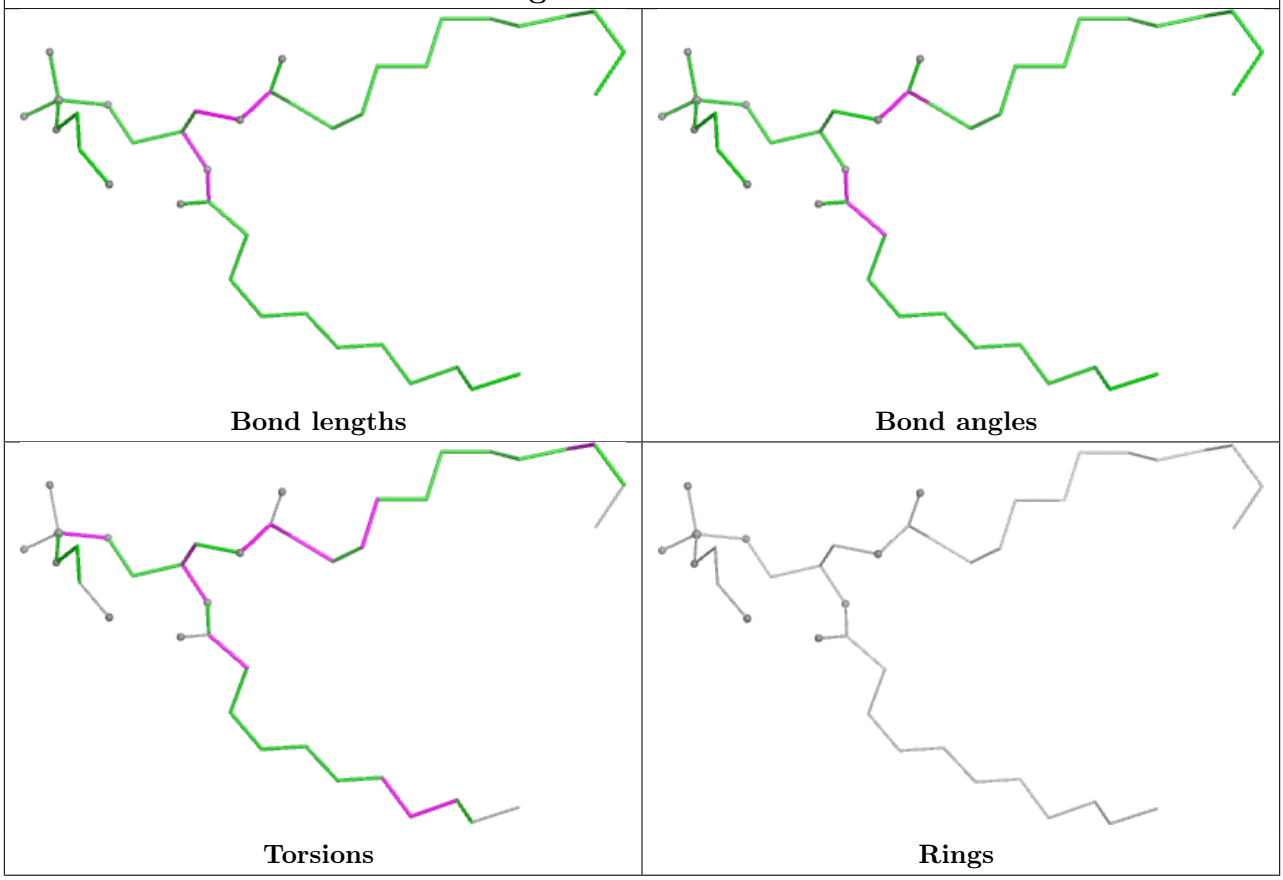
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

