wwPDB EM Validation Summary Report (i)

Aug 27, 2026 – 08:54 am BST

PDB ID	:	6ZKD / pdb_00006zkd
EMDB ID	:	EMD-11245
Title	:	Complex I during turnover, open1
Authors	:	Kampjut, D.; Sazanov, L.A.
Deposited on	:	2020-06-30
Resolution	:	2.70 Å(reported)
Based on initial model	:	5LNK

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

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

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

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

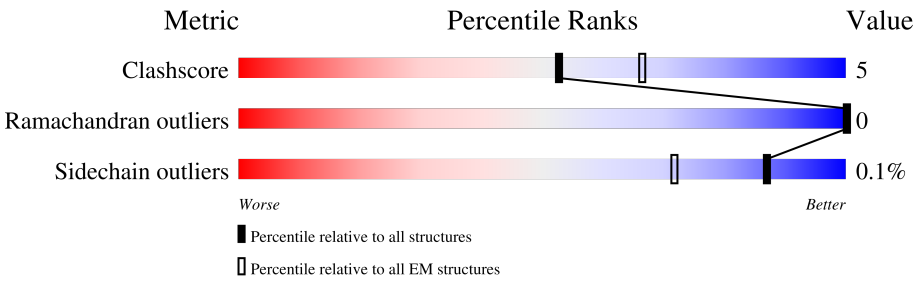
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

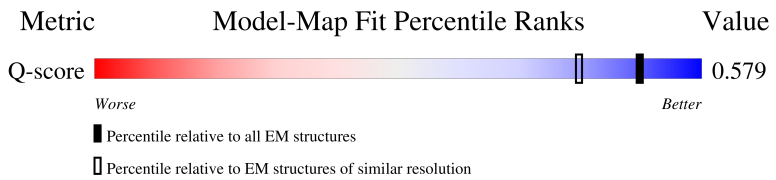
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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

Mol	Chain	Length	Quality of chain
1	1	464	78% 15% 7%
2	2	246	72% 15% 13%
3	3	727	79% 15% 5%
4	4	463	74% 17% 9%

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Mol	Chain	Length	Quality of chain
5	5	266	64% 15% 22%
6	6	223	61% 9% 30%
7	9	217	66% 15% 19%
8	A	115	5% 78% 17%
9	H	318	81% 17%
10	J	175	81% 15%
11	K	98	77% 23%
12	L	606	83% 17%
13	M	459	81% 19%
14	N	347	87% 13%
15	V	141	16% 84% 14%
16	W	189	65% 8% 26%
17	X	157	52% 45%
17	j	157	46% 6% 48%
18	Y	172	86% 13%
19	Z	175	84% 14%
20	a	109	34% 6% 60%
21	b	124	69% 8% 23%
22	c	170	66% 8% 26%
23	d	380	70% 8% 22%
24	e	99	76% 11% 13%
25	f	116	90% 8%
26	g	140	74% 8% 19%
27	h	114	75% 10% 16%
28	i	145	87% 13%

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Mol	Chain	Length	Quality of chain
29	k	355	82% 8% 10%
30	l	106	90% 9%
31	m	84	86% 10% 5%
32	n	98	77% 19%
33	o	122	81% 17%
34	p	130	90% 8%
35	q	144	85% 12%
36	r	128	70% 8% 23%
37	s	137	77% 12% 11%
38	t	179	5% 87% 12%
39	u	108	51% 9% 40%
40	v	186	70% 13% 17%
41	w	154	60% 6% 34%
42	x	76	58% 7% 36%
43	y	58	78% 9% 14%
44	z	70	93% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	CDL	L	1003	X	-	-	-
53	CDL	V	204	X	-	-	-
53	CDL	Y	201	X	-	-	-
53	CDL	o	201	X	-	-	-

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 67450 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	421	3390	2165	581	619	25	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	169	1294	870	185	226	13	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 17 is a protein called Acyl carrier protein.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

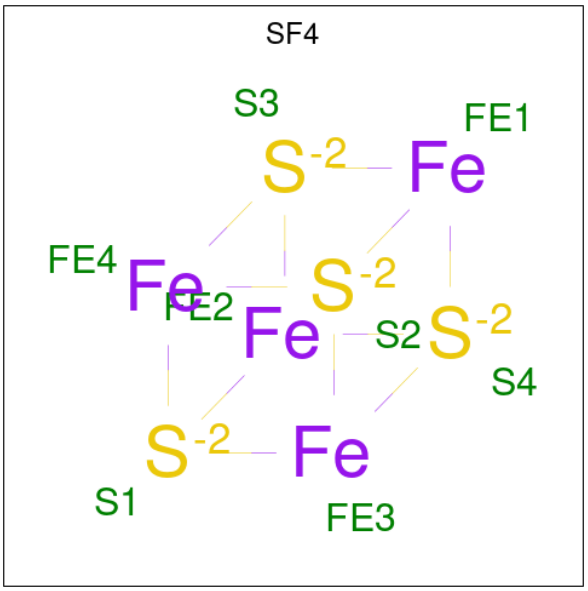
- Molecule 43 is a protein called Mitochondrial complex I, MNLL subunit.