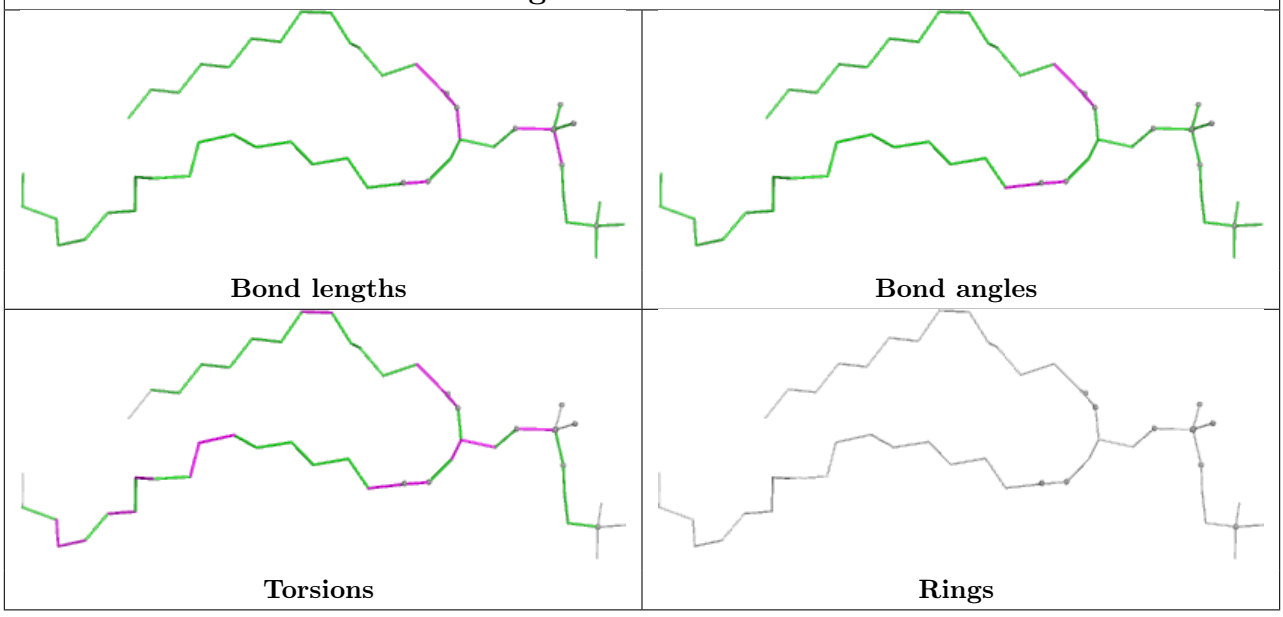
Ligand 3PE M 604



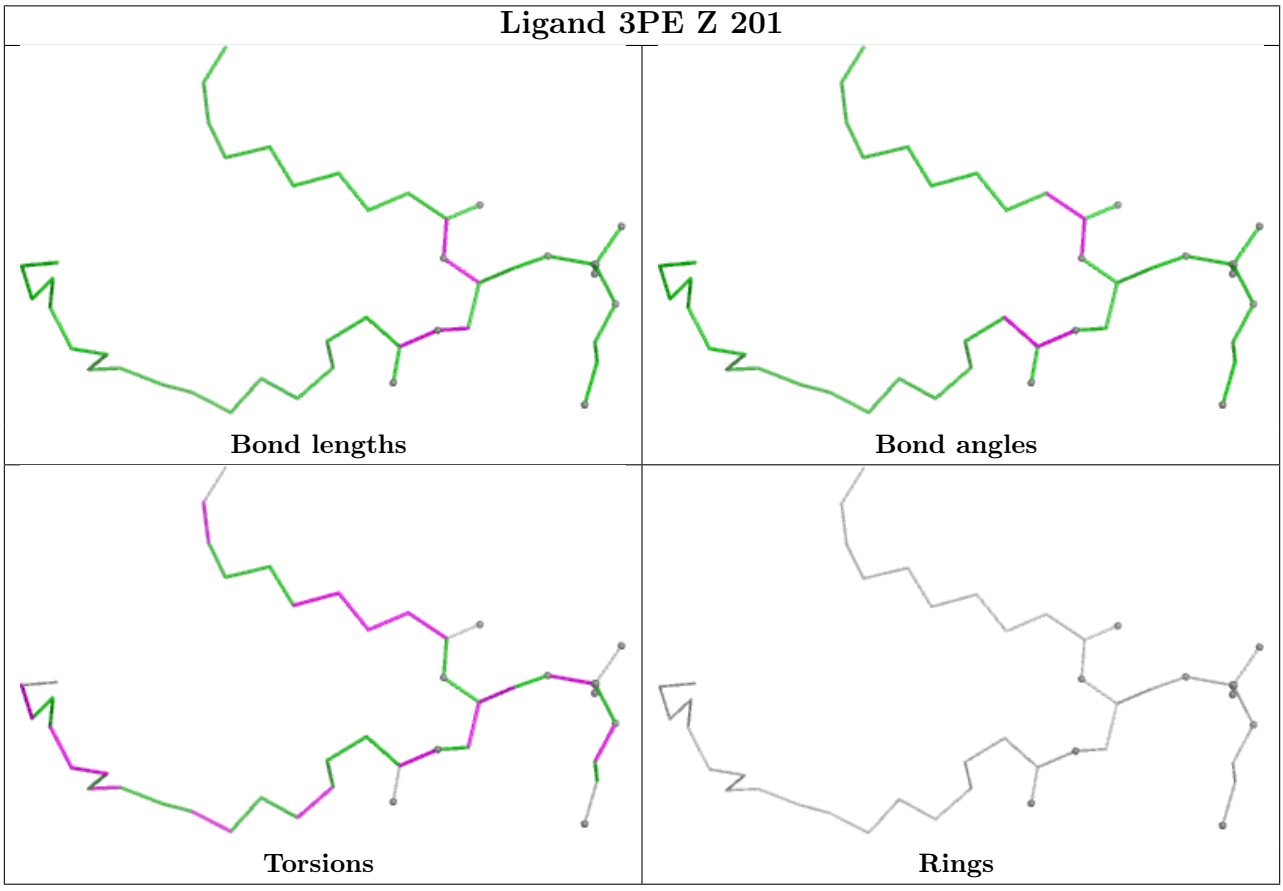
Ligand 3PE Y 203



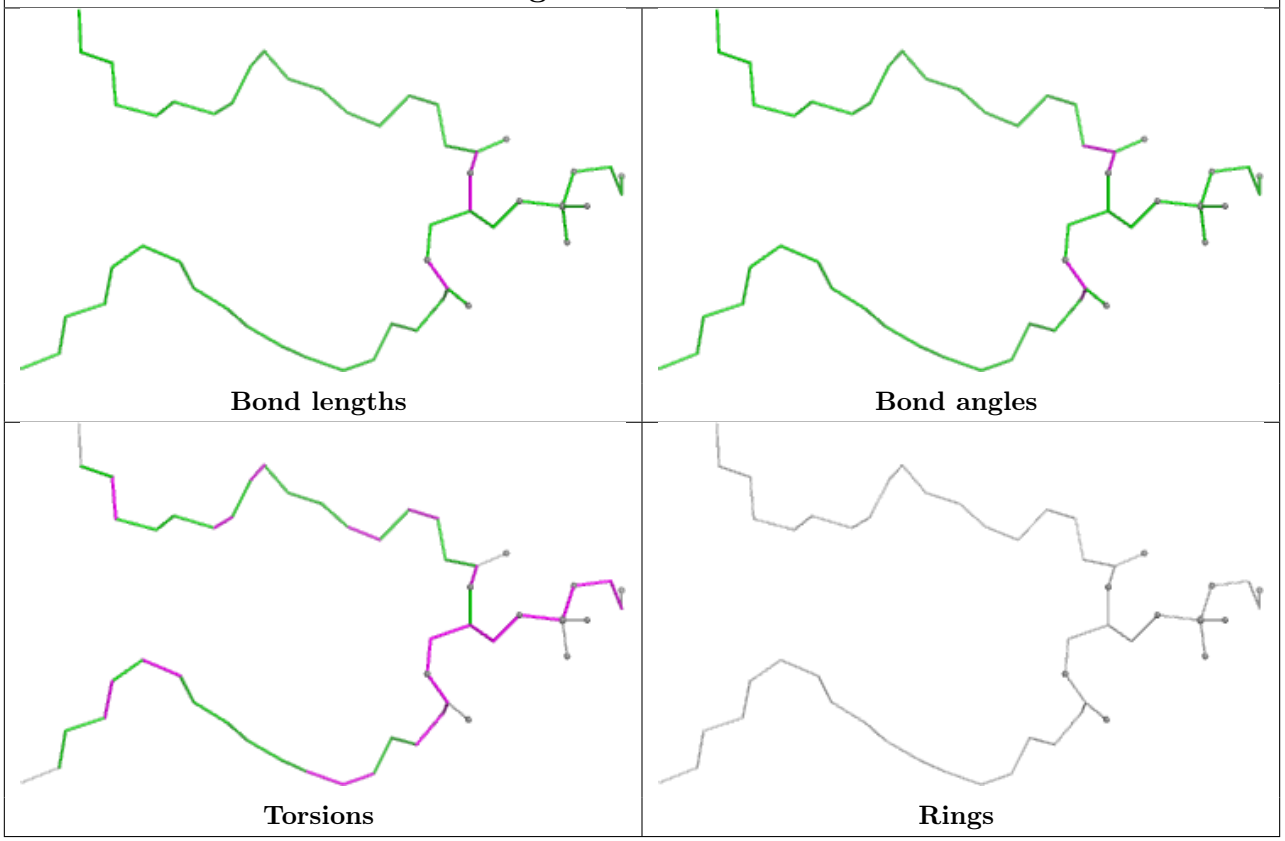
Ligand PC1 B 201



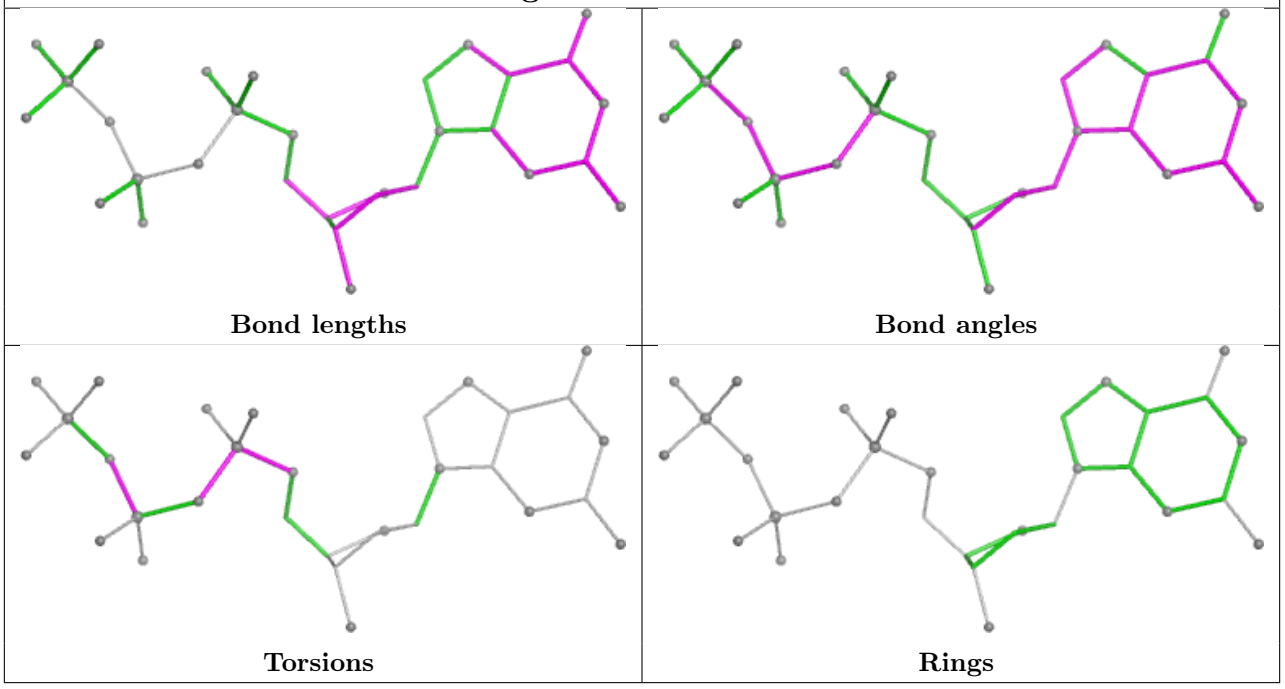
Ligand 3PE Z 201



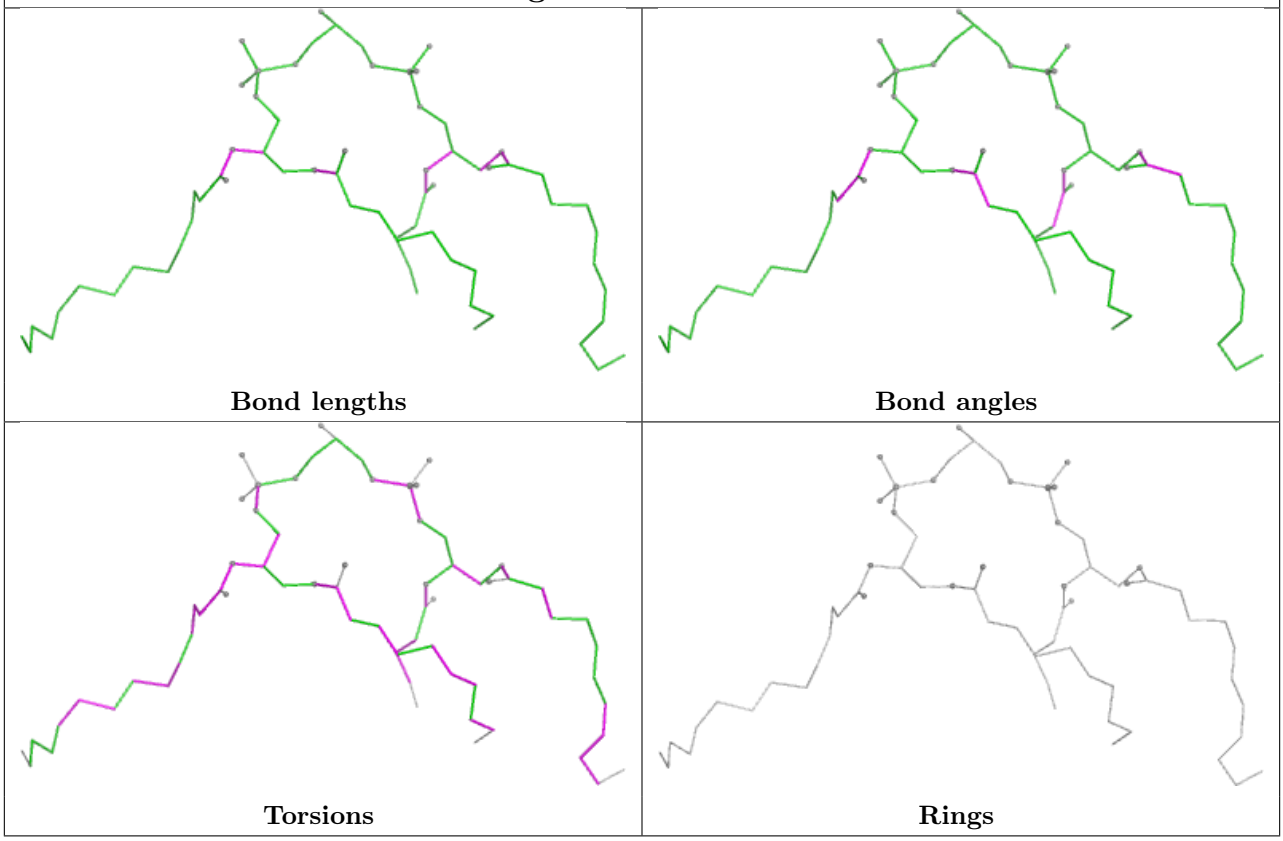
Ligand 3PE Y 201



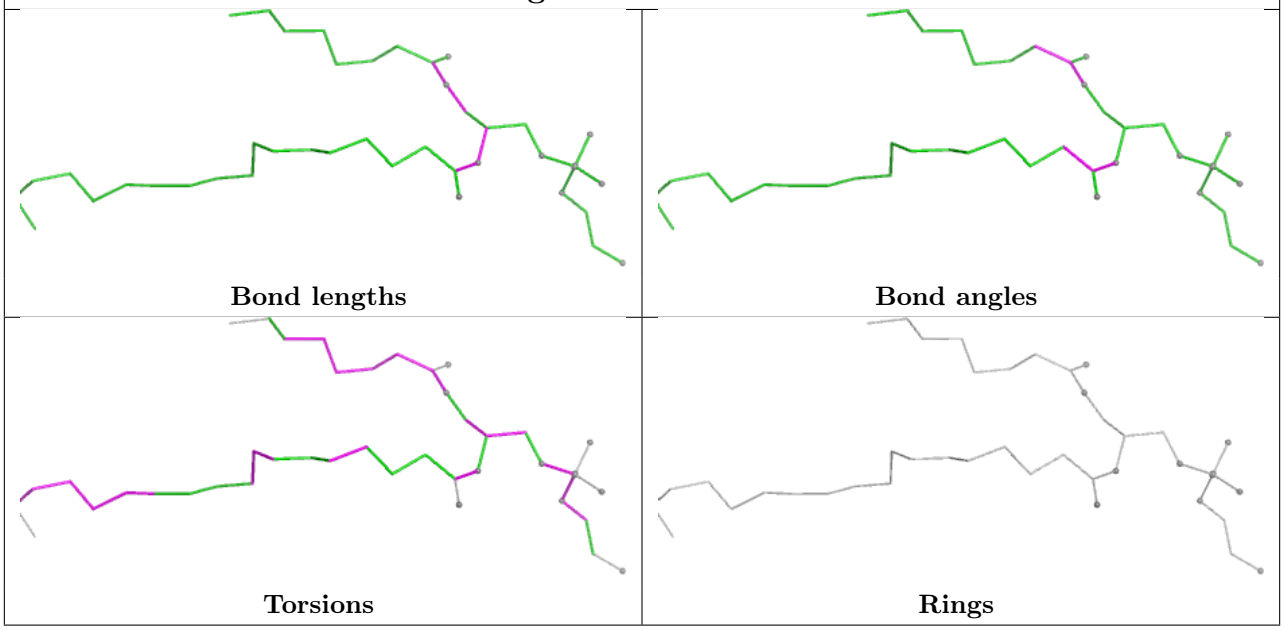
Ligand DGT O 401



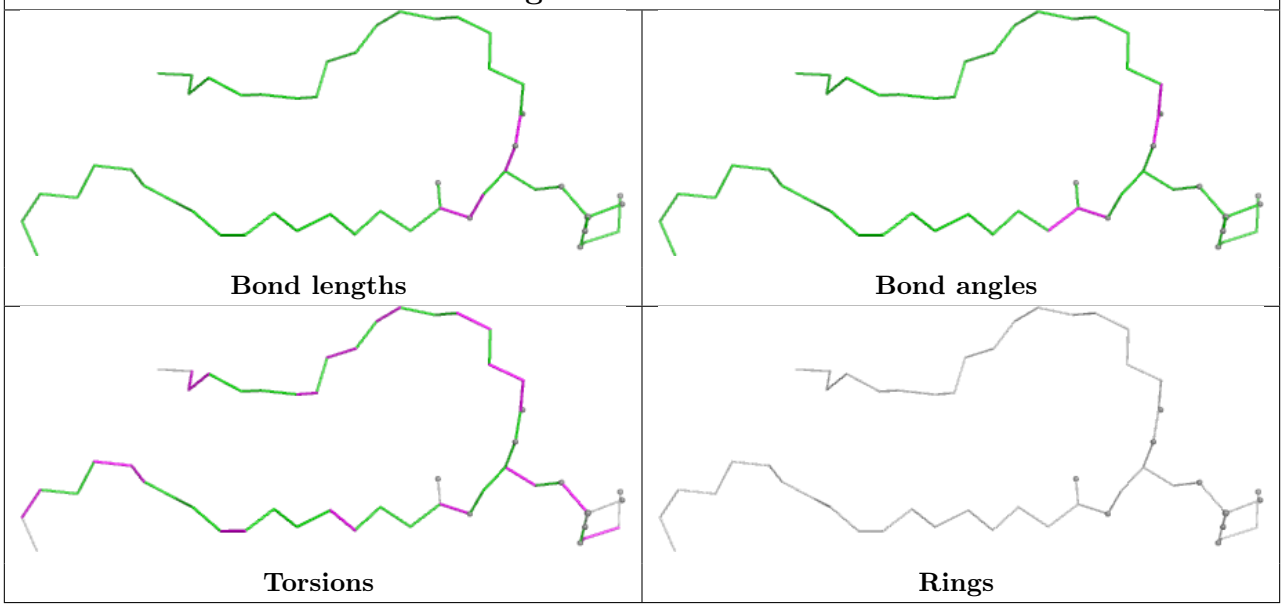
Ligand CDL h 201



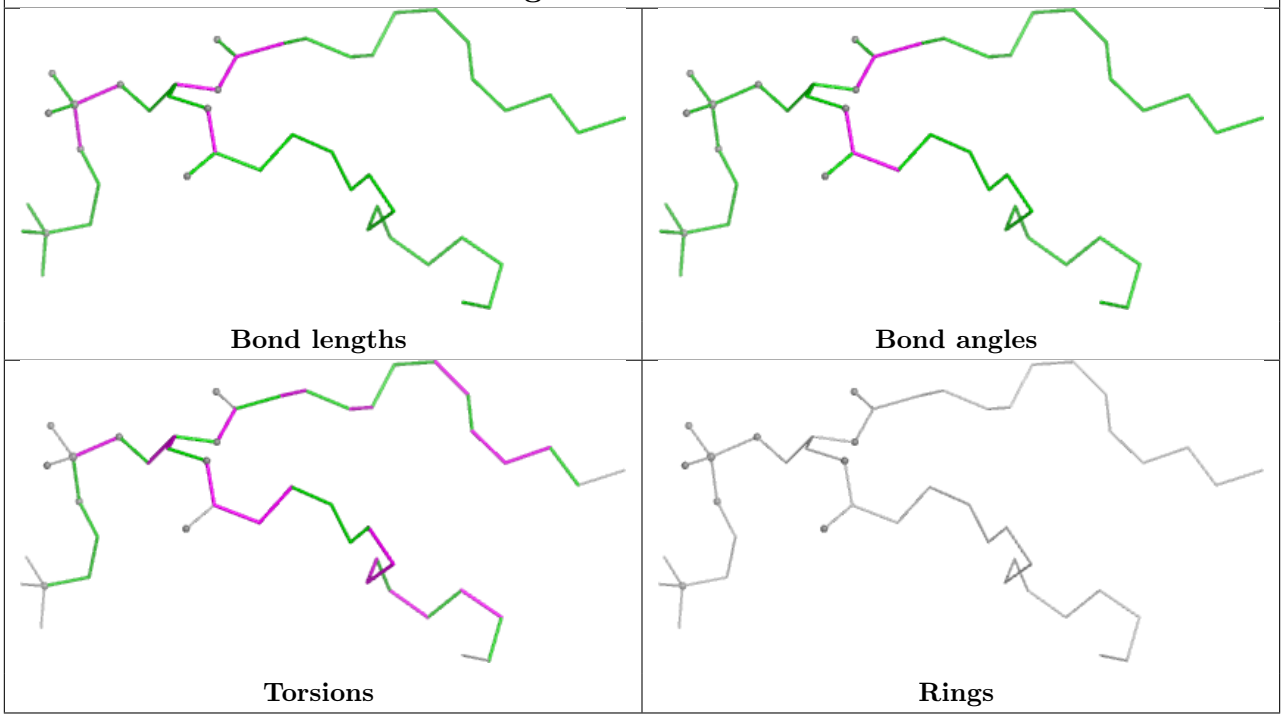
Ligand 3PE m 201



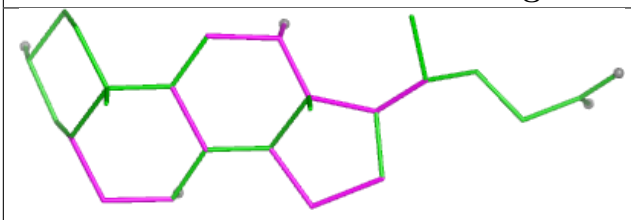
Ligand 3PE M 602



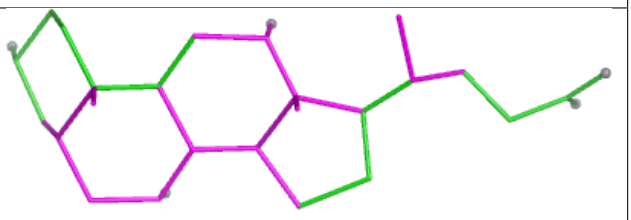
Ligand PC1 M 605



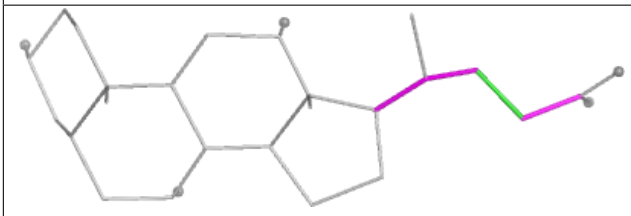
Ligand CHD L 704



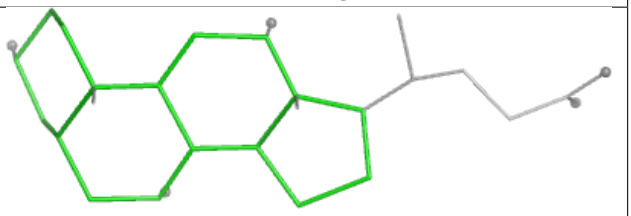
Bond lengths



Bond angles

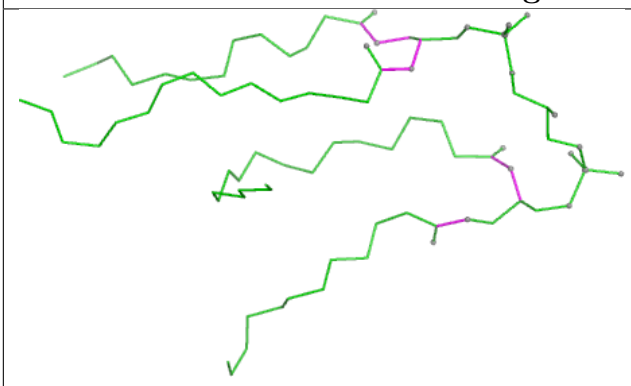


Torsions

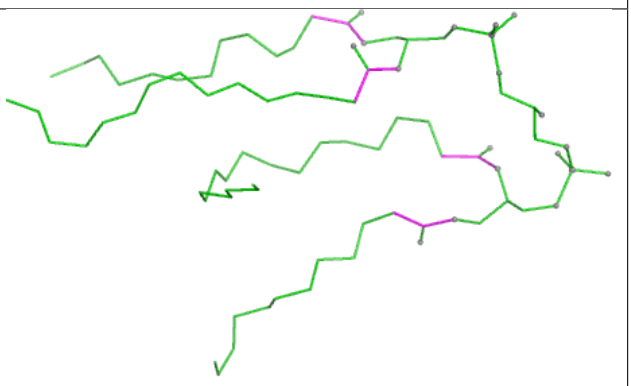


Rings

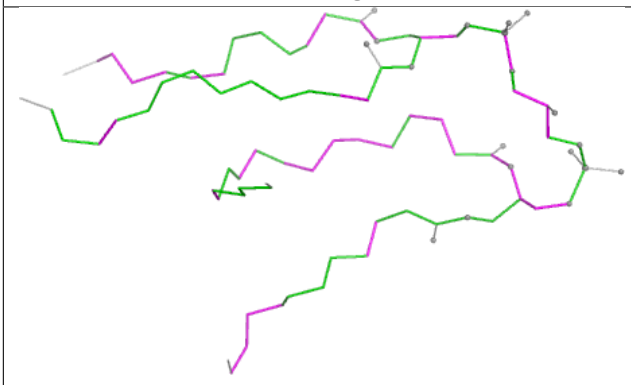
Ligand CDL N 401



Bond lengths



Bond angles

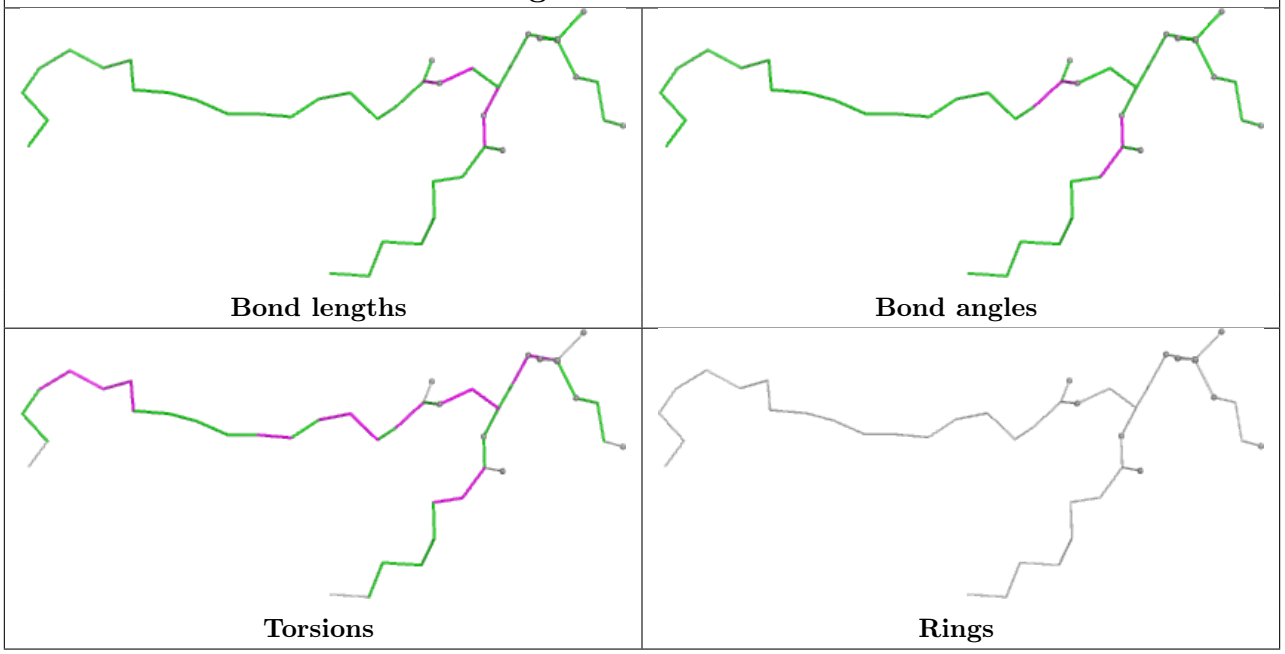


Torsions

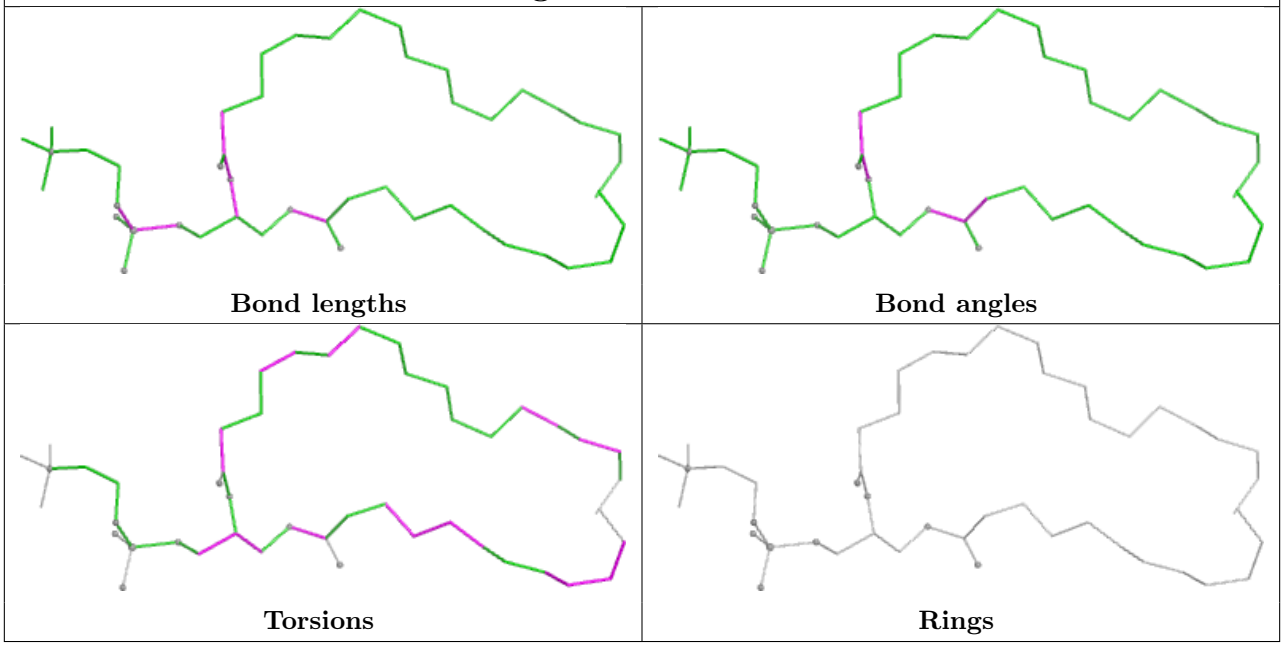


Rings

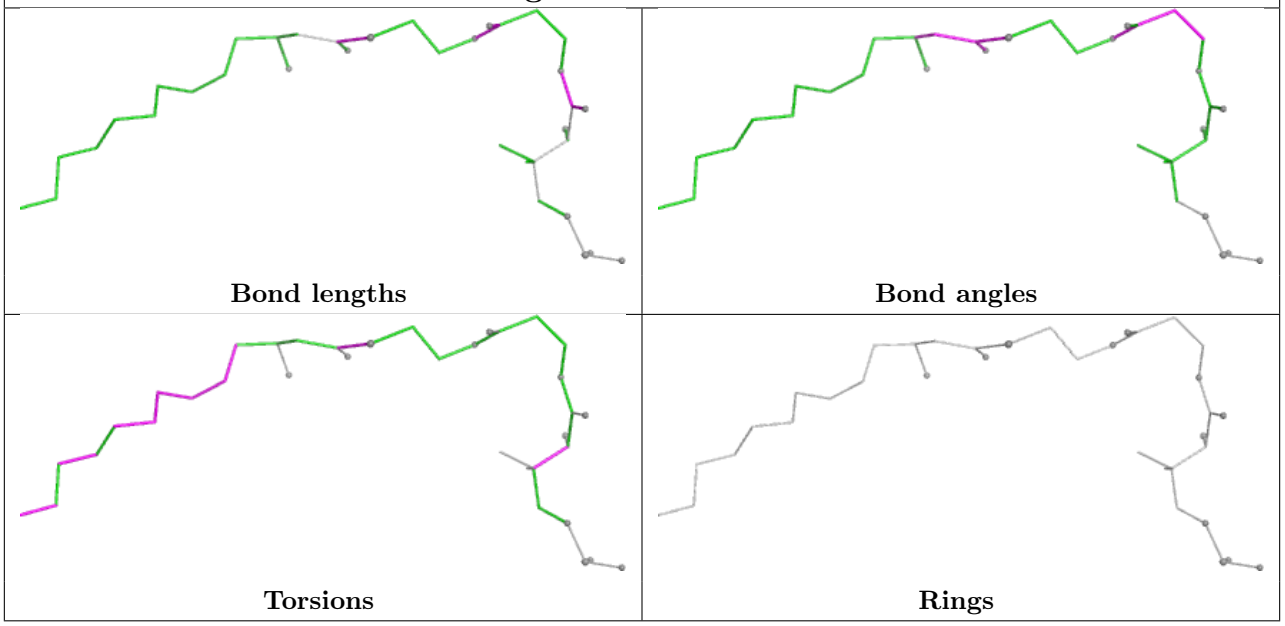
Ligand 3PE Y 204



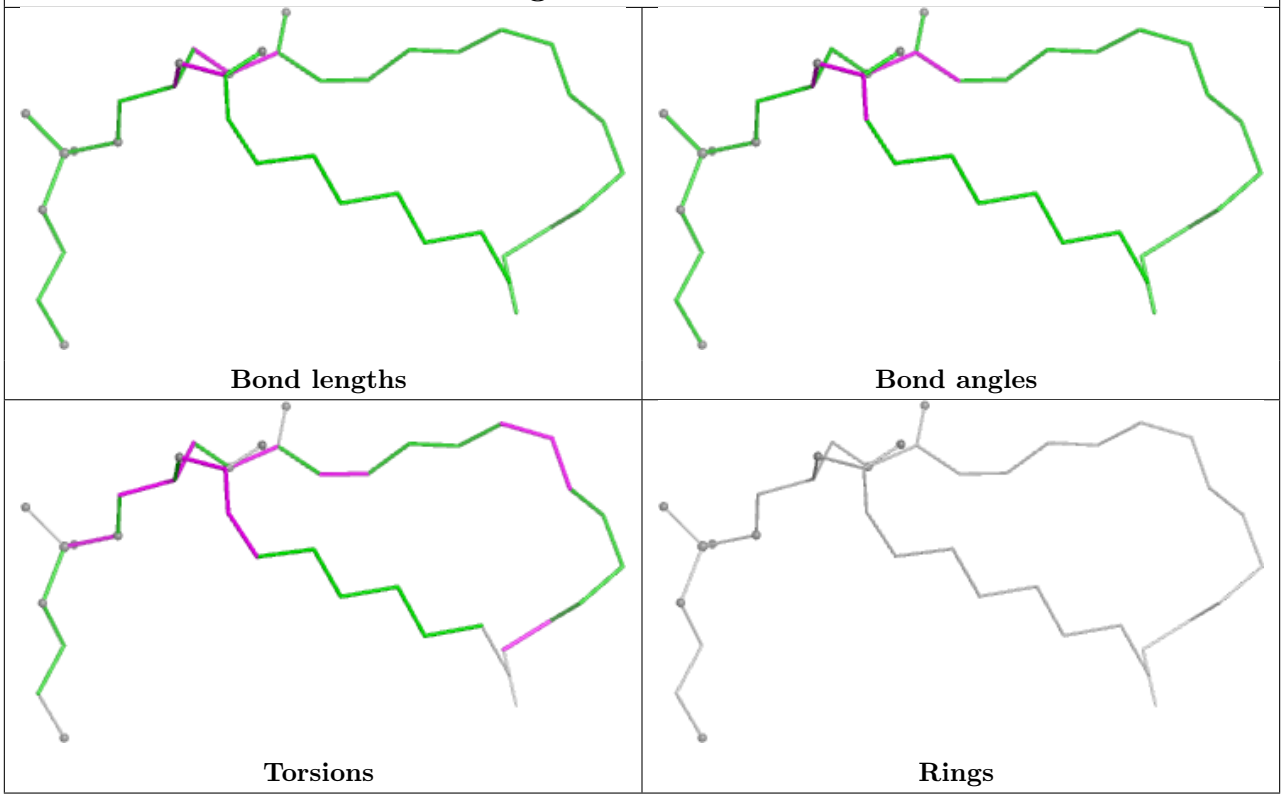
Ligand PC1 J 201