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

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

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

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



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

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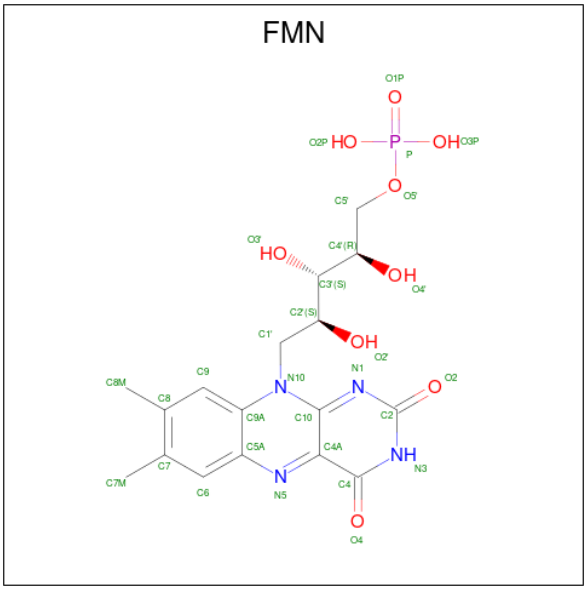
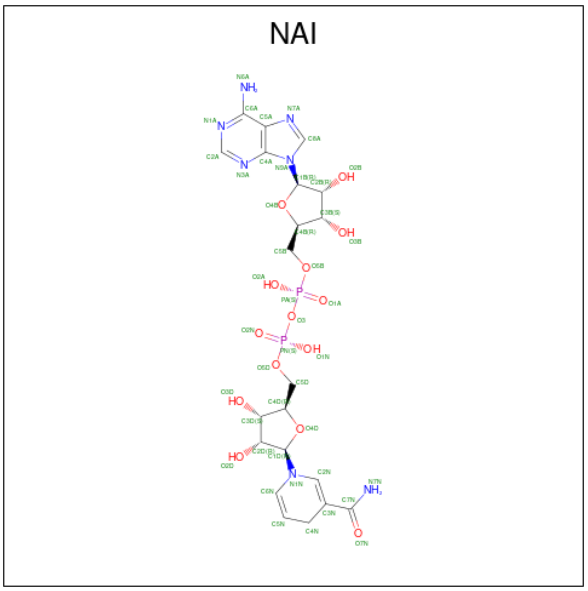
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	9	1	8	4	4	0
			Total	Fe	S	
45	9	1	8	4	4	0

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



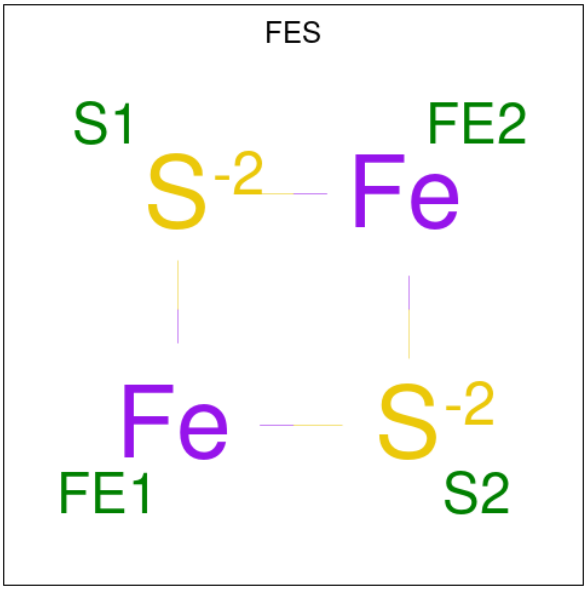
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	1	1	31	17	4	9	1	0

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



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

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

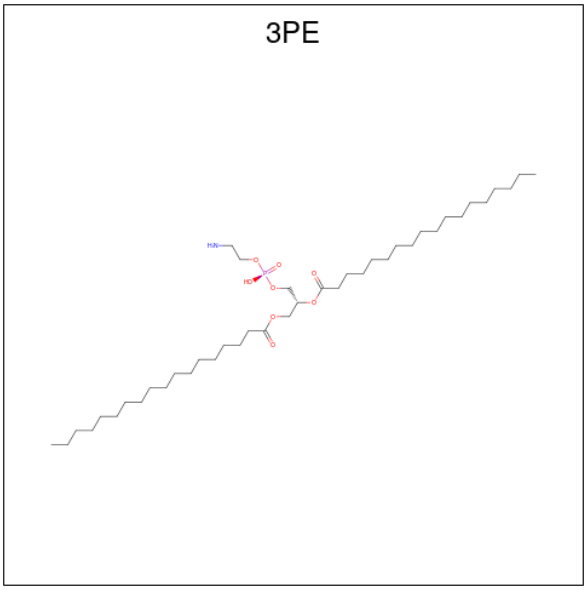


Mol	Chain	Residues	Atoms			AltConf
48	2	1	Total	Fe	S	0
			4	2	2	
48	3	1	Total	Fe	S	0
			4	2	2	

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

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

- Molecule 50 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
50	4	1	40	30	1	8	1	0
			Total	C	N	O	P	
50	A	1	51	41	1	8	1	0
			Total	C	N	O	P	
50	H	1	51	41	1	8	1	0
			Total	C	N	O	P	
50	K	1	40	30	1	8	1	0
			Total	C	N	O	P	
50	L	1	51	41	1	8	1	0
			Total	C	N	O	P	
50	L	1	31	21	1	8	1	0
			Total	C	N	O	P	
50	M	1	44	34	1	8	1	0
			Total	C	N	O	P	
50	N	1	51	41	1	8	1	0
			Total	C	N	O	P	
50	N	1	31	21	1	8	1	0
			Total	C	N	O	P	
50	V	1	35	25	1	8	1	0

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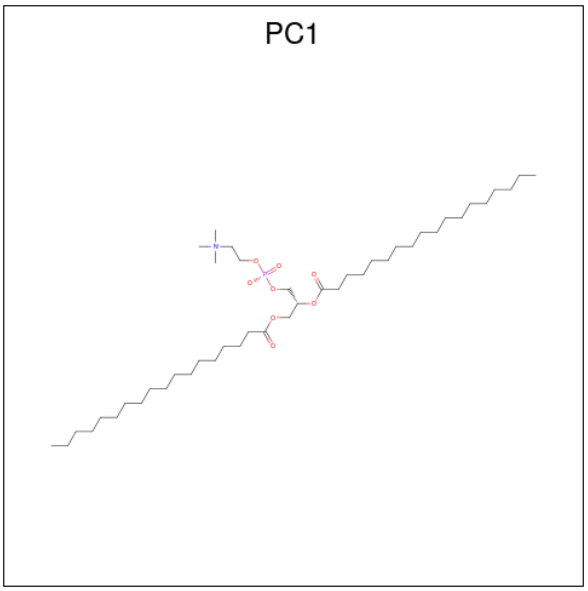
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
50	V	1	37	27	1	8	1	0
			Total	C	N	O	P	
50	i	1	51	41	1	8	1	0
			Total	C	N	O	P	
50	i	1	51	41	1	8	1	0
			Total	C	O	P		
50	p	1	27	18	8	1		0