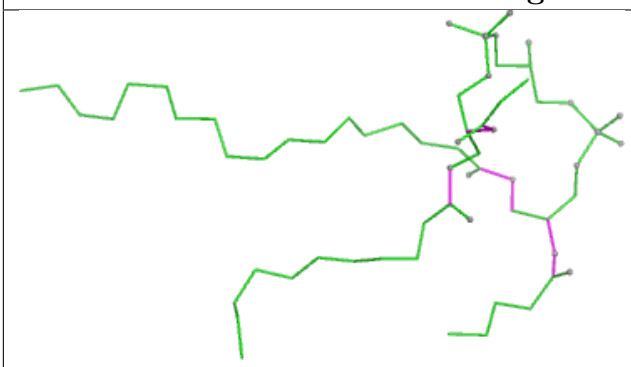
Ligand EHZ U 101



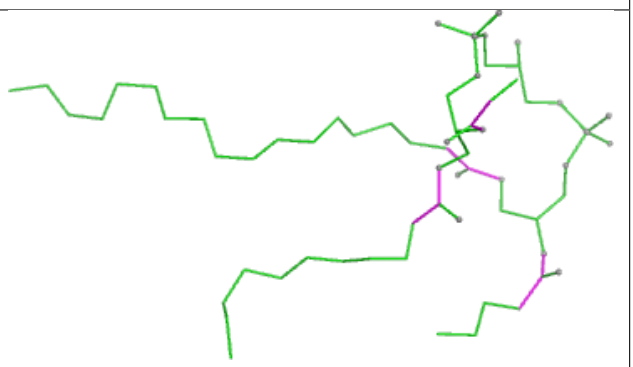
Ligand 3PE X 201



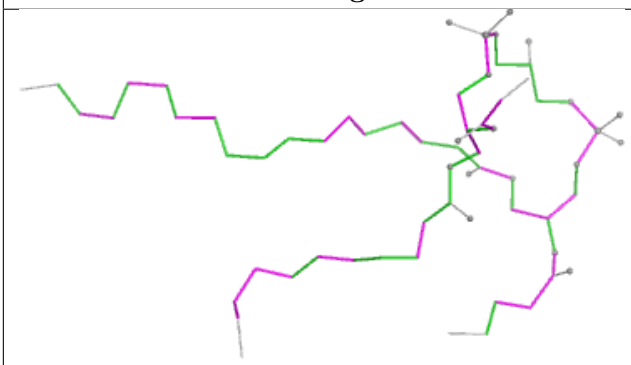
Ligand CDL d 203



Bond lengths



Bond angles

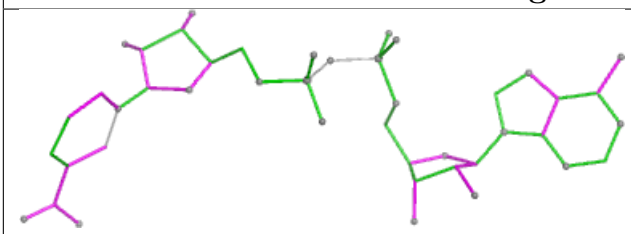


Torsions

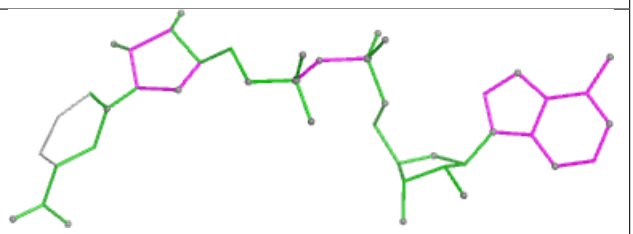


Rings

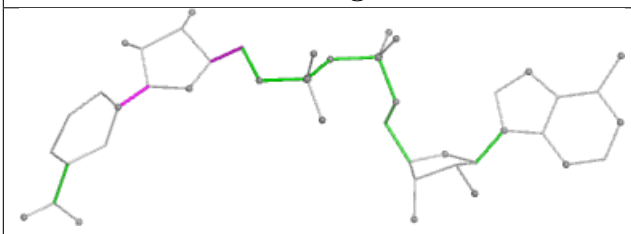
Ligand NAI F 503



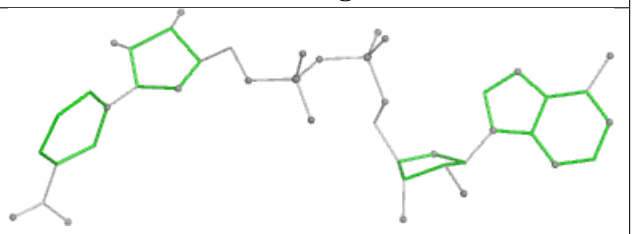
Bond lengths



Bond angles

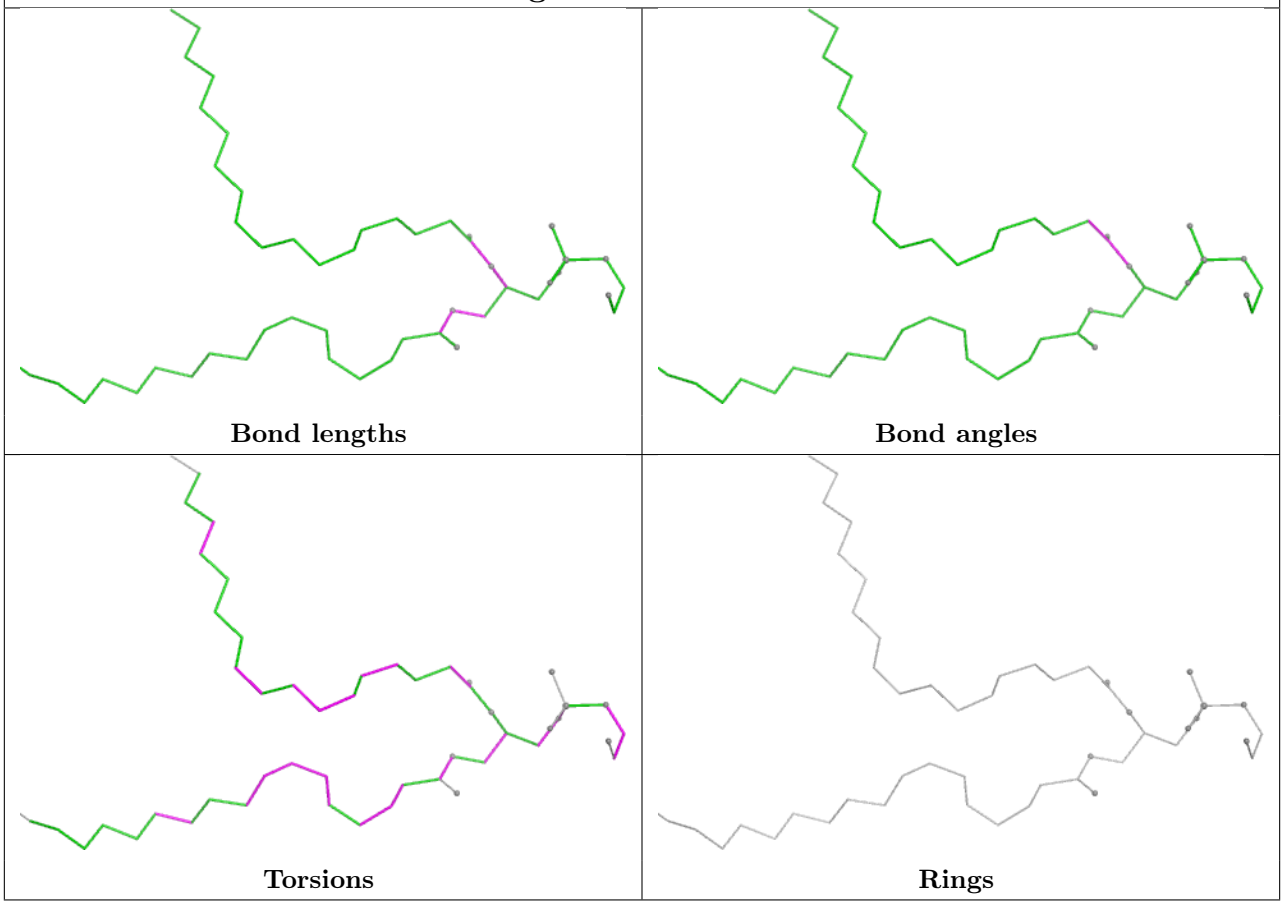


Torsions

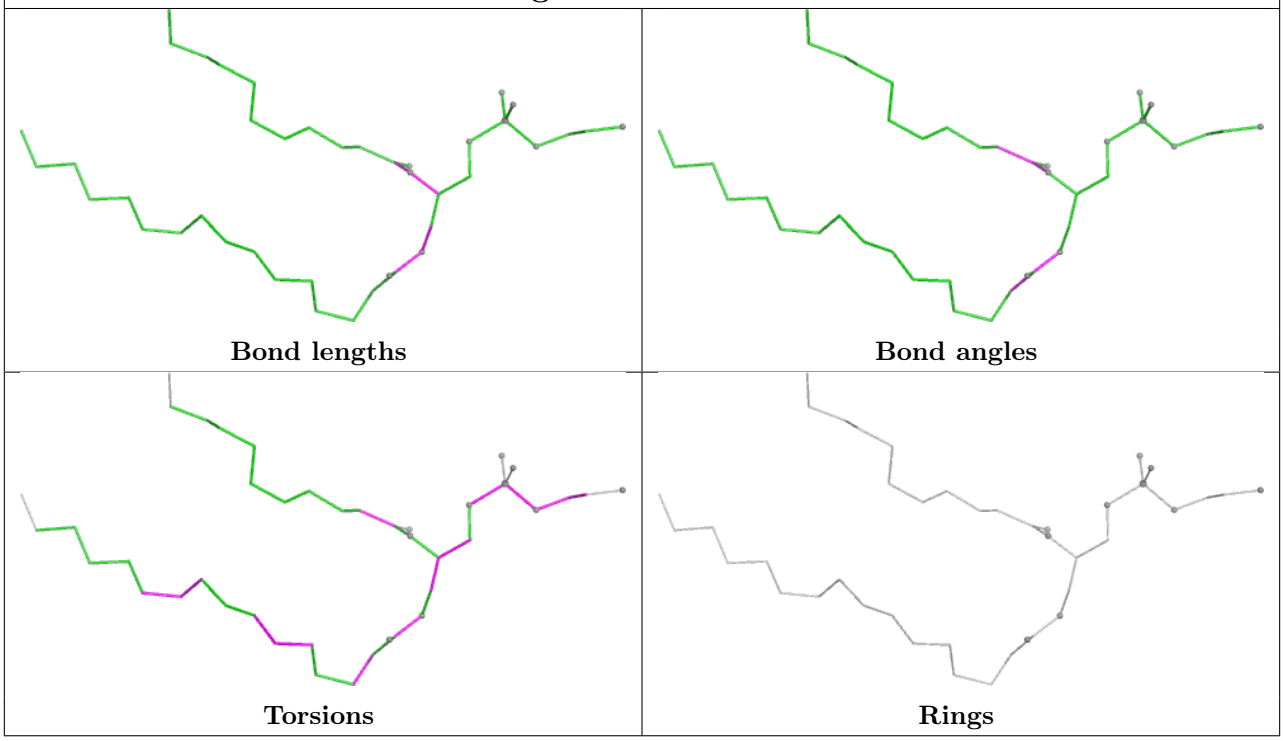


Rings

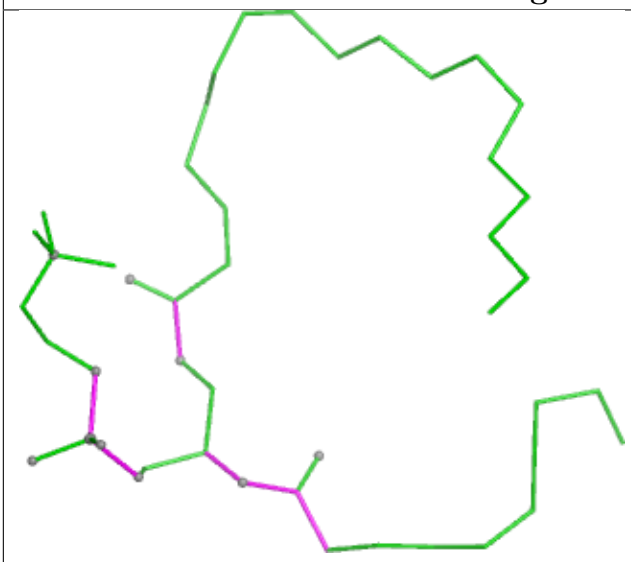
Ligand 3PE D 502



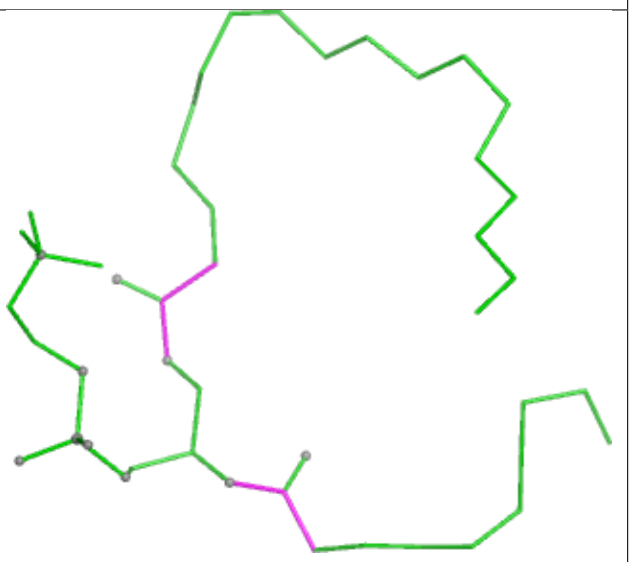
Ligand 3PE L 701



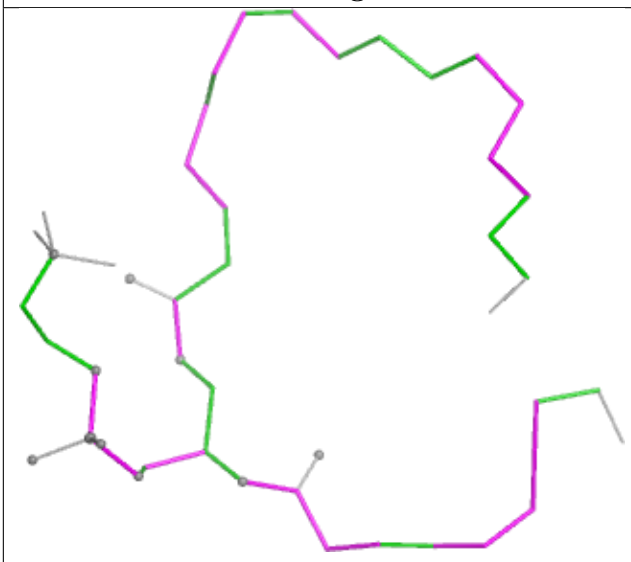
Ligand PC1 d 202



Bond lengths



Bond angles

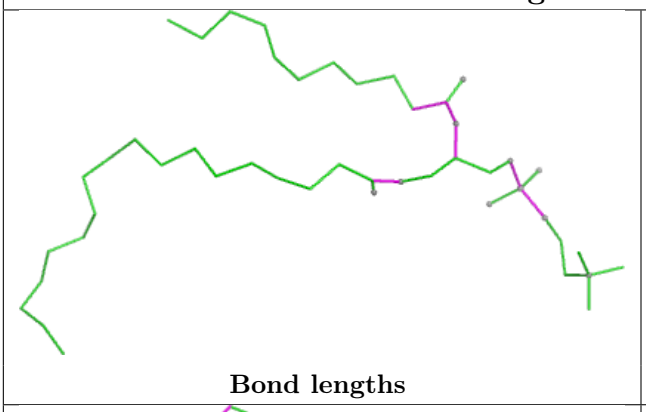


Torsions

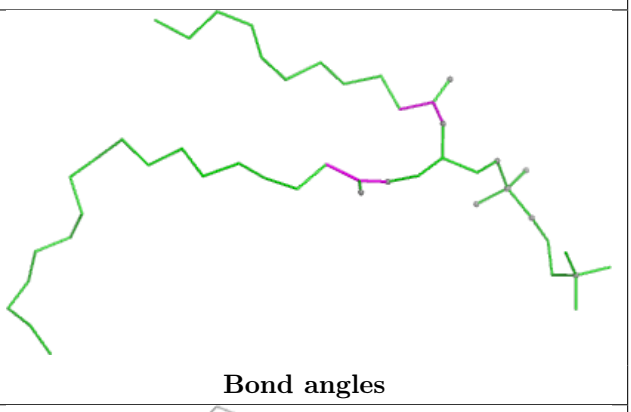


Rings

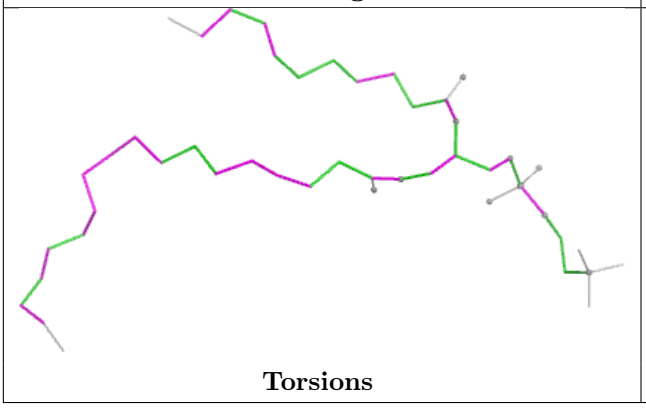
Ligand PC1 B 203



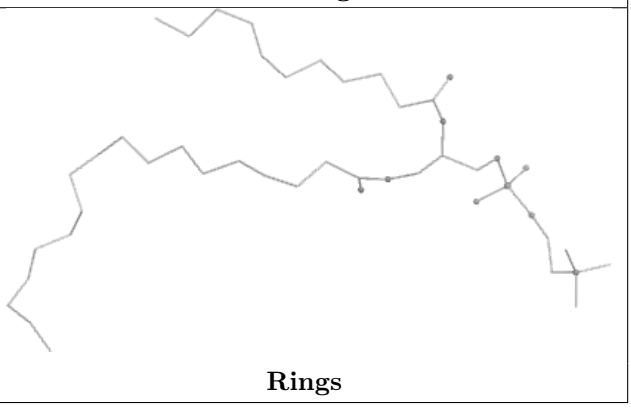
Bond lengths



Bond angles

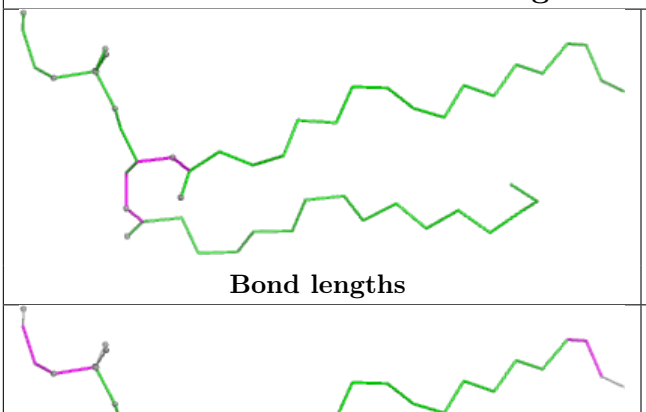


Torsions

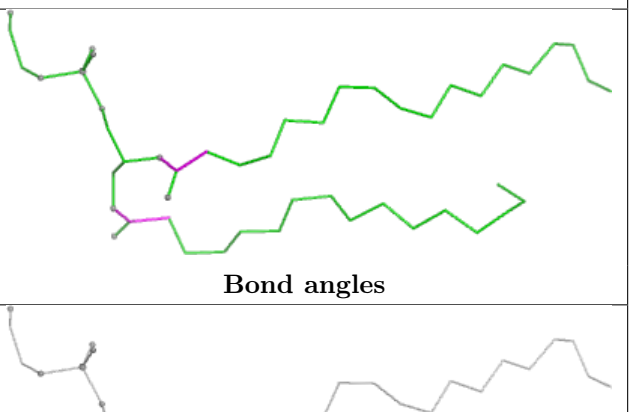


Rings

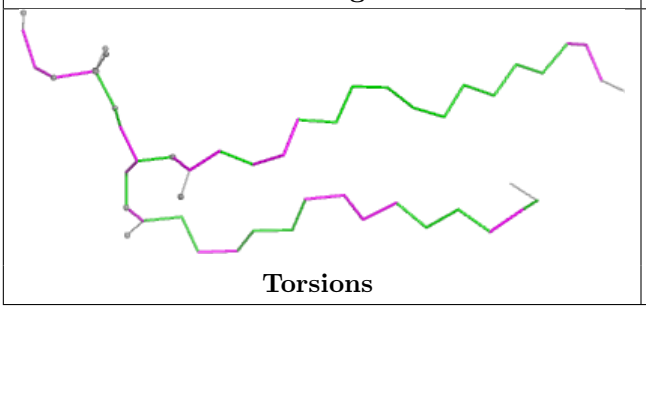
Ligand 3PE d 201



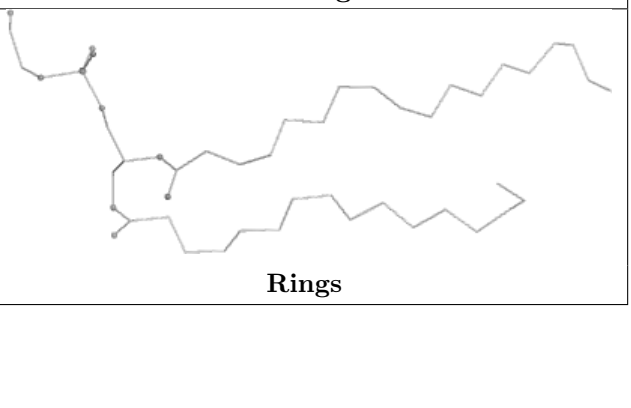