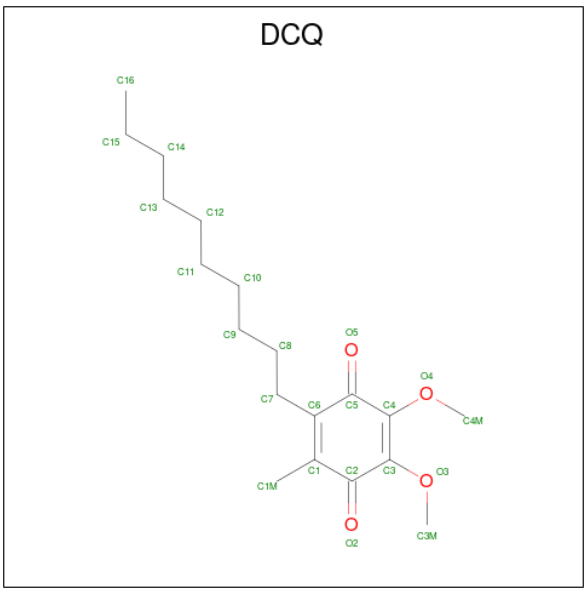
- Molecule 51 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
51	9	1	54	44	1	8	1	0
			Total	C	N	O	P	
51	A	1	46	36	1	8	1	0
			Total	C	N	O	P	
51	A	1	37	27	1	8	1	0
			Total	C	N	O	P	
51	L	1	54	44	1	8	1	0
			Total	C	N	O	P	
51	M	1	54	44	1	8	1	0
			Total	C	N	O	P	
51	w	1	54	44	1	8	1	0

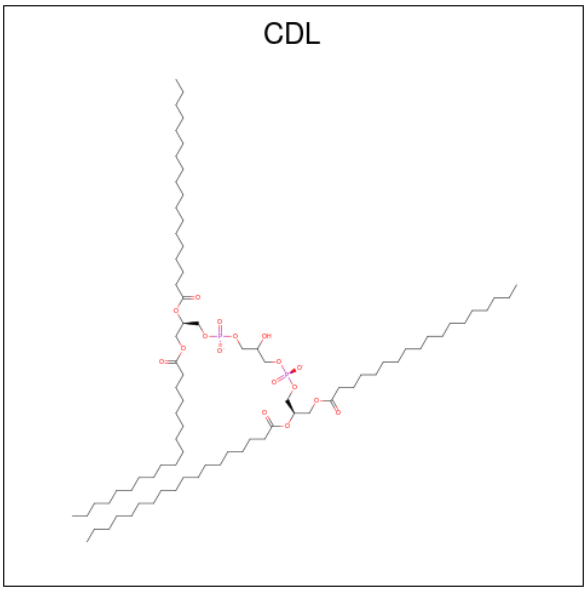
- Molecule 52 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (CCD ID:

DCQ) (formula: $C_{19}H_{30}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
52	H	1	23	19	4	0

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



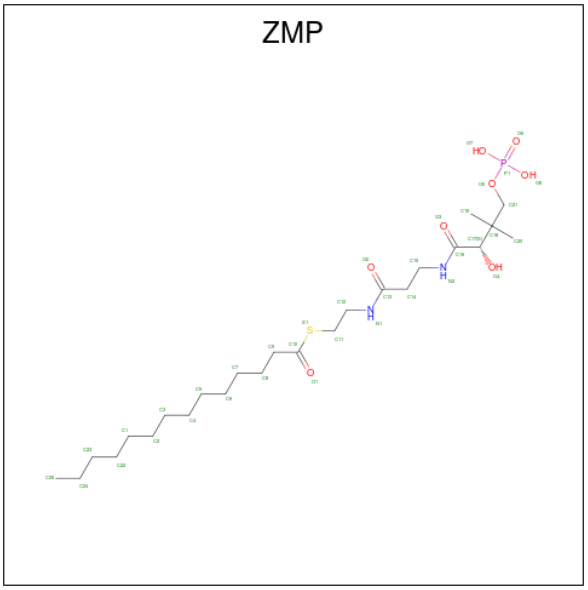
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
53	L	1	100	81	17	2	0
			Total	C	O	P	
53	V	1	94	75	17	2	0

Continued on next page...

Continued from previous page...

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

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

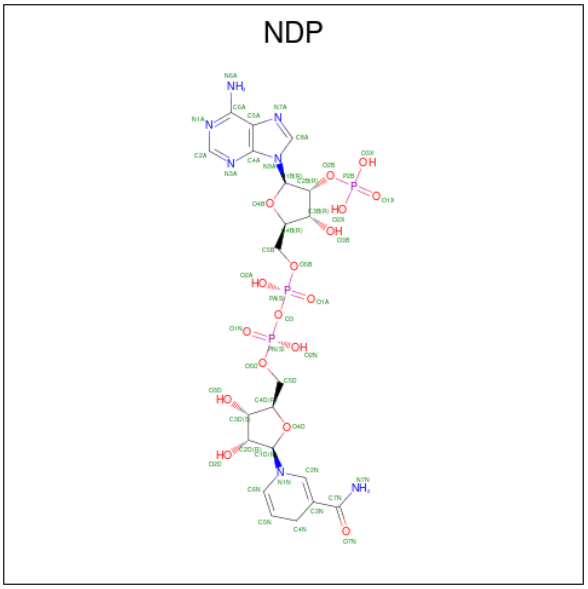


Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
54	X	1	31	20	2	7	1	1	0
			Total	C	N	O	P	S	
54	g	1	34	23	2	7	1	1	0

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

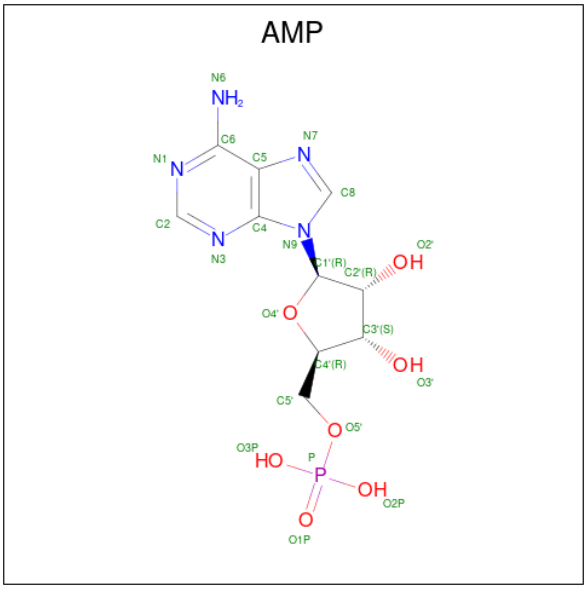
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
55	b	1	1	1	0

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



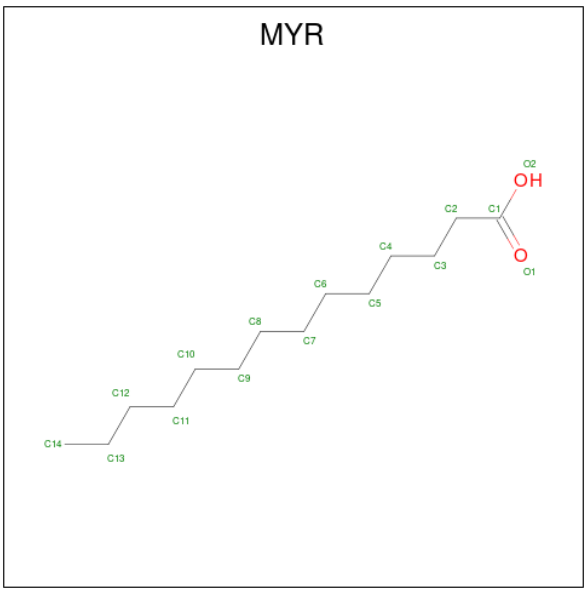
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	d	1	48	21	7	17	3	0

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



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

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



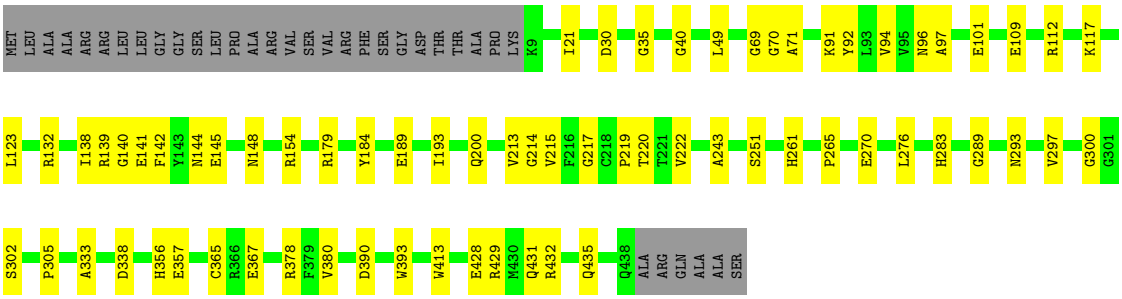
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
58	s	1	15	14	1	0

3 Residue-property plots (i)

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

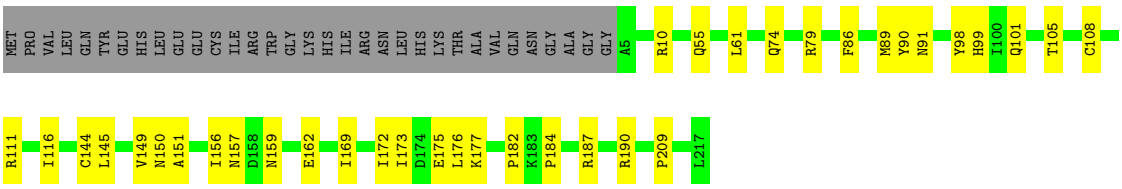
• Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1:



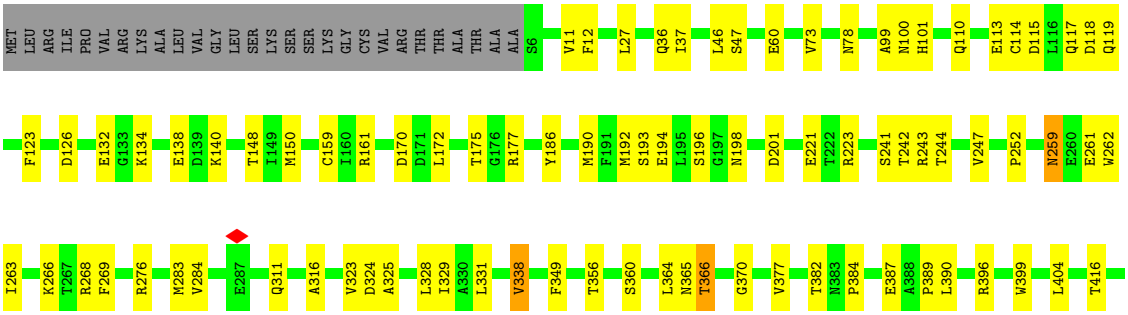
• Molecule 2: Mitochondrial complex I, 24 kDa subunit

Chain 2:



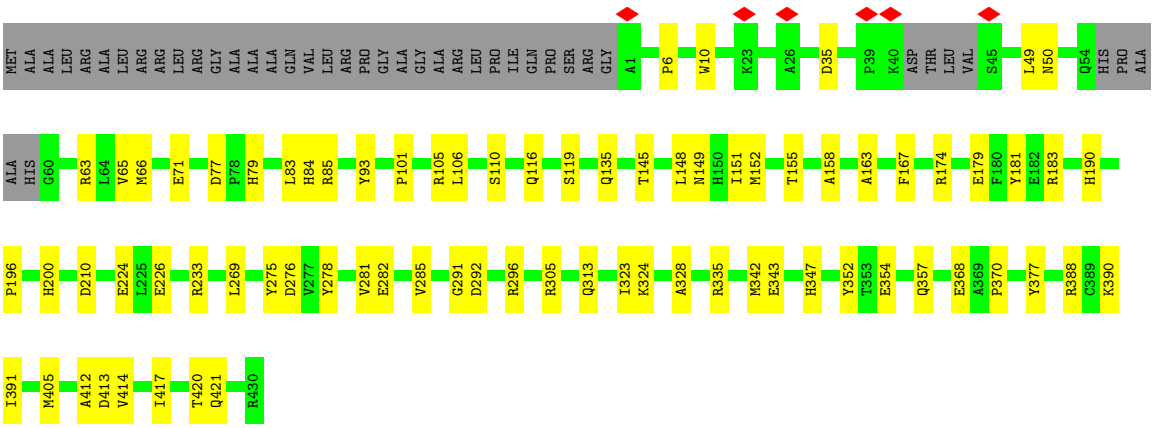
• Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