Bond lengths



Bond angles

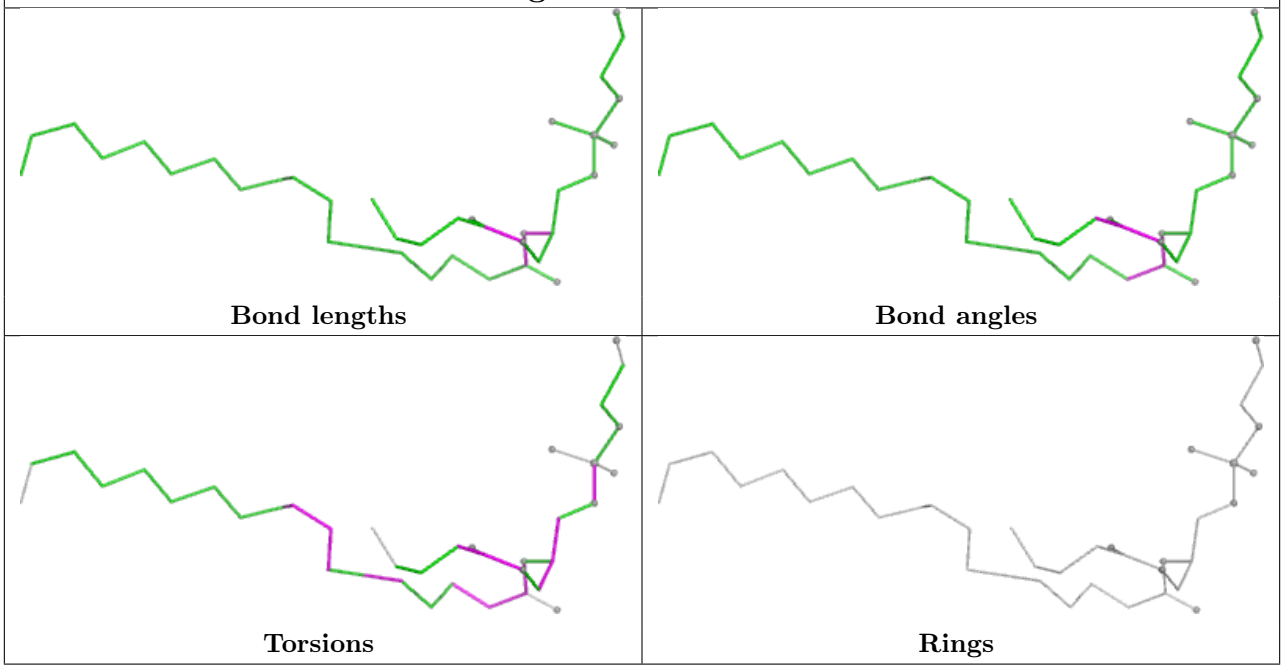


Torsions

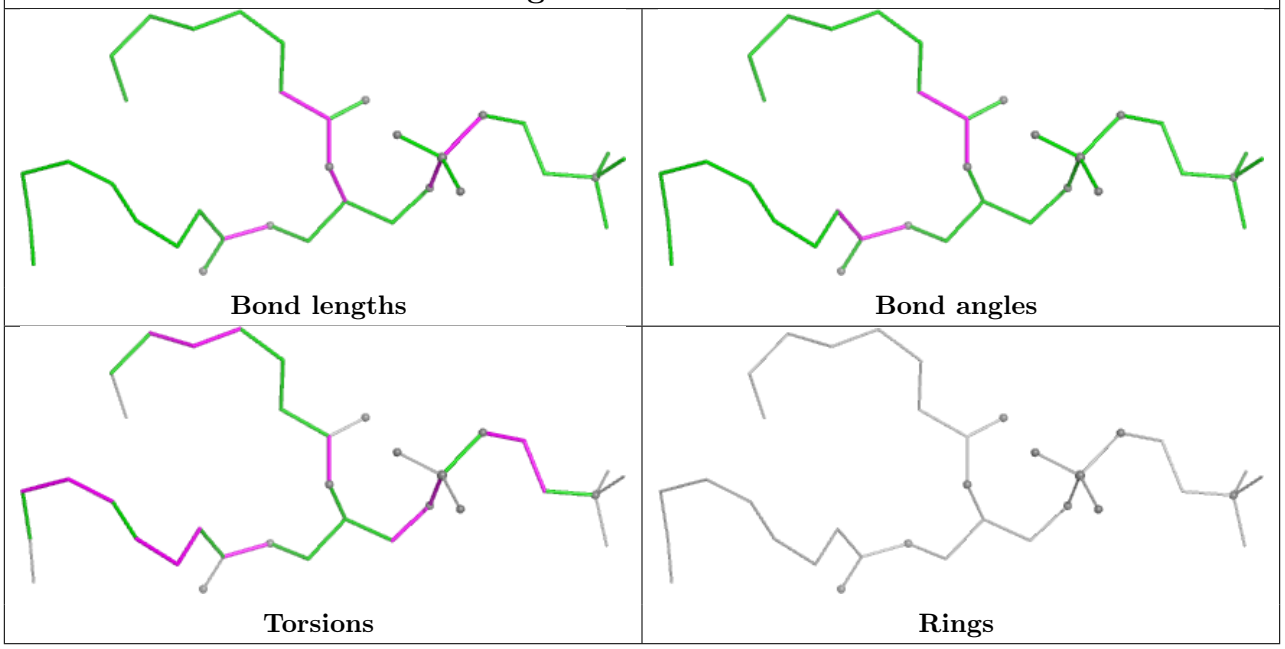


Rings

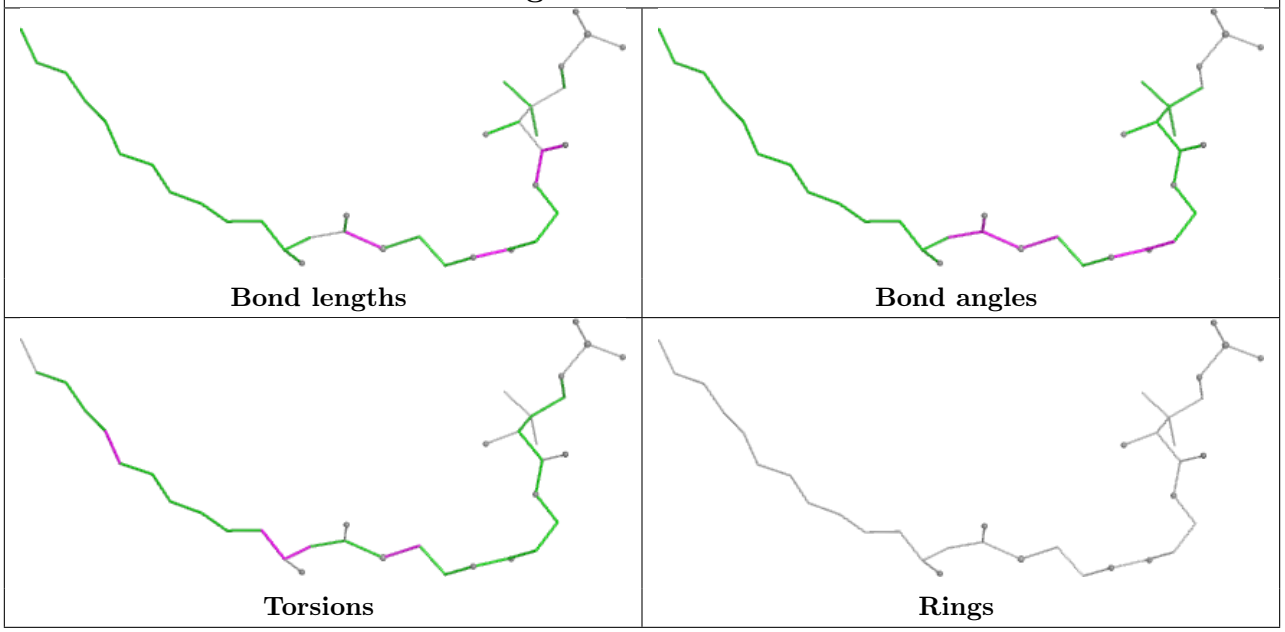
Ligand 3PE H 401



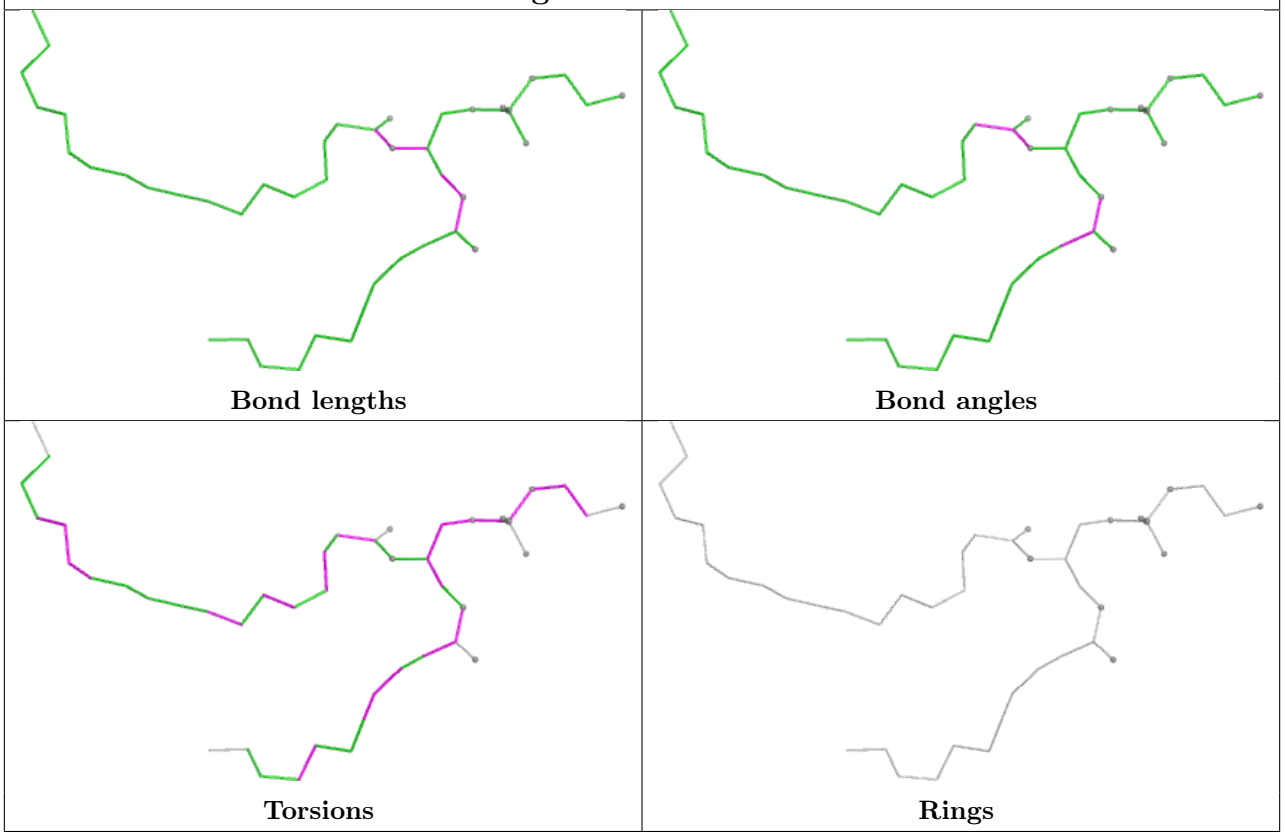
Ligand PC1 N 402



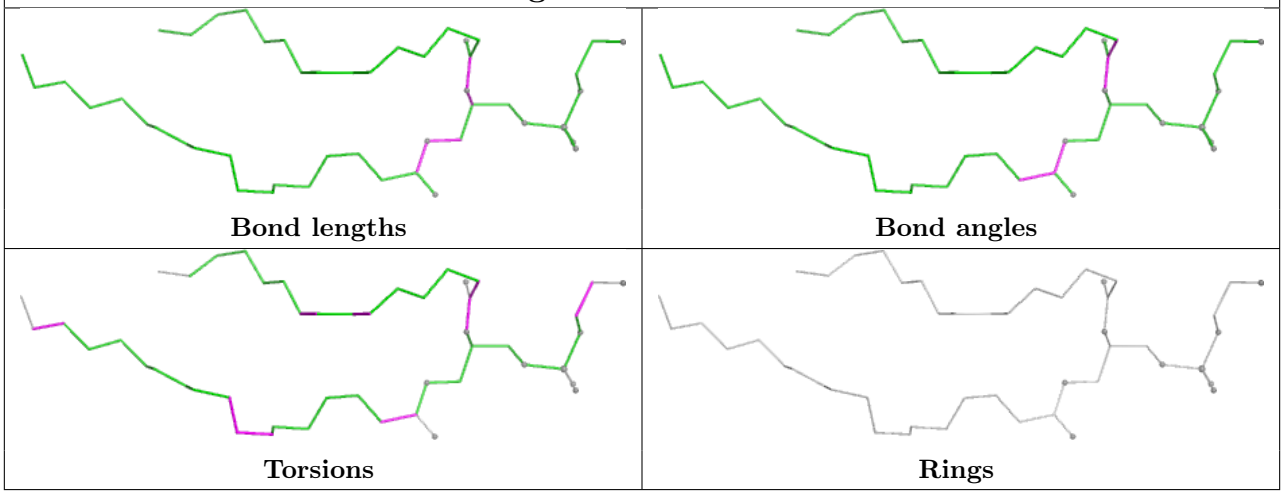
Ligand EHZ T 101



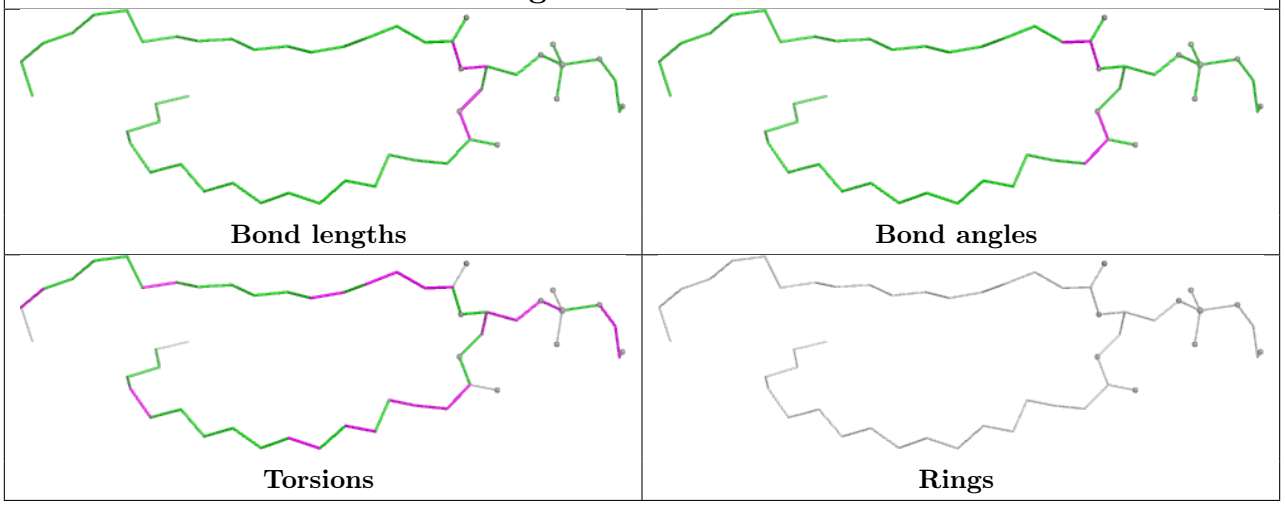
Ligand 3PE L 705



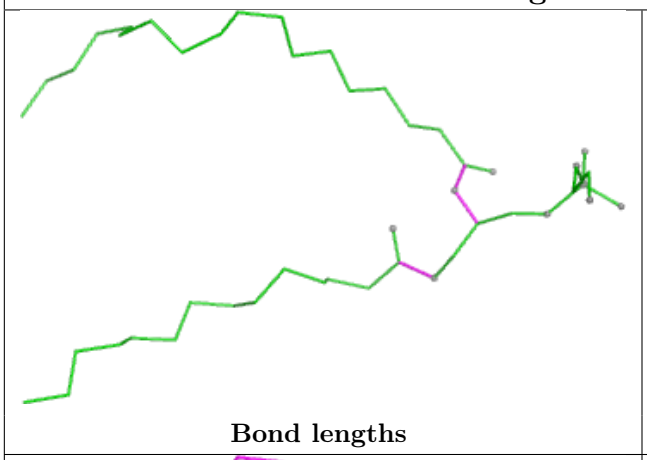
Ligand 3PE K 101



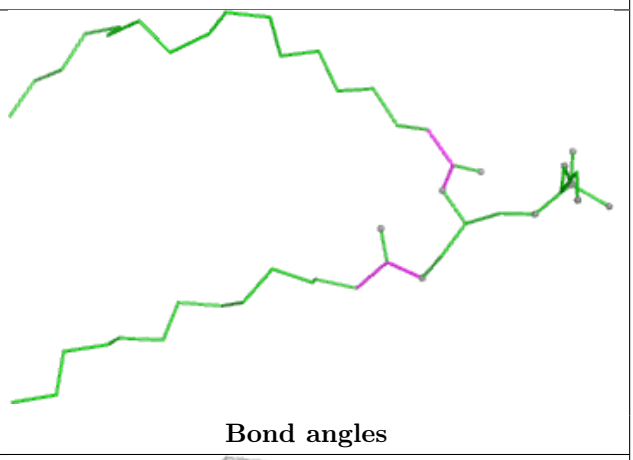
Ligand 3PE Y 202



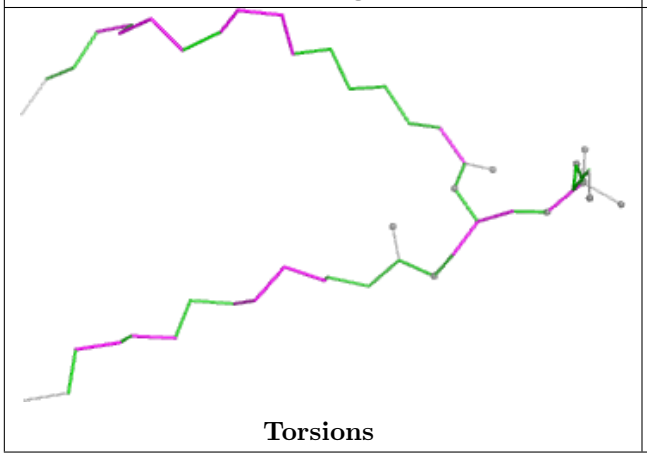
Ligand 3PE A 201



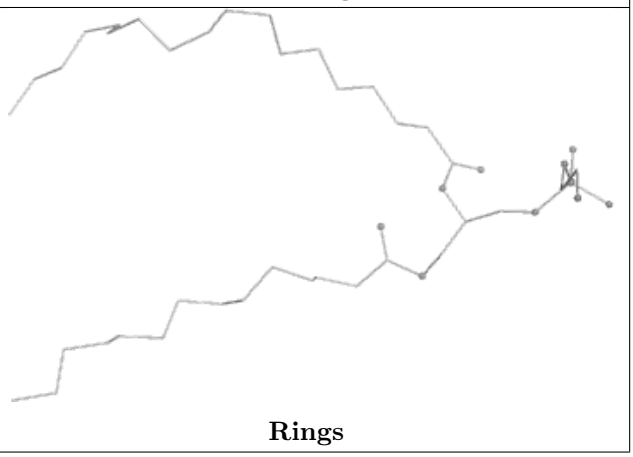
Bond lengths



Bond angles

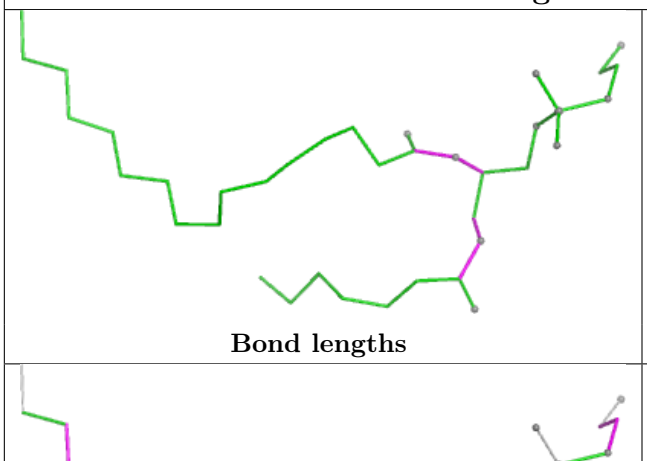


Torsions

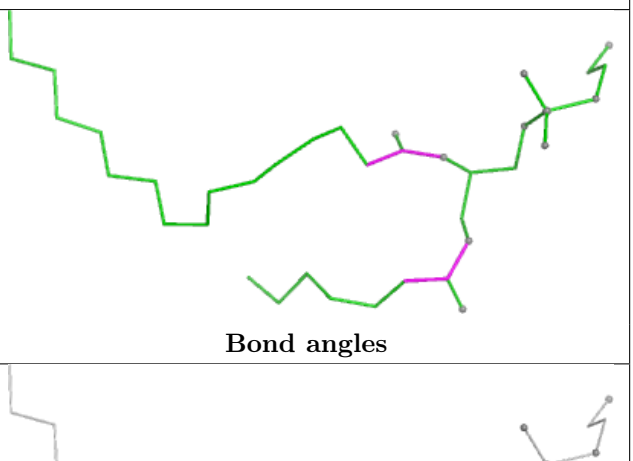


Rings

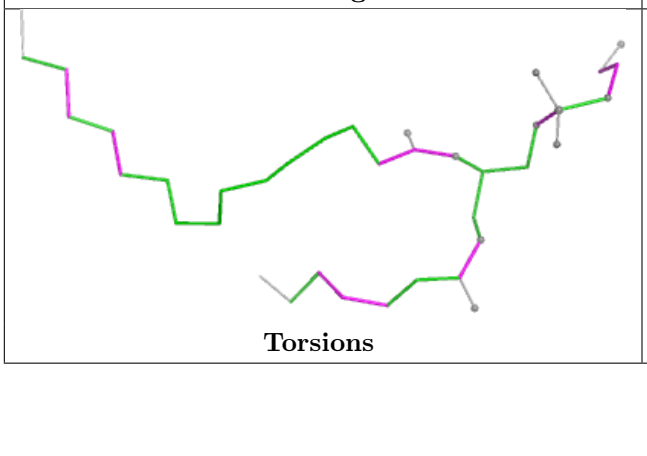
Ligand 3PE h 202



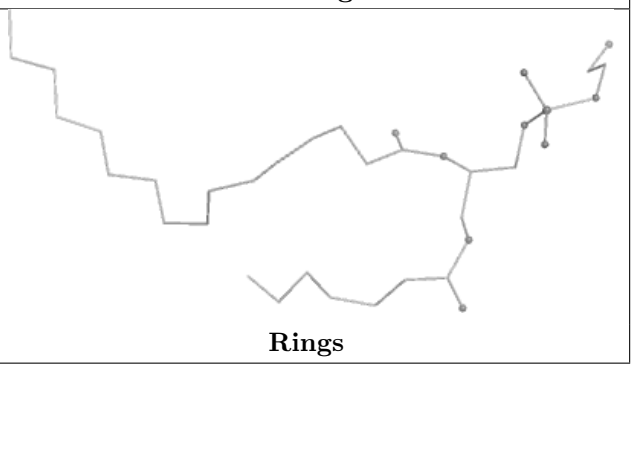
Bond lengths



Bond angles

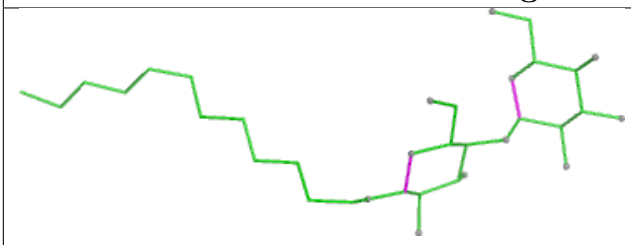


Torsions

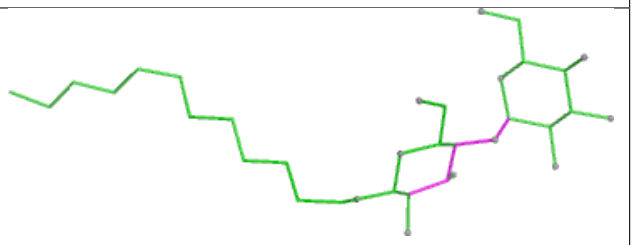


Rings

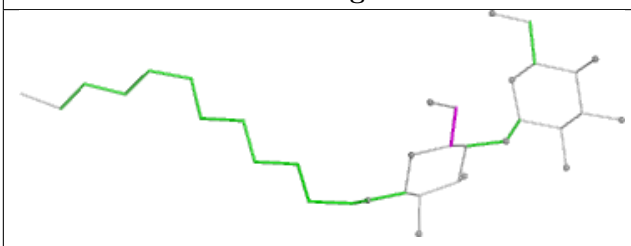
Ligand LMT D 501



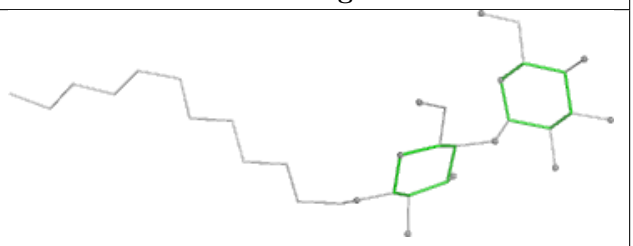
Bond lengths



Bond angles

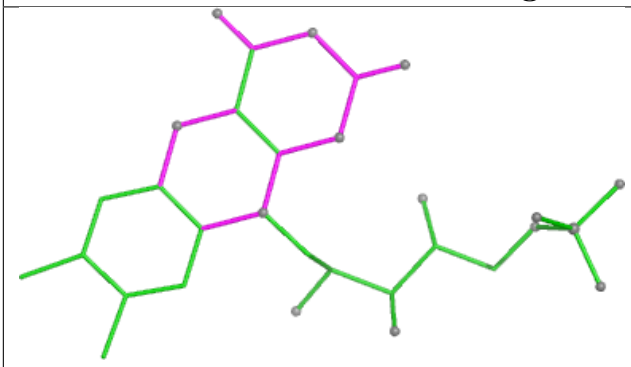


Torsions