Chain 3:



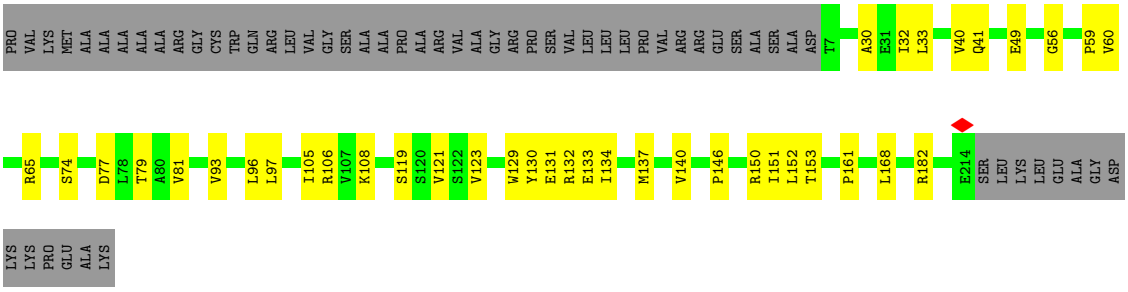
• Molecule 4: Mitochondrial complex I, 49 kDa subunit

Chain 4:



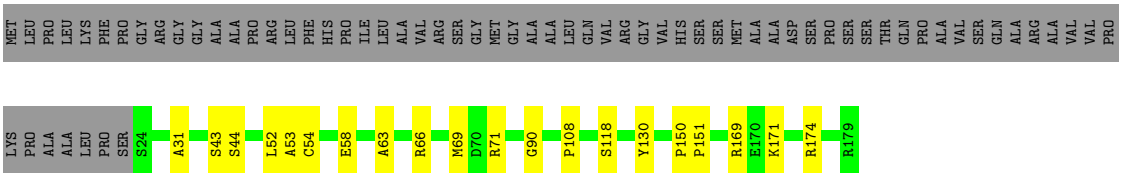
• Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3

Chain 5:



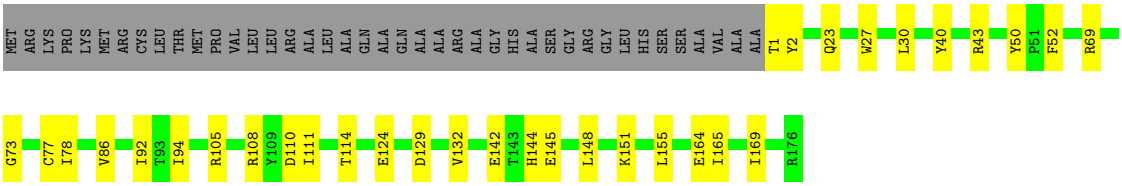
• Molecule 6: Mitochondrial complex I, PSST subunit

Chain 6:

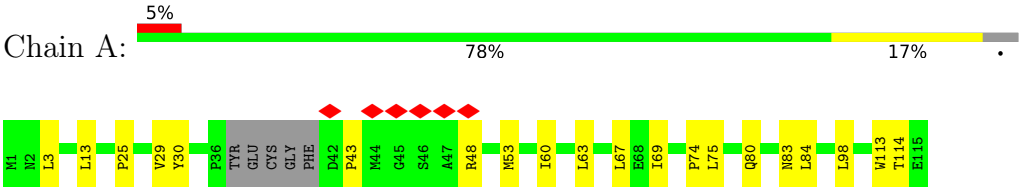


• Molecule 7: Mitochondrial complex I, TYKY subunit

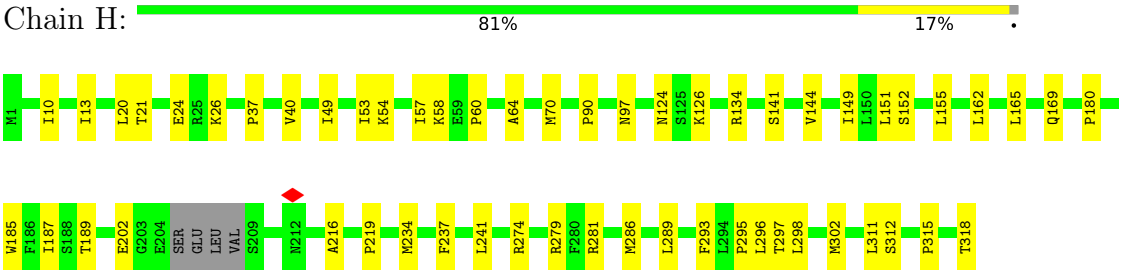
Chain 9:



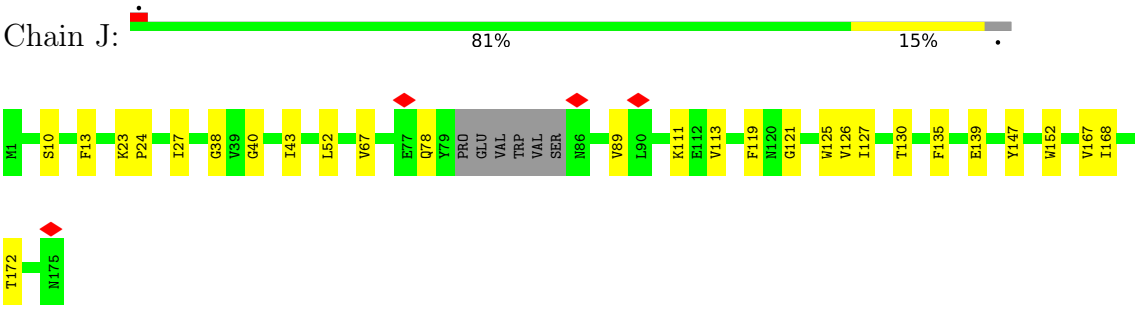
• Molecule 8: NADH-ubiquinone oxidoreductase chain 3