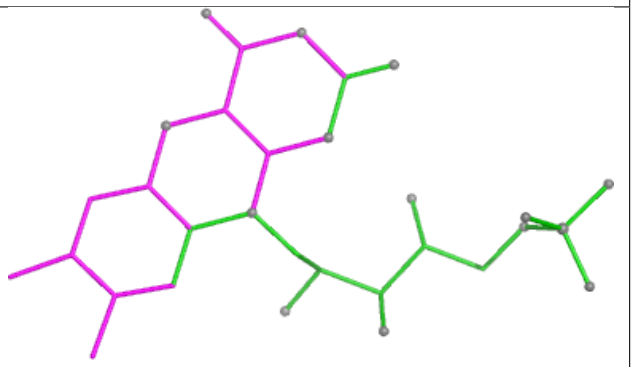


Rings

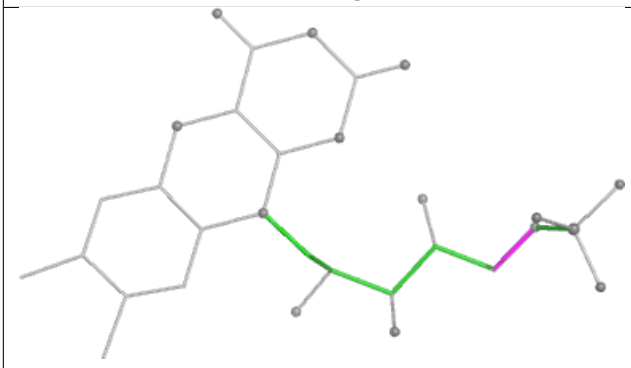
Ligand FMN F 501



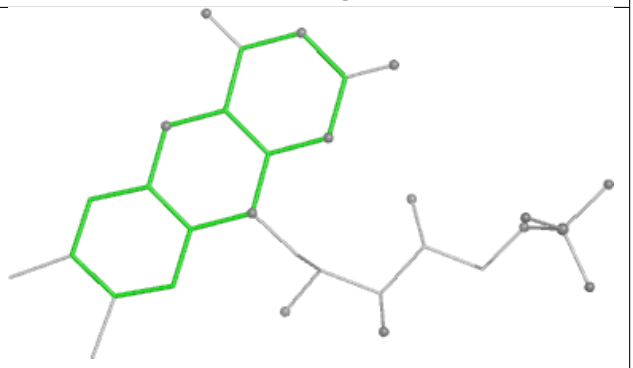
Bond lengths



Bond angles

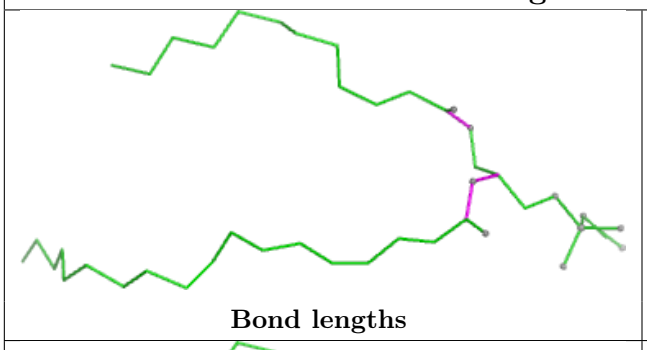


Torsions

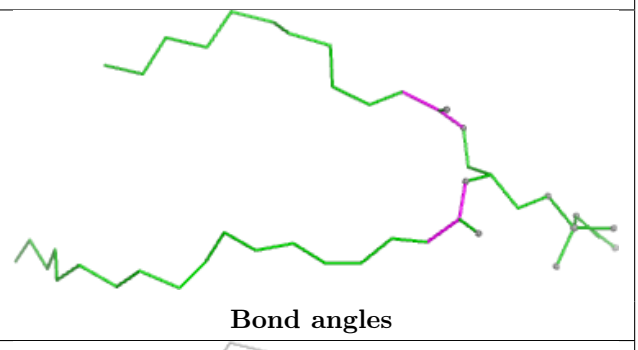


Rings

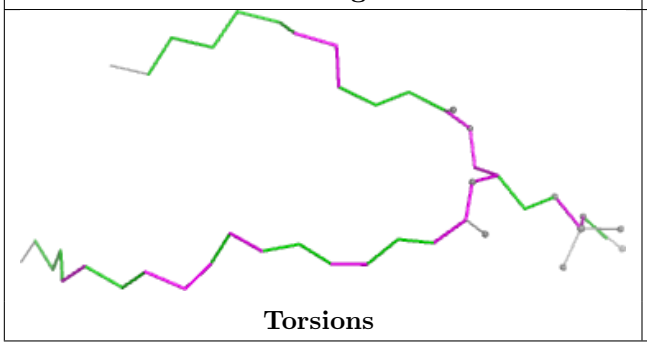
Ligand 3PE Y 205



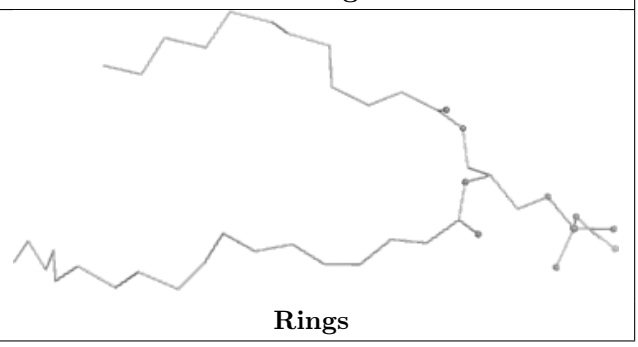
Bond lengths



Bond angles

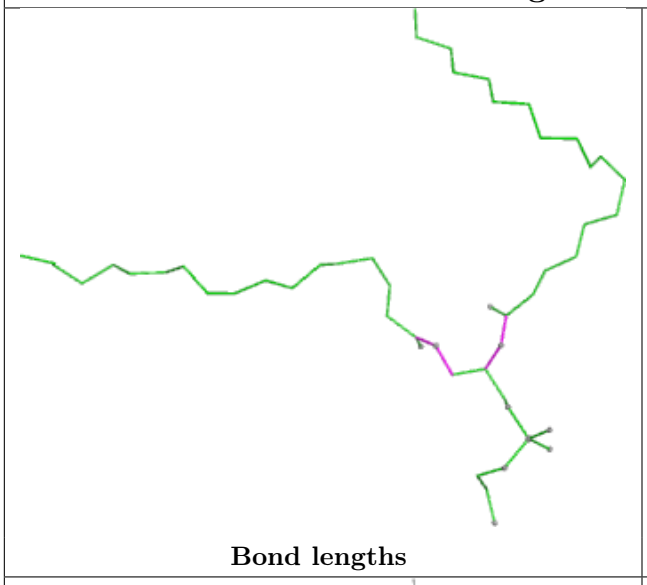


Torsions

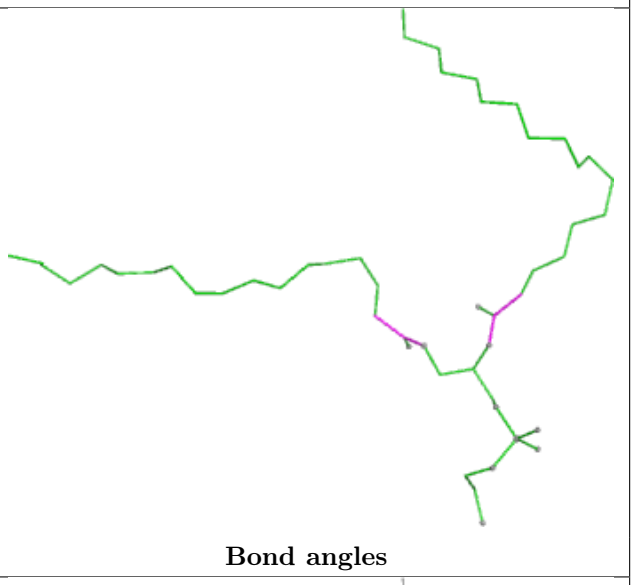


Rings

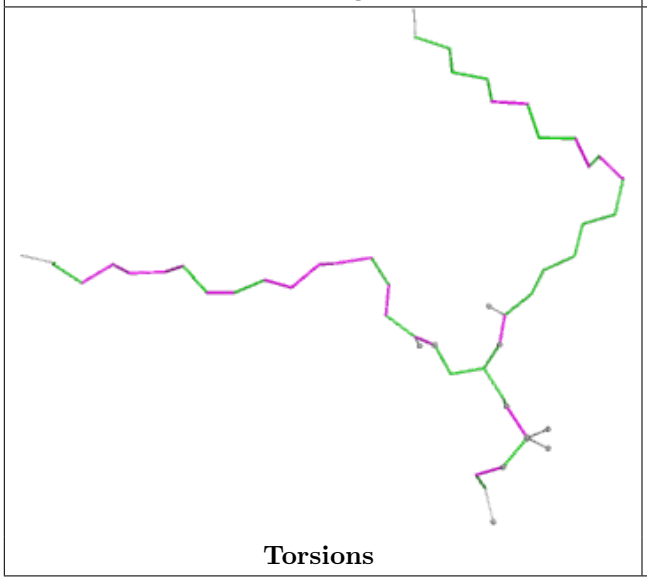
Ligand 3PE H 402



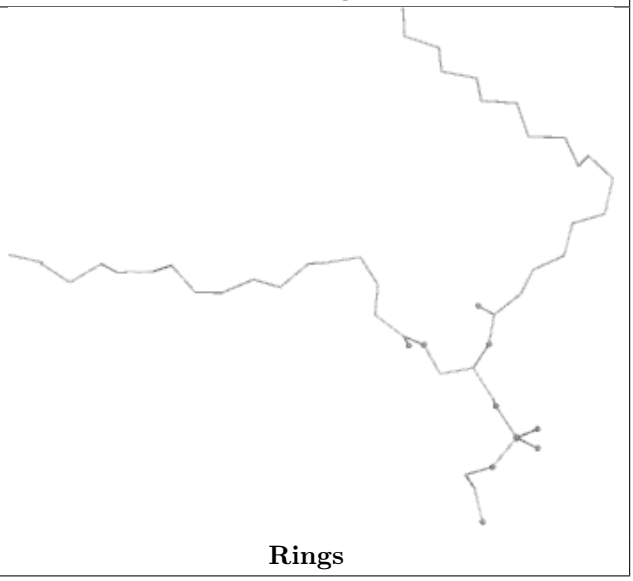
Bond lengths



Bond angles

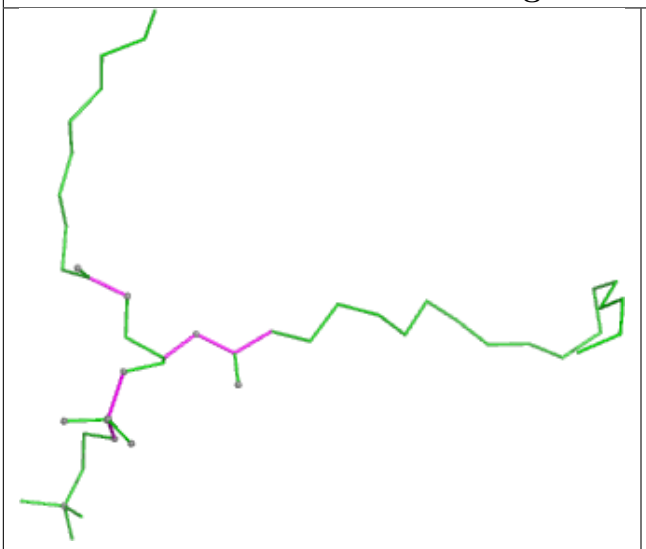


Torsions

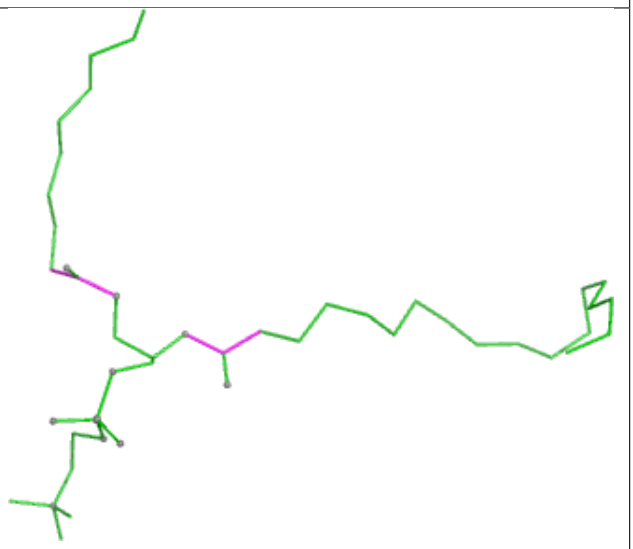


Rings

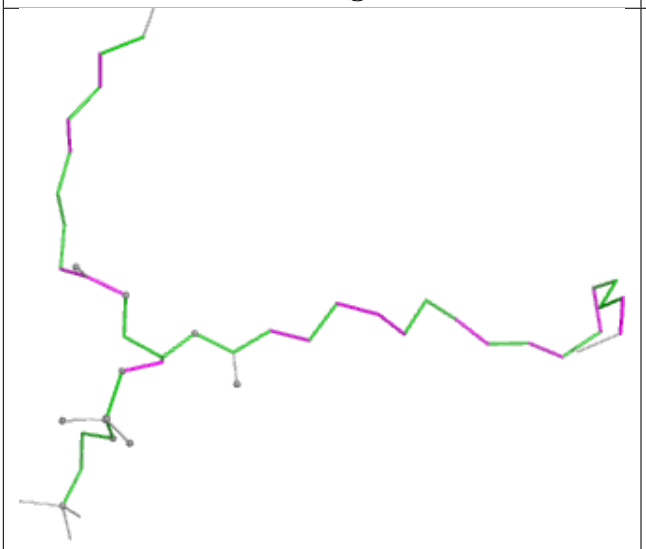
Ligand PC1 M 603



Bond lengths



Bond angles

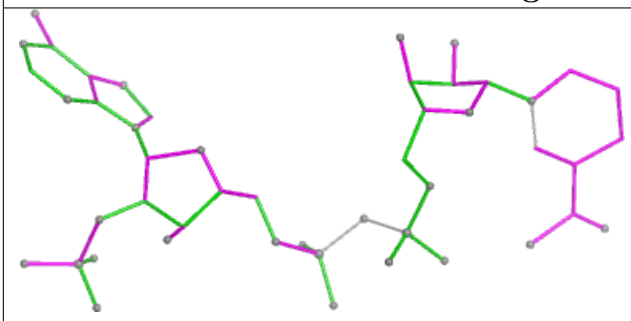


Torsions

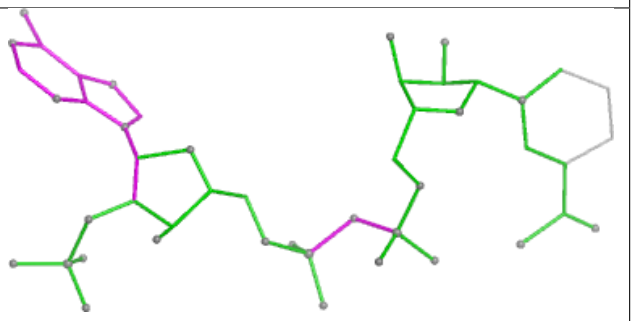


Rings

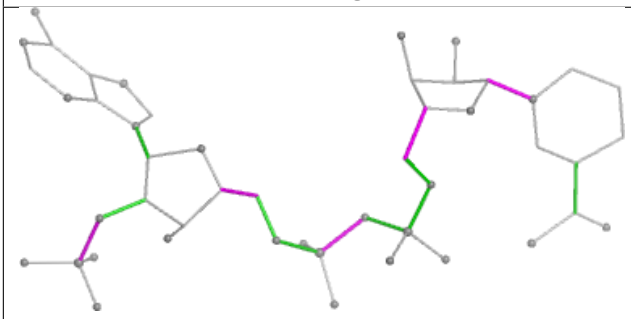
Ligand NDP P 501



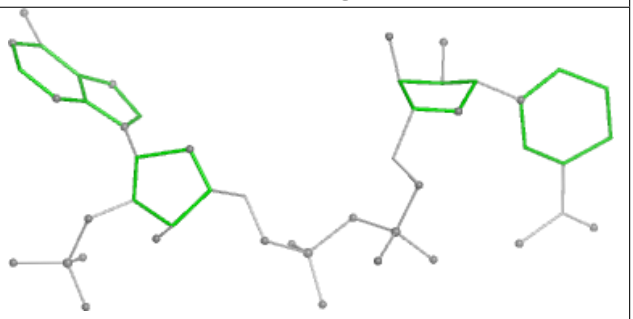
Bond lengths



Bond angles

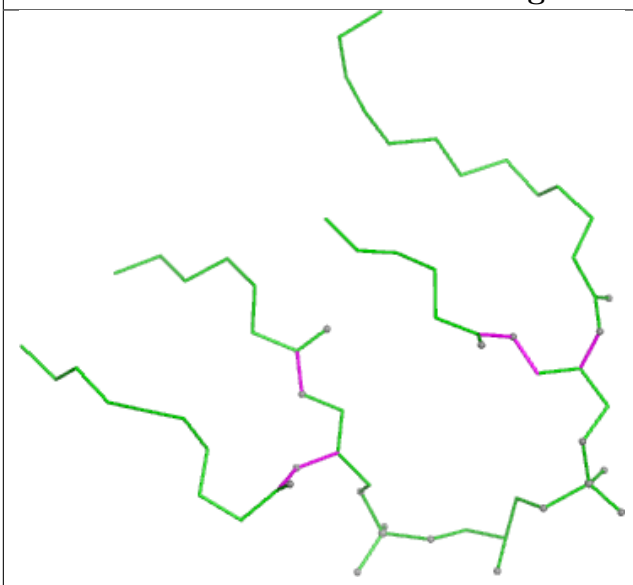


Torsions

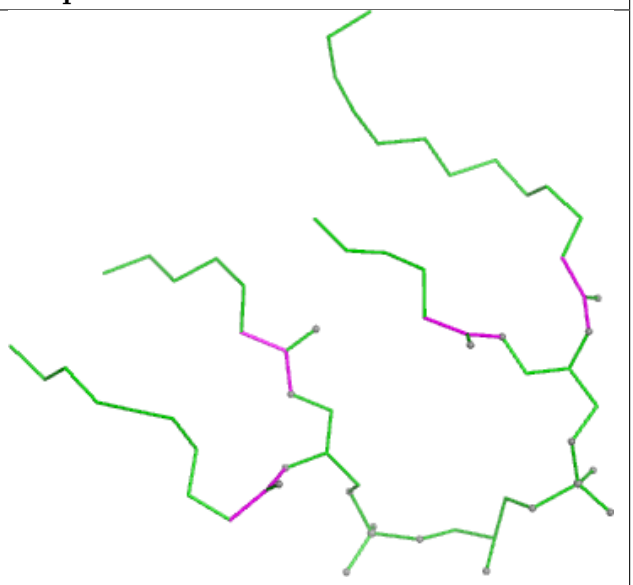


Rings

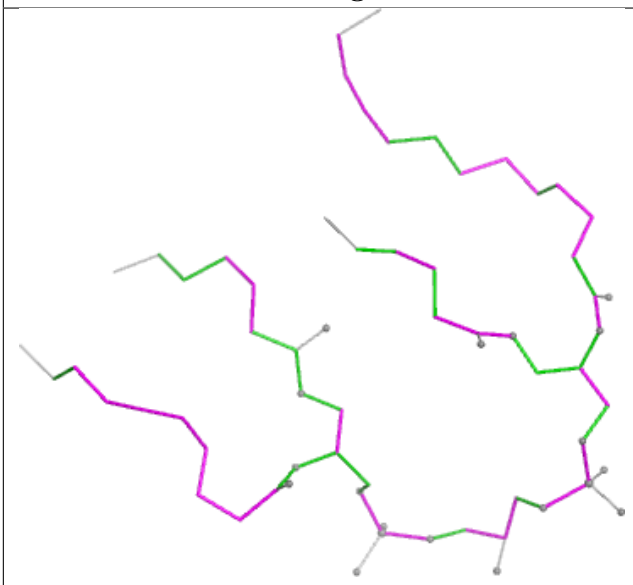
Ligand CDL q 201



Bond lengths



Bond angles

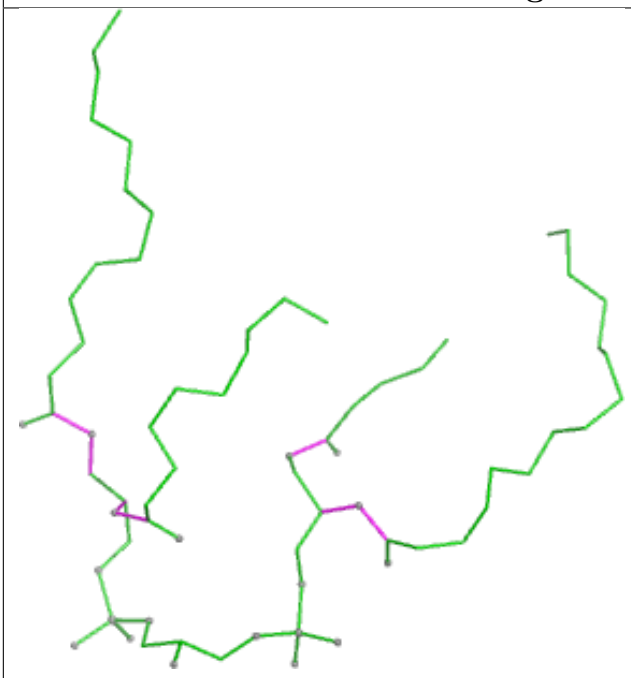


Torsions

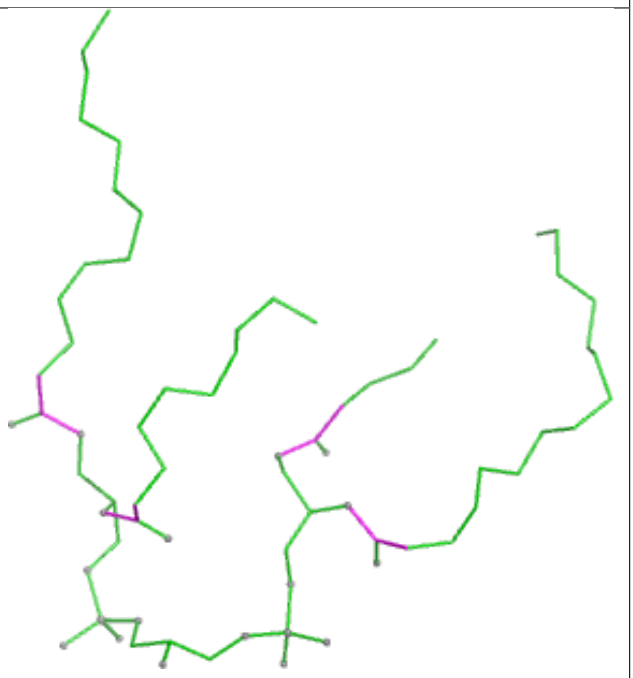


Rings

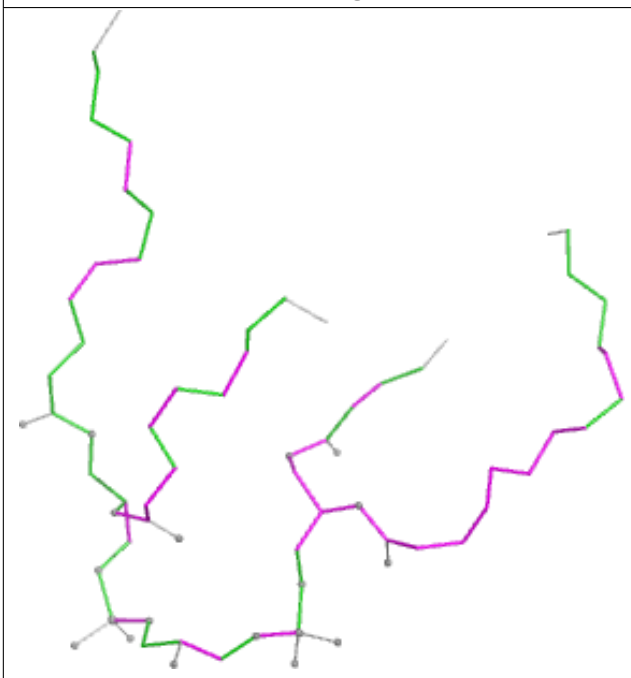
Ligand CDL L 702



Bond lengths



Bond angles

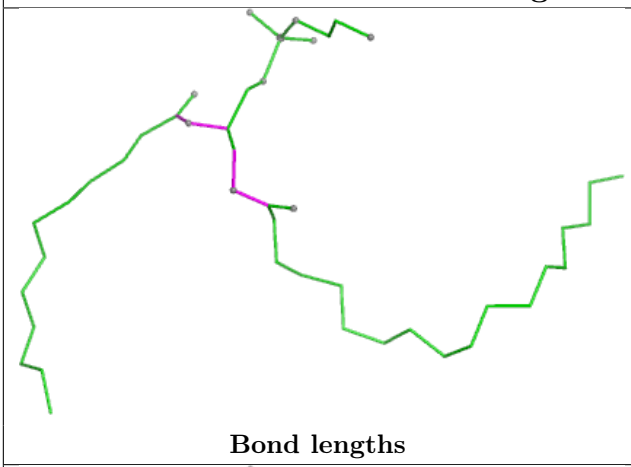


Torsions

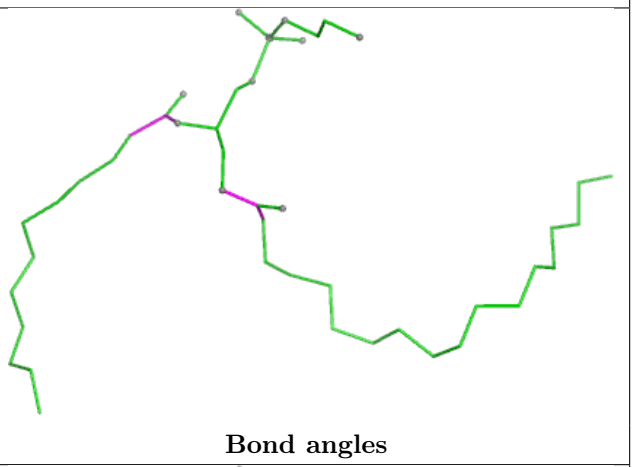


Rings

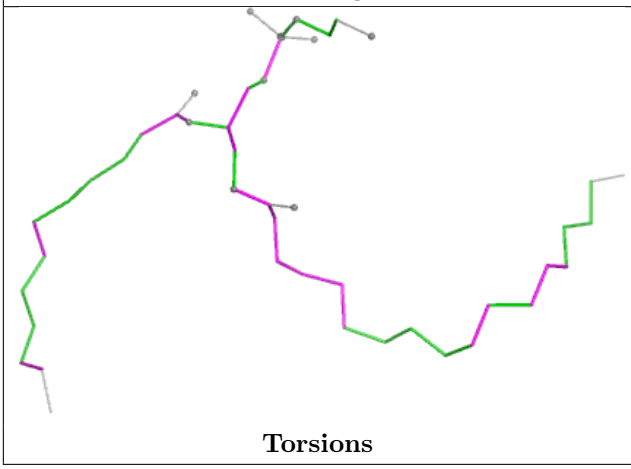
Ligand 3PE L 703



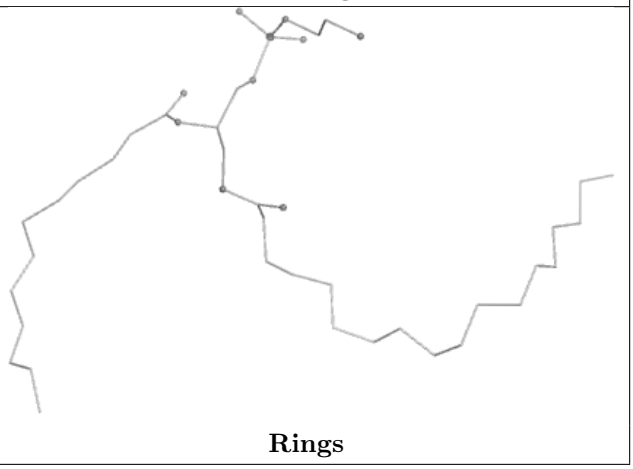
Bond lengths



Bond angles

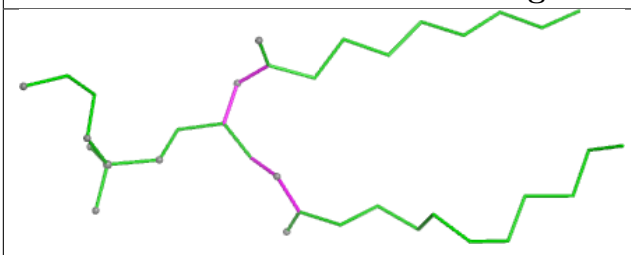


Torsions

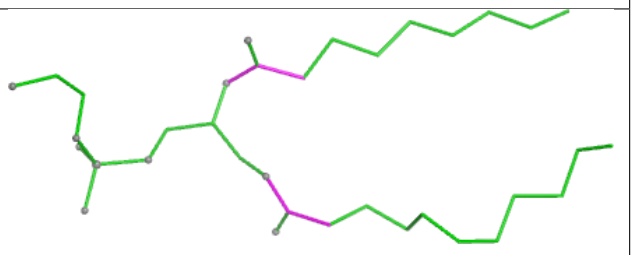


Rings

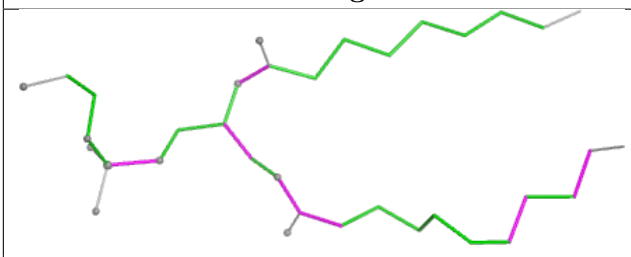
Ligand 3PE A 202



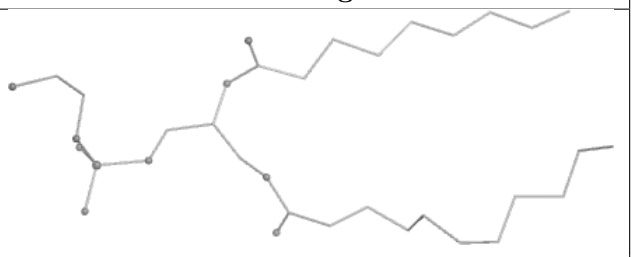
Bond lengths



Bond angles

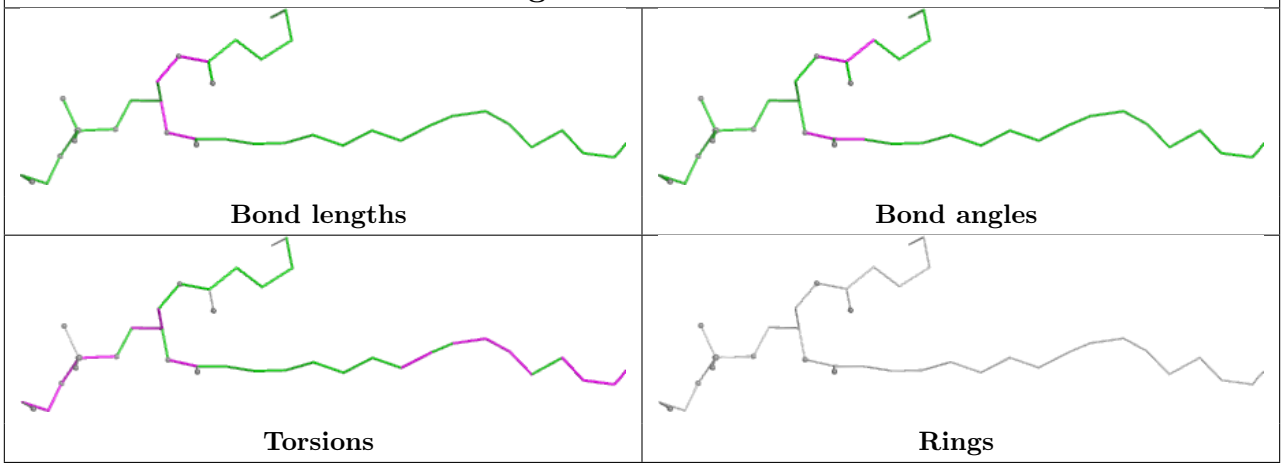


Torsions

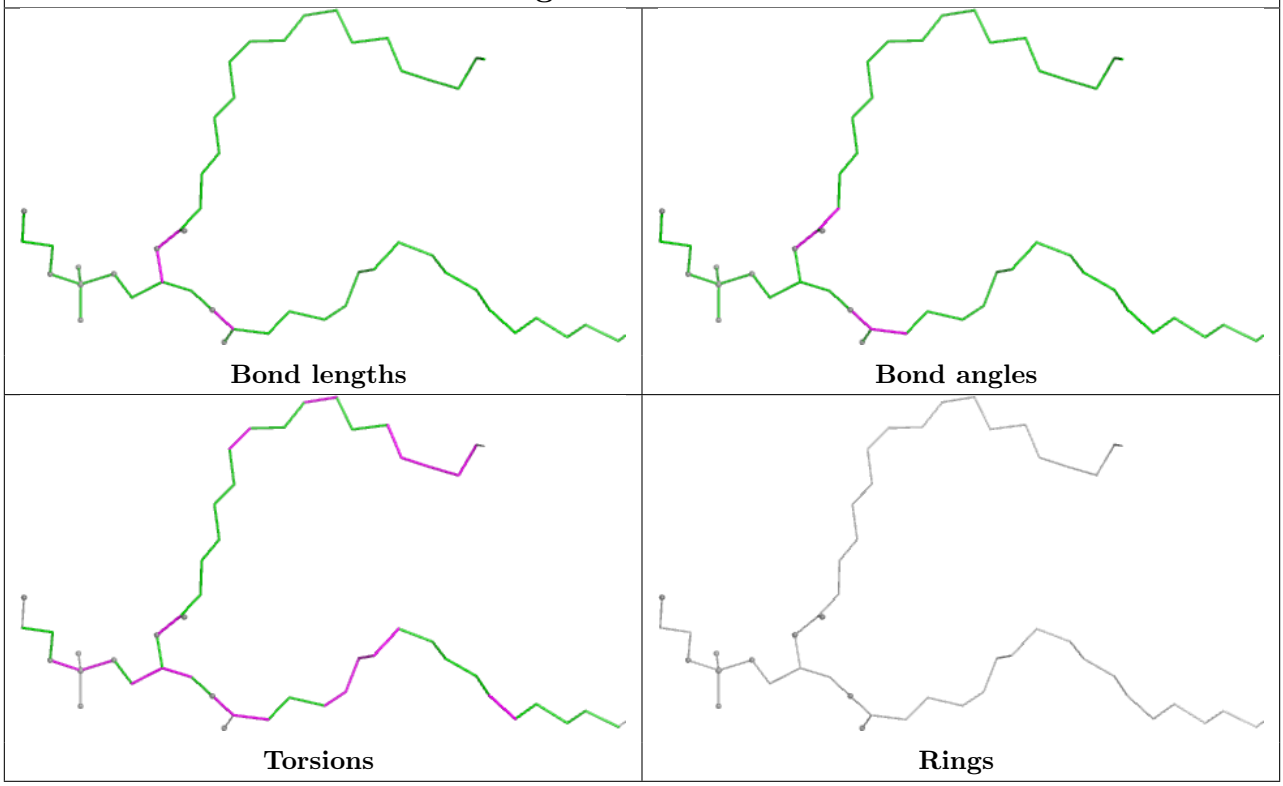


Rings

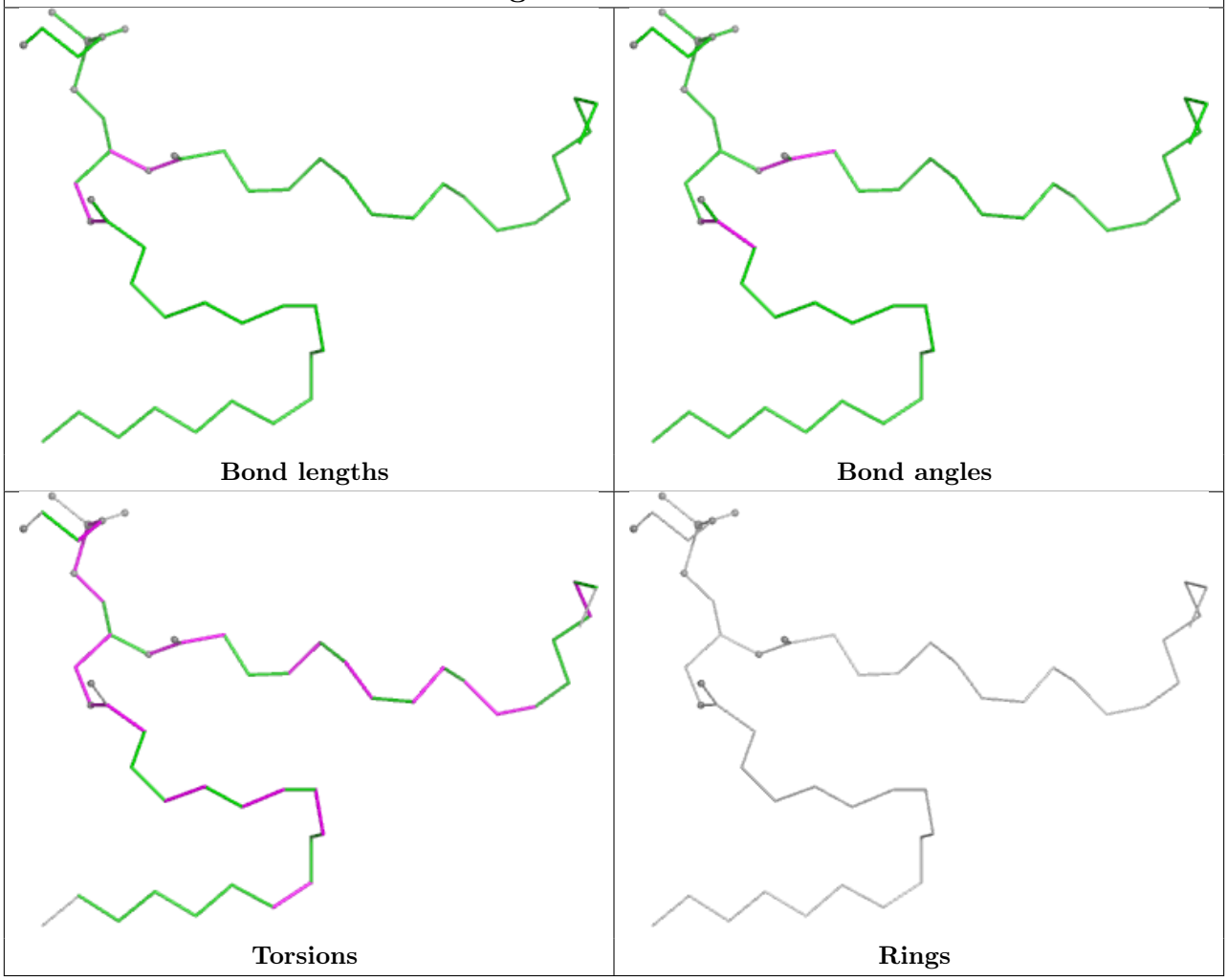
Ligand 3PE N 403



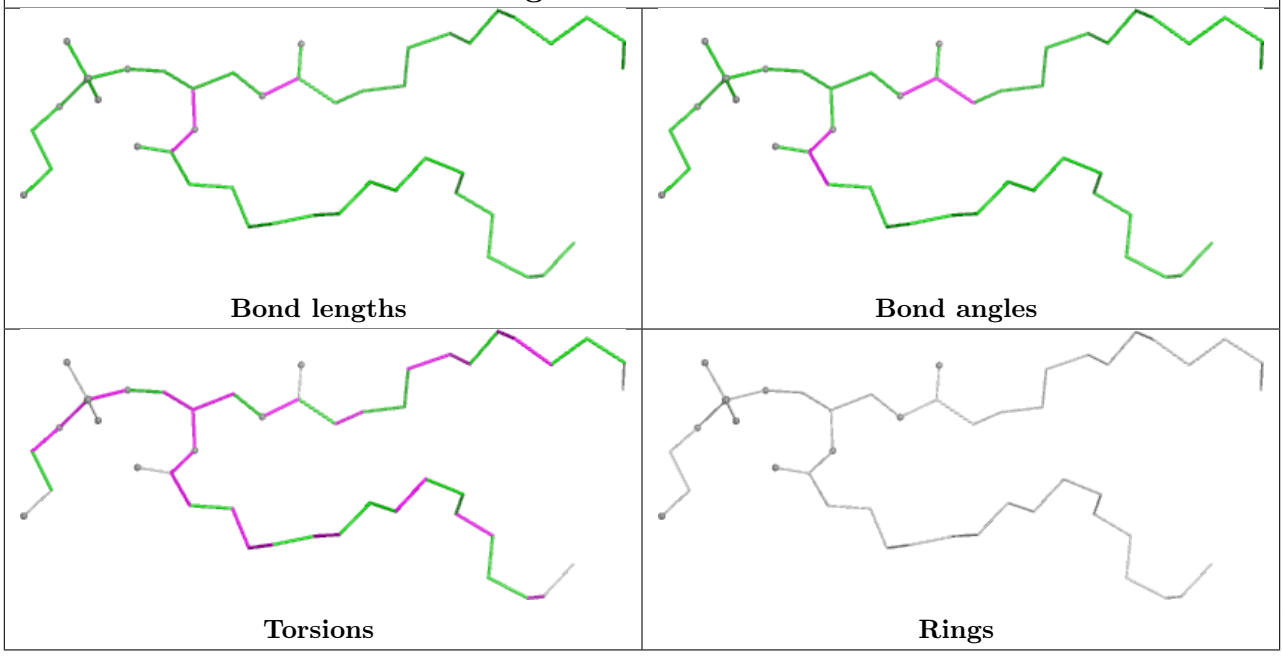
Ligand 3PE I 203



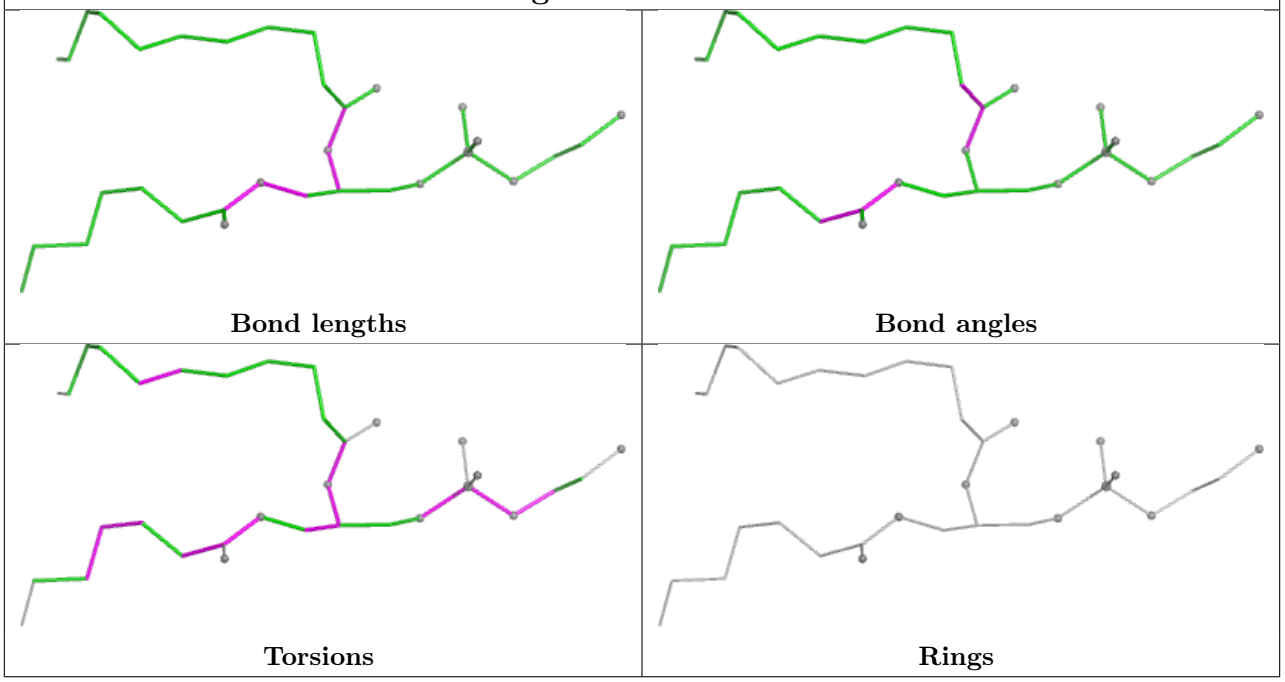
Ligand 3PE h 203



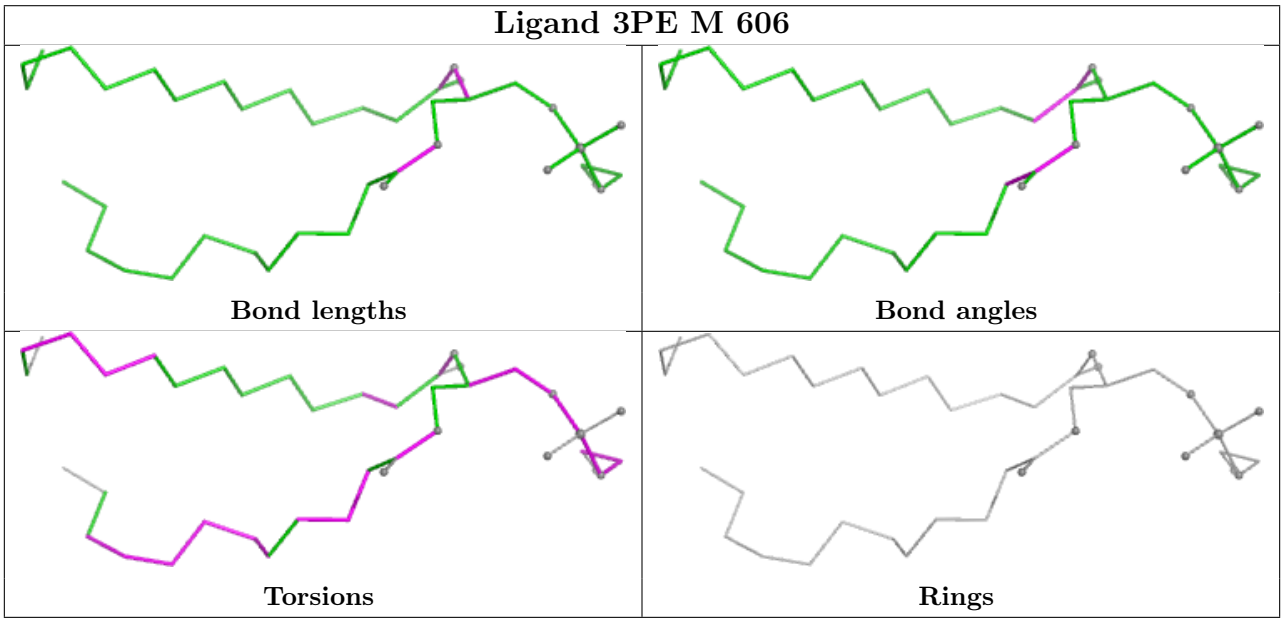
Ligand 3PE M 601



Ligand 3PE Z 202



Ligand 3PE M 606



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.

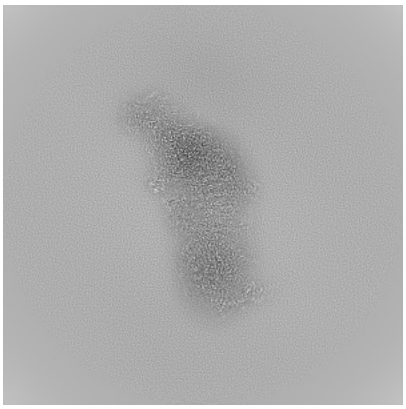
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-55033. These allow visual inspection of the internal detail of the map and identification of artifacts.

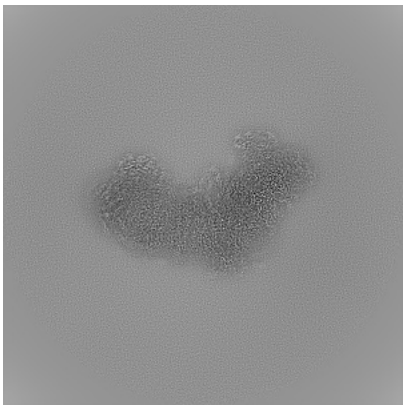
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

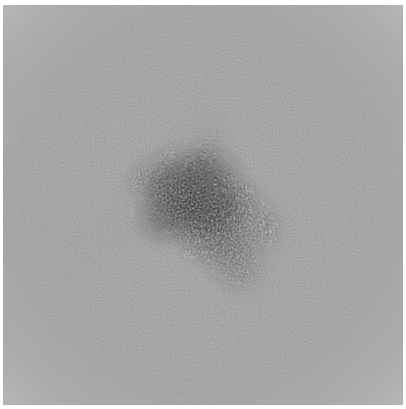
6.1.1 Primary map



X

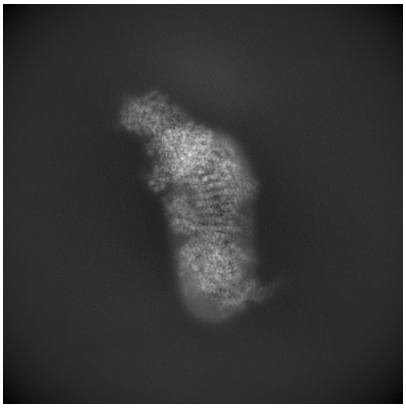


Y

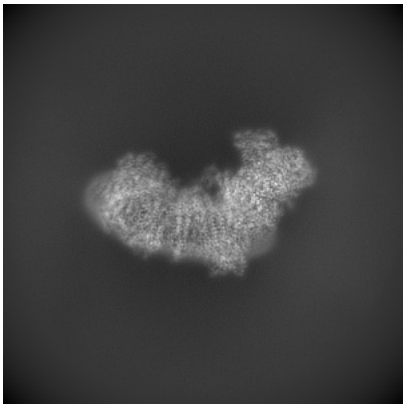


Z

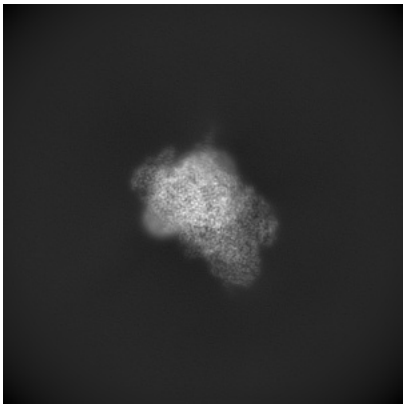
6.1.2 Raw map



X



Y

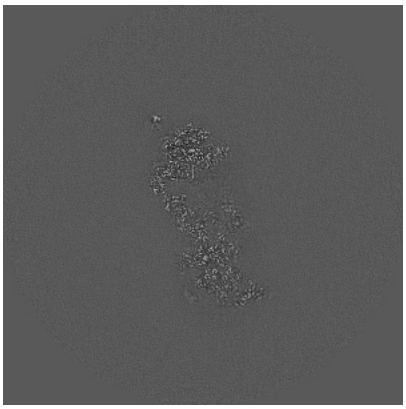


Z

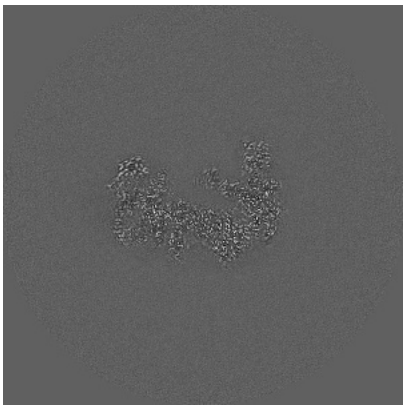
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

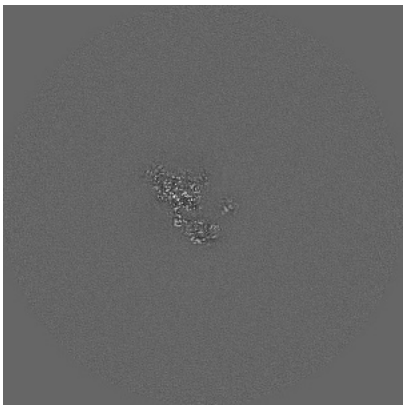
6.2.1 Primary map



X Index: 320

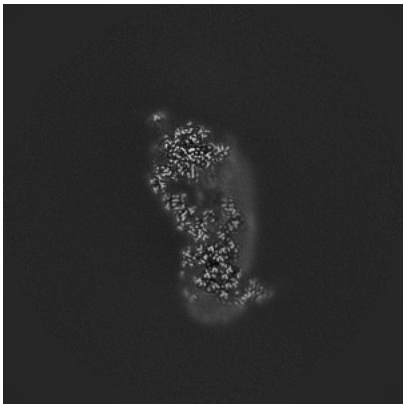


Y Index: 320

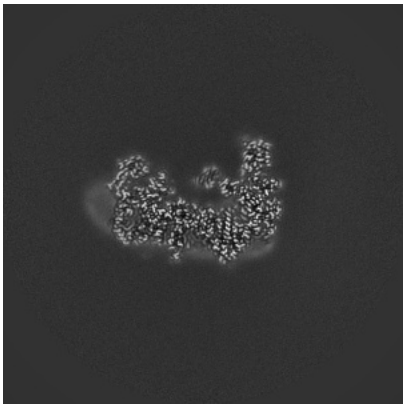


Z Index: 320

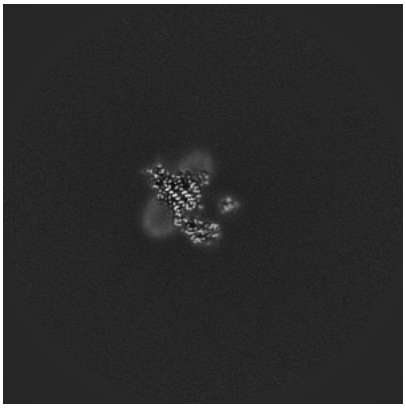
6.2.2 Raw map



X Index: 320



Y Index: 320

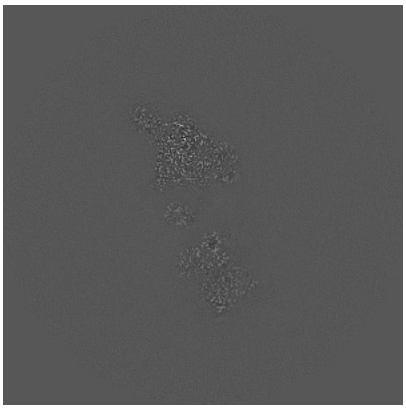


Z Index: 320

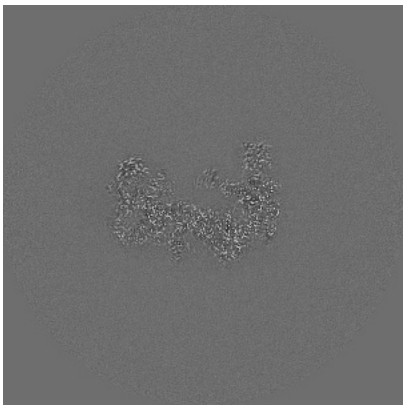
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

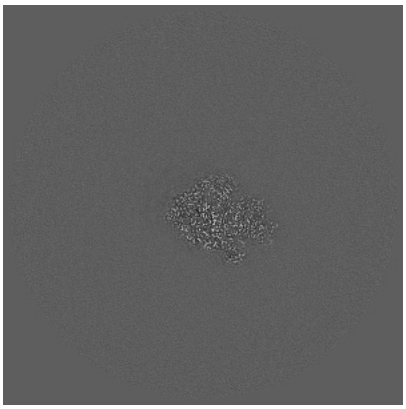
6.3.1 Primary map



X Index: 342

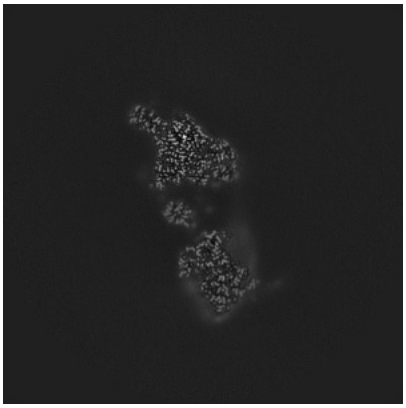


Y Index: 321

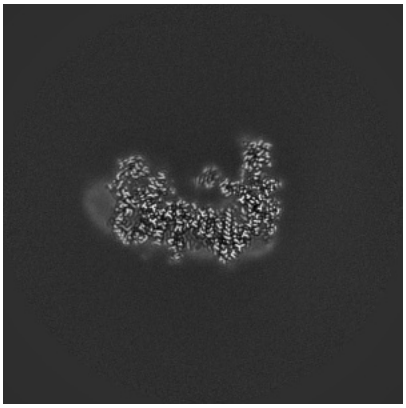


Z Index: 407

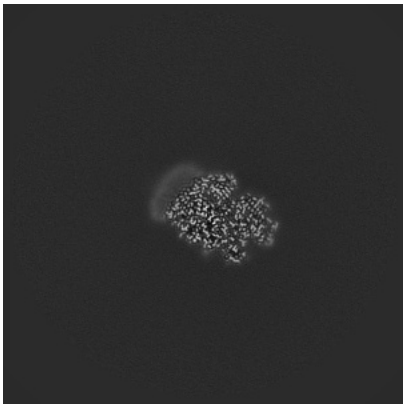
6.3.2 Raw map



X Index: 341



Y Index: 321

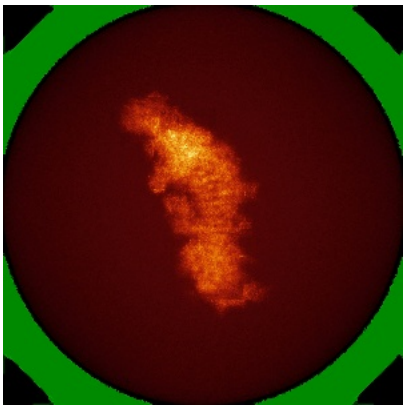


Z Index: 408

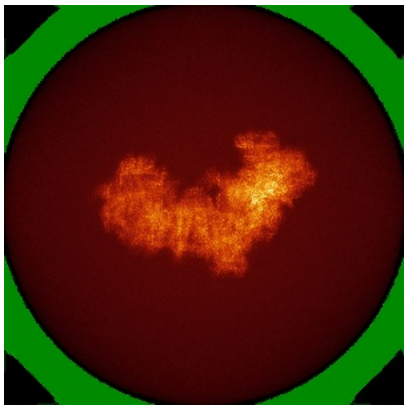
The images above show the largest variance slices of the map in three orthogonal directions.

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

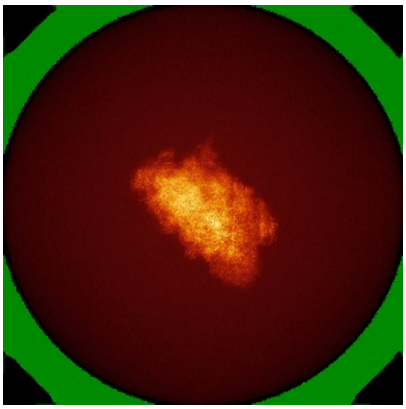
6.4.1 Primary map



X

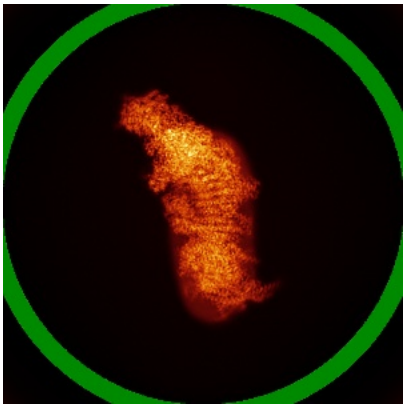


Y

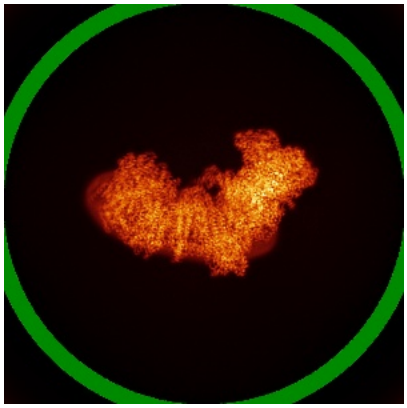


Z

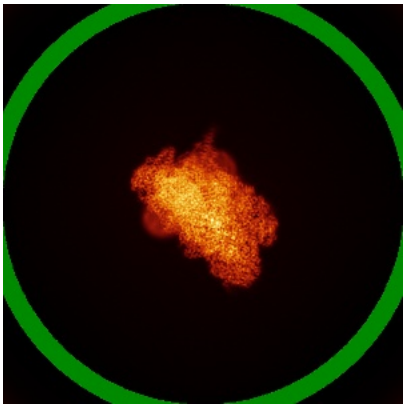
6.4.2 Raw map



X



Y

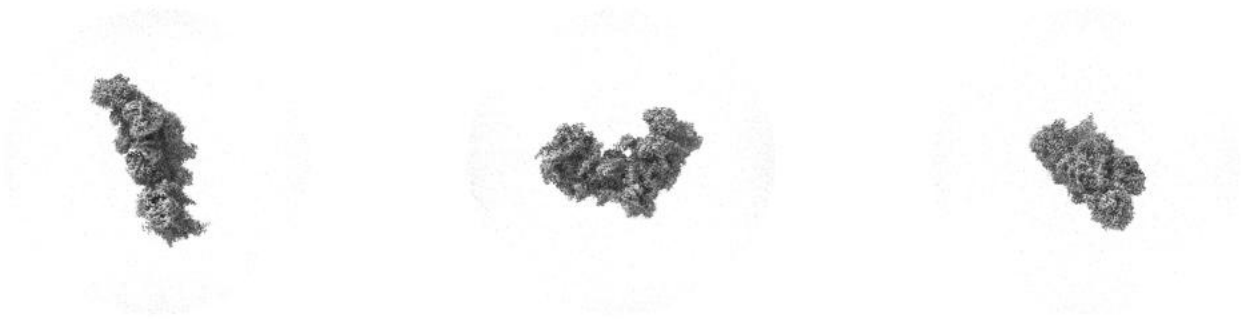


Z

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)

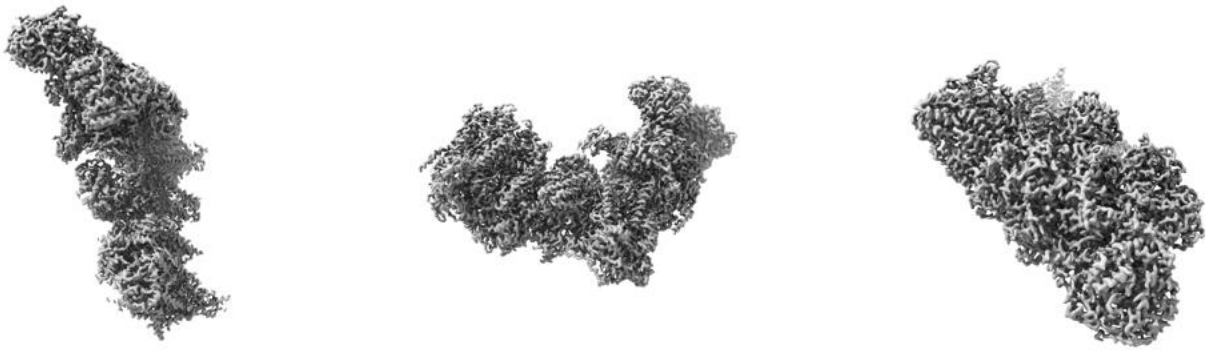
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

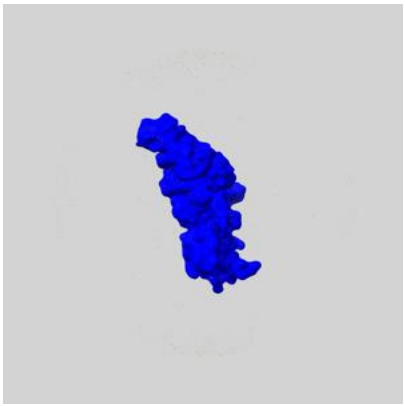
6.6 Mask visualisation

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

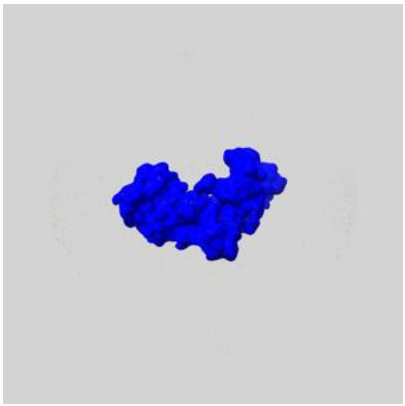
A mask typically either:

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

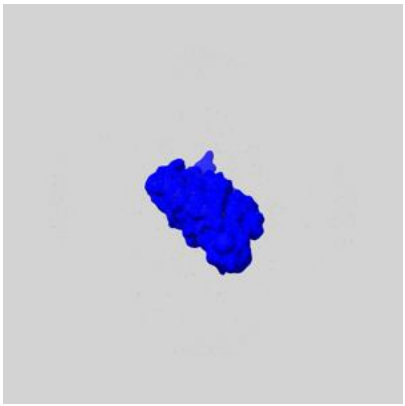
6.6.1 emd_55033_msk_1.map



X



Y

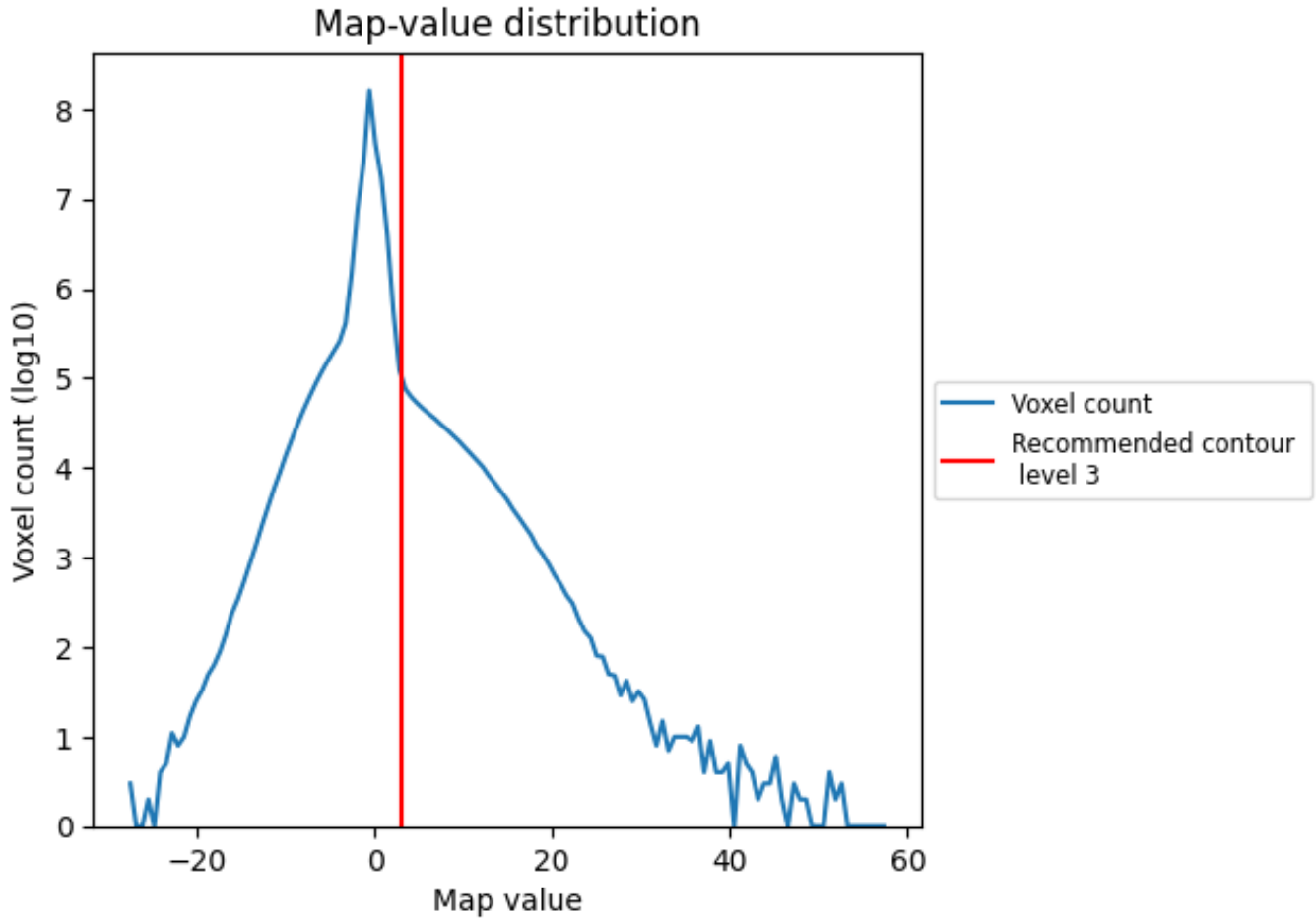


Z

7 Map analysis

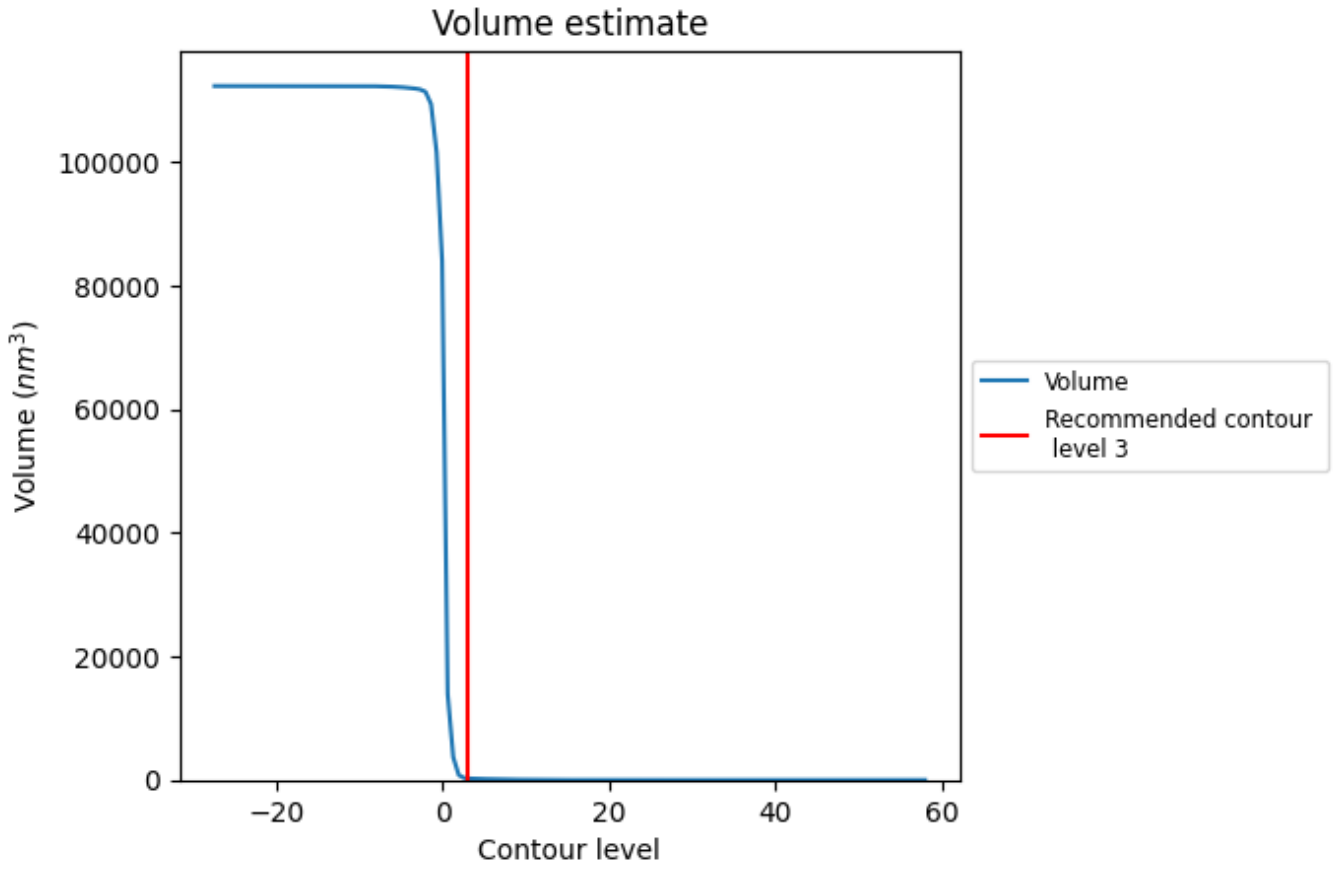
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

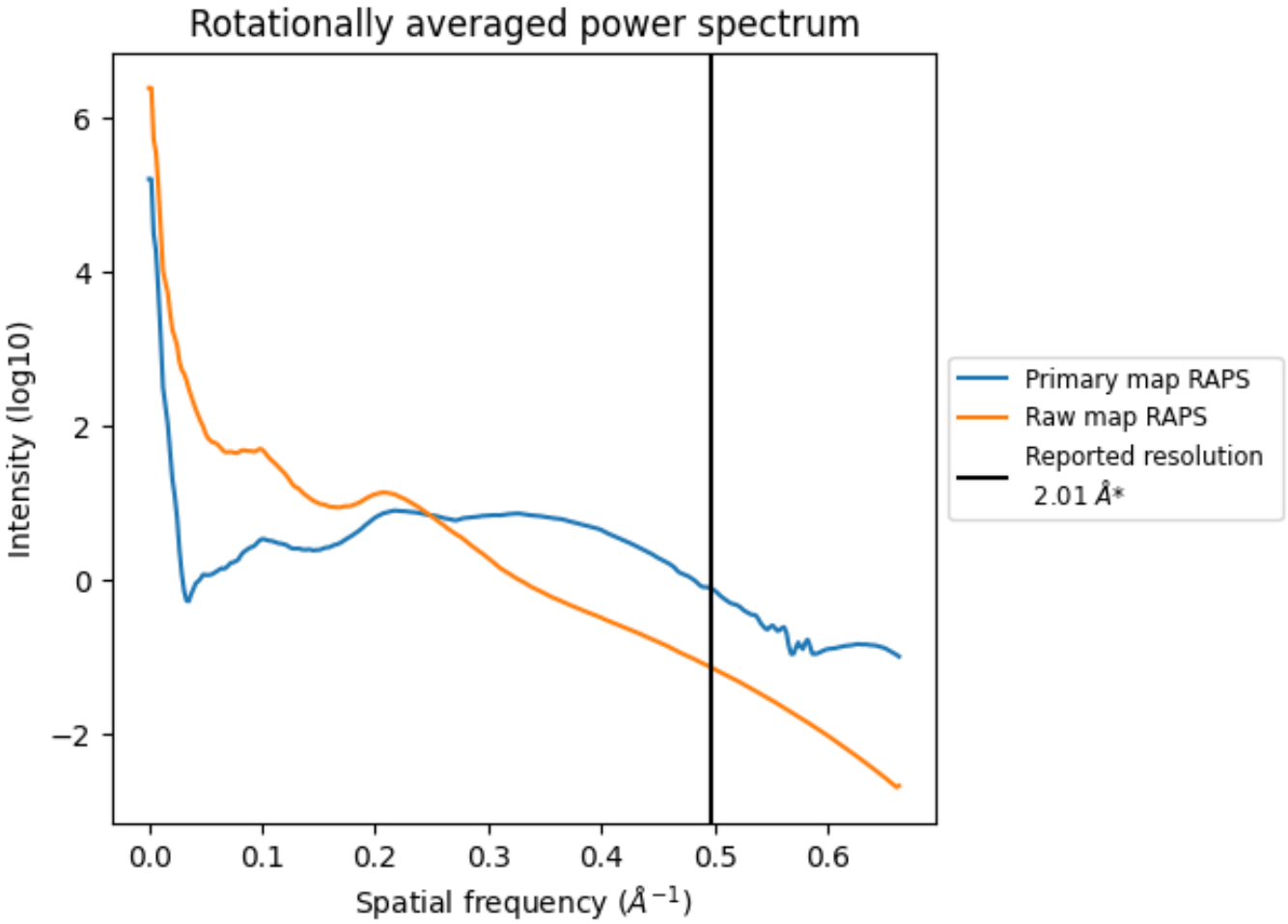
7.2 Volume estimate (i)



The volume at the recommended contour level is 259 nm^3; this corresponds to an approximate mass of 234 kDa.

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

7.3 Rotationally averaged power spectrum (i)

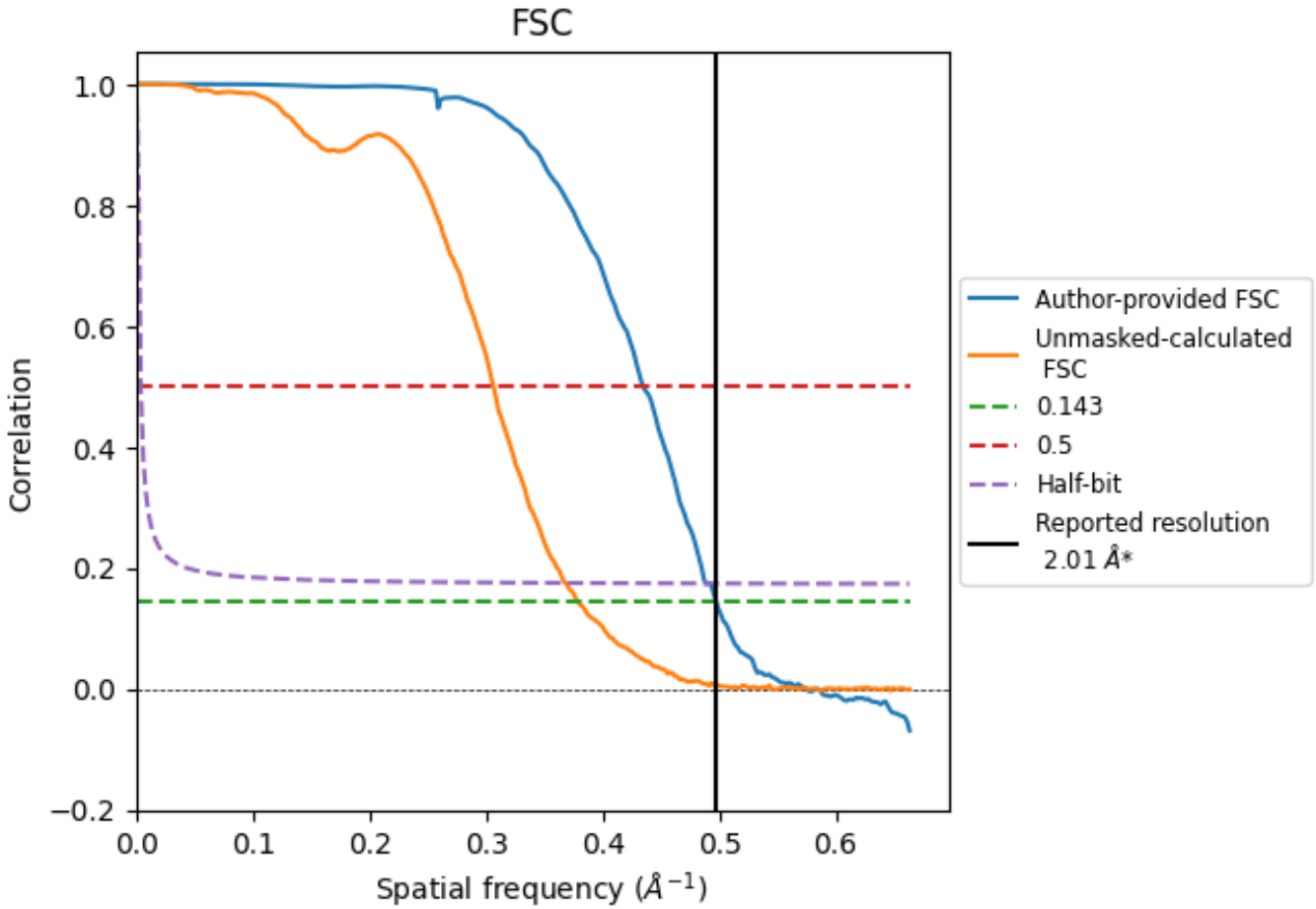


*Reported resolution corresponds to spatial frequency of 0.498 Å^{-1}

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 0.498 Å^{-1}

8.2 Resolution estimates (i)

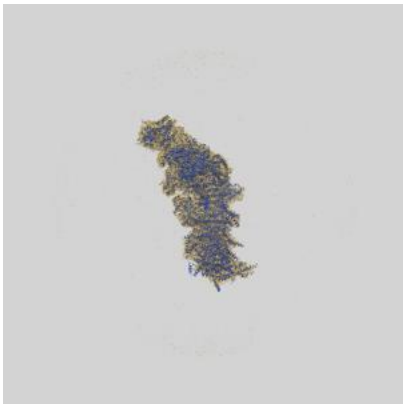
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.01	-	-
Author-provided FSC curve	2.01	2.30	2.05
Unmasked-calculated*	2.64	3.26	2.71

*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 2.64 differs from the reported value 2.01 by more than 10 %

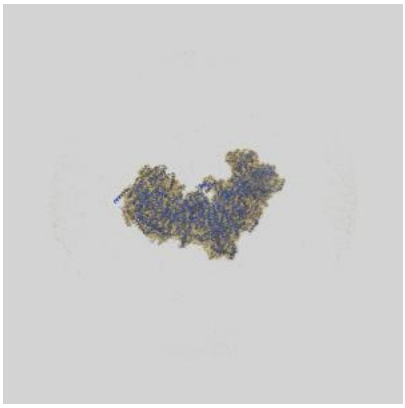
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-55033 and PDB model 9SMI. Per-residue inclusion information can be found in section 3 on page 26.

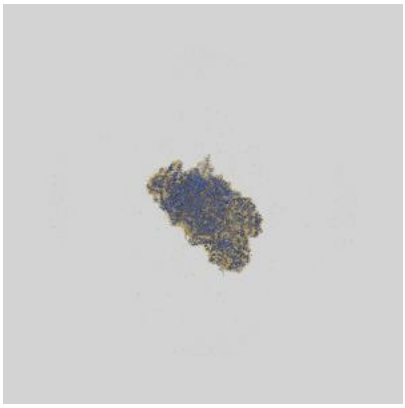
9.1 Map-model overlay



X



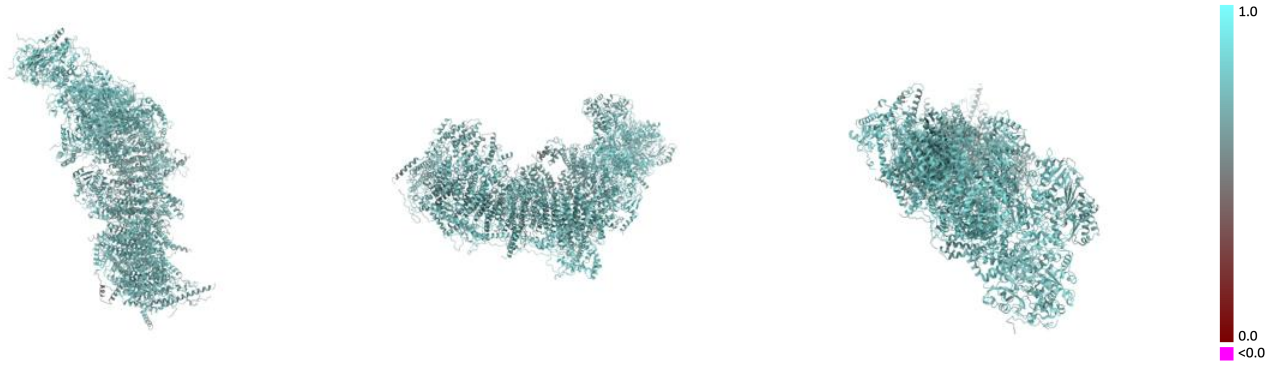
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 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.

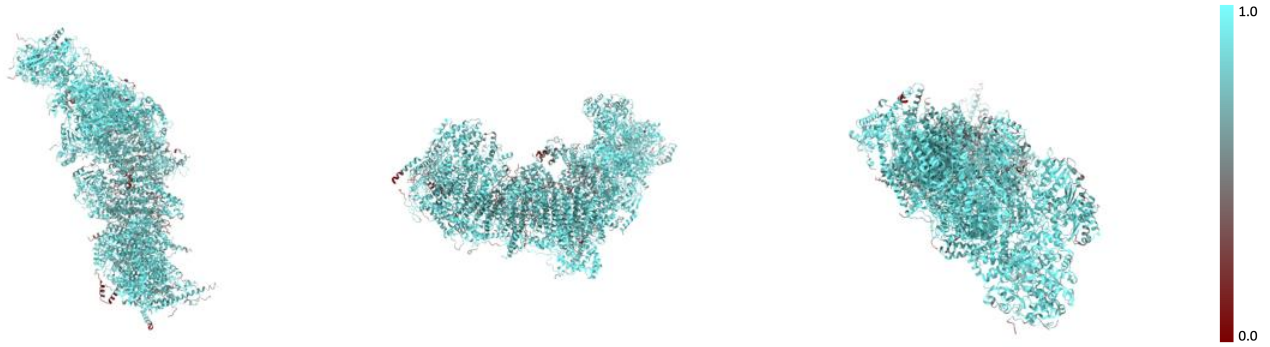
9.2 Q-score mapped to coordinate model (i)



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.

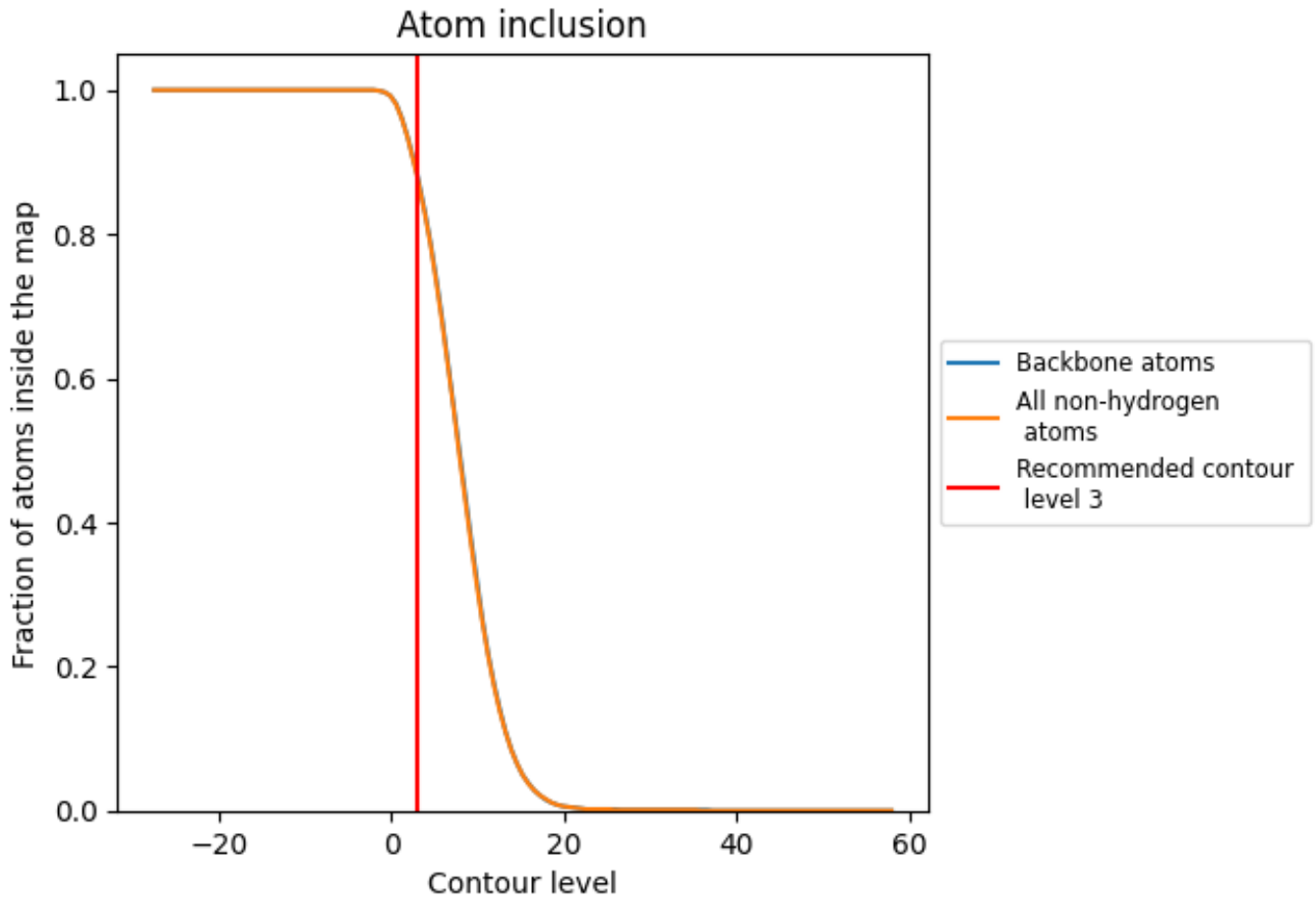
9.3 Atom inclusion mapped to coordinate model (i)



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 (3).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 88% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8810	0.7410
A	0.8400	0.7310
B	0.9320	0.7880
C	0.9700	0.7960
D	0.9440	0.7920
E	0.8630	0.7200
F	0.9210	0.7430
G	0.9240	0.7540
H	0.9550	0.7850
I	0.9720	0.8020
J	0.8460	0.7360
K	0.9490	0.7780
L	0.8870	0.7430
M	0.9430	0.7780
N	0.9400	0.7870
O	0.8880	0.7150
P	0.8000	0.6970
Q	0.9240	0.7800
R	0.8710	0.7530
S	0.8530	0.6670
T	0.6170	0.6040
U	0.8590	0.6790
V	0.8980	0.7290
W	0.8680	0.7260
X	0.8880	0.7430
Y	0.7360	0.6920
Z	0.8800	0.7380
a	0.9470	0.7630
b	0.8650	0.7380
c	0.8250	0.7120
d	0.8400	0.7330
e	0.8590	0.7390
f	0.7100	0.6950
g	0.8420	0.7280
h	0.8530	0.7440



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.6690	0.6540
j	0.7750	0.6530
k	0.7550	0.6460
l	0.8510	0.7110
m	0.8290	0.7160
n	0.8790	0.7000
o	0.7600	0.6470
p	0.8510	0.7230
q	0.9060	0.7570
r	0.9250	0.7680
s	0.8430	0.7180