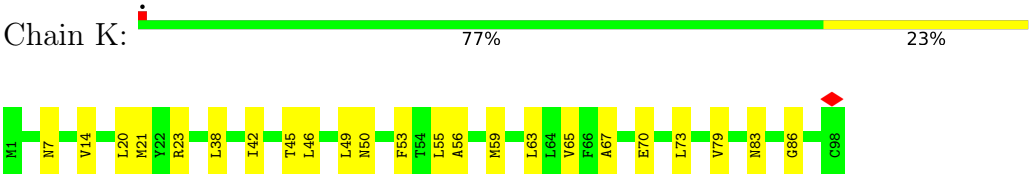
• Molecule 9: NADH-ubiquinone oxidoreductase chain 1



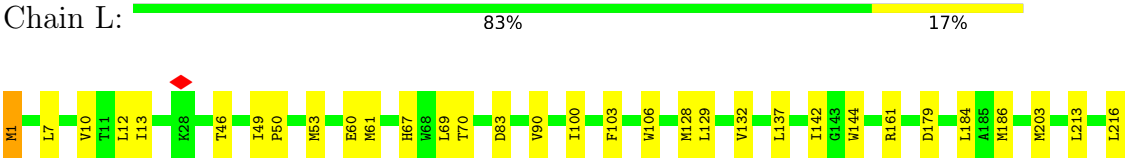
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6



• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

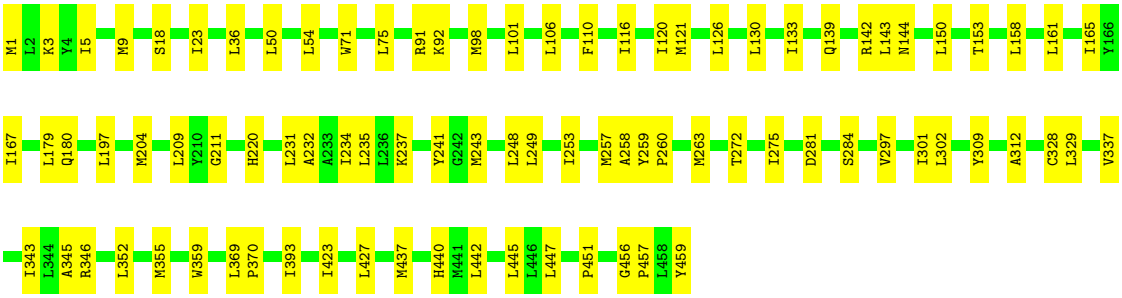


• Molecule 12: NADH-ubiquinone oxidoreductase chain 5



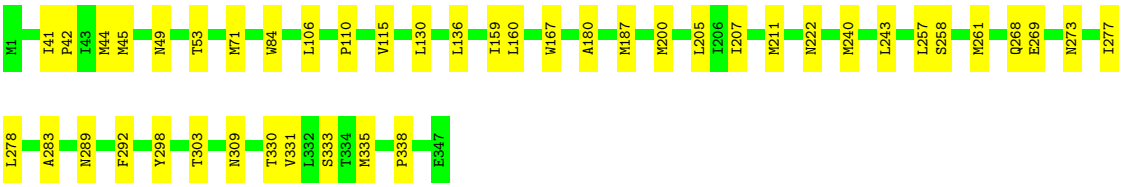
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:



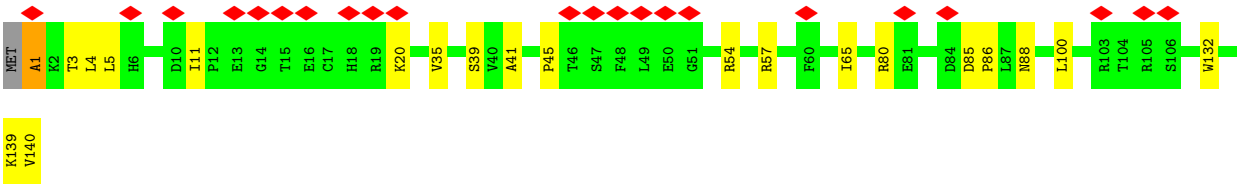
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:



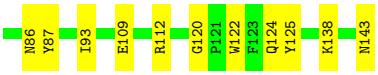
• Molecule 15: Mitochondrial complex I, B14.7 subunit

Chain V:



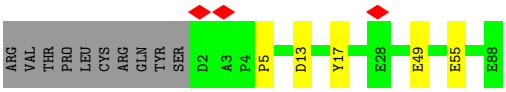
• Molecule 16: NADH:ubiquinone oxidoreductase subunit B5

Chain W:



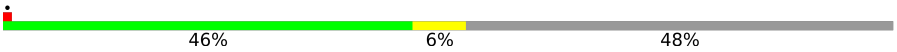
• Molecule 17: Acyl carrier protein

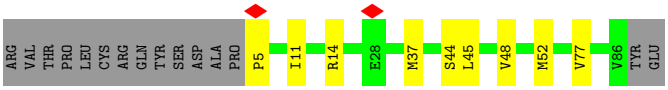
Chain X:



• Molecule 17: Acyl carrier protein

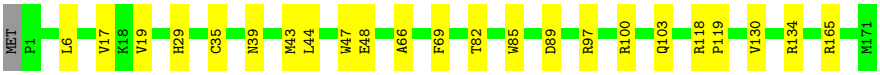
Chain j:





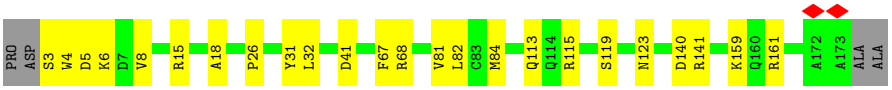
• Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain Y:



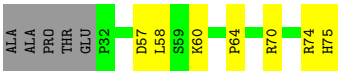
• Molecule 19: Mitochondrial complex I, PDSW subunit

Chain Z:



• Molecule 20: Mitochondrial complex I, 10 kDa subunit

Chain a:



• Molecule 21: Mitochondrial complex I, 13 kDa subunit

Chain b: 69% 8% 23%

MET ALA ALA ALA VAL THR PHE LEU ARG LEU LEU GLY ARG GLY GLY ALA VAL THR ARG GLY LEU PRO GLY GLY ALA ARG CYS PHE G1 D20 R25 Q32 K33 E34 N38 V49 C84 G85 Y86 C87 Q90 H95 HIS

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

Chain c: 66% 8% 26%

MET SER VAL ALA LEU ARG GLN ALA LEU TRP GLY ARG ARG VAL GLY THR VAL ALA ALA VAL SER VAL SER LYS VAL SER THR ARG SER LEU SER THR SER THR TRP ARG LEU ALA GLN ASP GLN THR ARG ASP T8 E28 H29 T32 R33 R42 Q46 S47 G48 F59 D60

M70 A73 D77 L82 K116 K133

• Molecule 23: NADH:ubiquinone oxidoreductase subunit A9

Chain d: 70% 8% 22%

MET ALA ALA ALA VAL HIS LEU ARG VAL VAL ARG VAL LEU PRO MET SER ARG SER SER VAL PRO ALA LEU ALA ALA SER VAL PHE HIS SER PRO PRO GLN ARG GLN L1 K10 T22 A26 G31 V47 P48 M71 D72 R83 V91 E100 D105 K128

F129 I130 L135 E155 E158 T164 K167 R186 TRP PHE GLY GLY VAL PRO LEU ILE S195 L196 G197 K198 V201 I218 A229 F230 L237 P252 PHE LEU PRO TYR PRO MET PRO HIS PHE ALA TYR ARG TRP ILE GLY ARG LEU PHE GLU ILE SER PRO PHE

GLU PRO W278 T279 T280 K283 L300 V305 E311 T323 TYR ARG TRP LEU SER SER GLU ILE GLU ASP V334 Q335 P336 V340 PRO ALA SER GLY PRO

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

Chain e: 76% 11% 13%

MET ALA ALA ALA ALA ALA ILE ARG GLY VAL ARG GLY LYS L13 E17 I18 R19 C23 Q24 Y40 L43 C57 S58 D59 W65 A66 R67 E73 A98

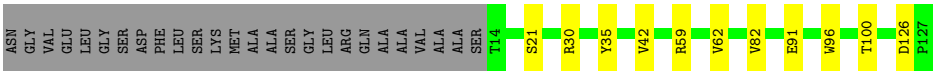
• Molecule 25: Mitochondrial complex I, B13 subunit

Chain f: 90% 8%

MET ALA GLY L3 L4 K5 L34 I37 Y43 R44 Q49 E68 L71 V79 I115

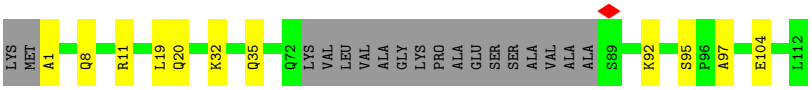
• Molecule 26: NADH:ubiquinone oxidoreductase subunit A6

Chain g: 74% 8% 19%



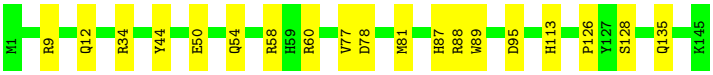
• Molecule 27: Mitochondrial complex I, B14.5a subunit

Chain h:



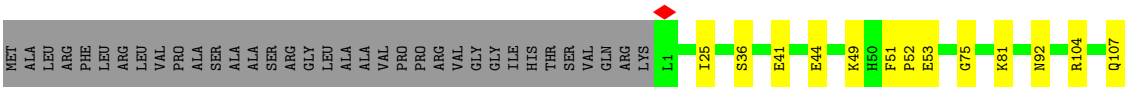
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain i:



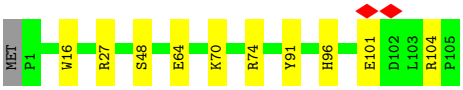
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain k:



• Molecule 30: NADH:ubiquinone oxidoreductase subunit S5

Chain l:

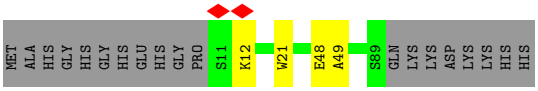


• Molecule 31: NADH:ubiquinone oxidoreductase subunit A3

Chain m:

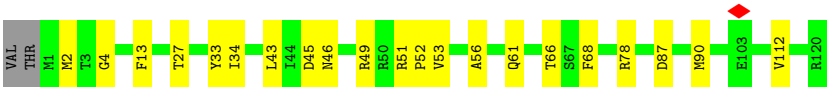
• Molecule 32: NADH:ubiquinone oxidoreductase subunit B3

Chain n:



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

Chain o:

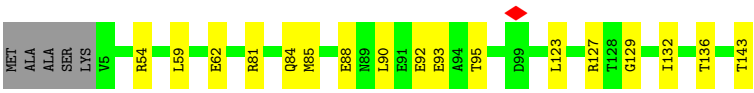


• Molecule 34: NADH:ubiquinone oxidoreductase subunit B4

Chain p:

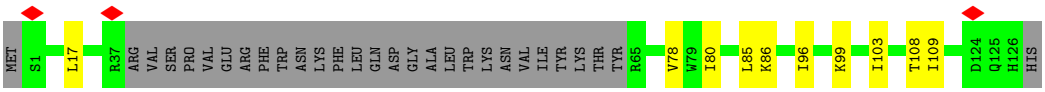
• Molecule 35: Mitochondrial complex I, B16.6 subunit

Chain q:



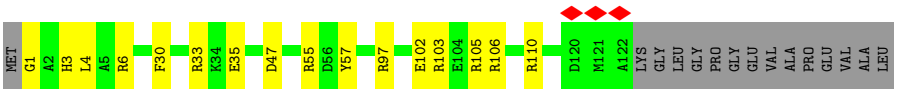
• Molecule 36: Mitochondrial complex I, B17 subunit

Chain r:



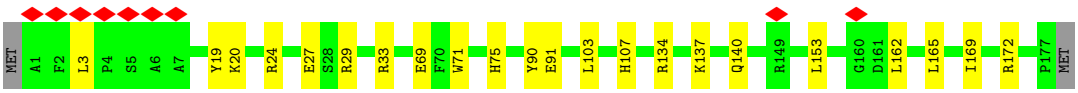
• Molecule 37: NADH:ubiquinone oxidoreductase subunit B7

Chain s:



• Molecule 38: NADH:ubiquinone oxidoreductase subunit B9

Chain t:



• Molecule 39: NADH:ubiquinone oxidoreductase subunit B2

Chain u: 51% 9% 40%

MET ALA GLY MET SER ALA LEU LYS ARG LEU ALA PRO PHE ALA HIS VAL GLY GLY HIS LEU PHE ARG GLY ARG CYS ALA ARG ALA VAL GLY ALA GLY GLY VAL ARG ARG ALA GLY GLY GLY **A5 H6** I7 R10 P15 Q16 L17 T18 R19 S20 G49 D61 I66 D69

ASP GLU ASP

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

Chain v: 70% 13% 17%

MET ALA ALA ARG ALA GLY VAL LEU GLY ILE ARG TRP LEU GLN LYS ALA ALA ARG ASN VAL VAL PRO LEU GLY ALA ARG THR ALA SER HIS **I4** M8 Y44 Y47 P48 D52 **R53** S54 D68 L71 M77 H78 **W79** D80 M83 Y84 **I85** R86 **N87** R88 V89

D90 M112 T124 P127 V128 D145 **E149 P150 E151** H155 Y156 **E157 I158**

• Molecule 41: Mitochondrial complex I, ESSS subunit

Chain w: 60% 6% 34%

MET ALA ALA GLY MET LEU GLY LEU CYS GLY ARG ARG LEU LEU ALA VAL ALA ALA THR ARG GLY LEU PRO ALA ALA SER VAL ARG TRP GLU SER SER SER SER ARG ALA VAL ILE ALA PRO SER THR LEU ALA GLY LYS ARG PRO SER GLU PRO **T23 L24** **E33** D43 V69

R84 R100 L105 **P106** L107 C112 **F113** D114 K117 **D123** GLU ASP

• Molecule 42: Mitochondrial complex I, KFYI subunit

Chain x: 58% 7% 36%

MET ALA PRO SER ALA PHE LEU ARG PRO PHE TRP LYS LEU LEU ALA PRO ALA ARG PHE PRO SER VAL SER SER SER ARG SER **K1** P7 P8 W28 E41 R44 **E49**

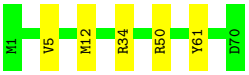
• Molecule 43: Mitochondrial complex I, MNLL subunit

Chain y: 78% 9% 14%

MET MET ASN LEU LEU GLN VAL VAL R8 **D9 H10** P17 F20 L43 **Q51** **K57**

• Molecule 44: Mitochondrial complex I, MWFE subunit

Chain z: 93% 7%


M1
V5
M12
R34
R50
Y61
D70

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81780	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.370	Depositor
Minimum map value	-0.140	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	170.821, 196.285, 286.47	wwPDB
Map dimensions	270, 185, 161	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	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: PC1, CDL, NDP, AYA, K, ZN, SEP, FMN, NAI, MYR, FES, 2MR, DCQ, ZMP, SF4, 3PE, AMP, FME

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	1	0.33	0/3386	0.58	0/4575
2	2	0.32	0/1695	0.58	0/2306
3	3	0.34	0/5362	0.57	3/7266 (0.0%)
4	4	0.36	0/3463	0.57	0/4687
5	5	0.36	0/1776	0.56	0/2417
6	6	0.40	0/1278	0.56	0/1728
7	9	0.41	0/1445	0.58	0/1956
8	A	0.31	0/902	0.64	0/1234
9	H	0.37	0/2572	0.65	2/3517 (0.1%)
10	J	0.31	0/1324	0.63	0/1790
11	K	0.36	0/749	0.62	0/1014
12	L	0.29	0/4924	0.57	0/6698
13	M	0.34	0/3731	0.59	0/5085
14	N	0.35	0/2787	0.58	0/3795
15	V	0.19	0/1041	0.45	0/1412
16	W	0.26	0/1188	0.49	0/1607
17	X	0.19	0/713	0.43	0/963
17	j	0.22	0/670	0.48	0/902
18	Y	0.28	0/1440	0.53	0/1942
19	Z	0.25	0/1475	0.48	0/1989
20	a	0.23	0/383	0.40	0/518
21	b	0.29	0/749	0.46	0/1009
22	c	0.33	0/1047	0.48	0/1415
23	d	0.29	0/2424	0.50	0/3276
24	e	0.25	0/702	0.50	0/945
25	f	0.26	0/937	0.51	0/1271
26	g	0.28	0/993	0.53	0/1336
27	h	0.32	0/779	0.53	0/1053
28	i	0.30	0/1250	0.47	0/1698
29	k	0.25	0/2646	0.45	0/3579
30	l	0.28	0/896	0.51	0/1200

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	m	0.25	0/647	0.50	0/890
32	n	0.18	0/653	0.39	0/882
33	o	0.25	0/1035	0.48	0/1398
34	p	0.22	0/1085	0.47	0/1467
35	q	0.26	0/1171	0.49	0/1579
36	r	0.23	0/874	0.49	0/1188
37	s	0.20	0/1072	0.48	0/1436
38	t	0.22	0/1573	0.52	0/2130
39	u	0.19	0/590	0.45	0/810
40	v	0.22	0/1361	0.46	0/1861
41	w	0.25	0/872	0.53	0/1185
42	x	0.21	0/425	0.41	0/576
43	y	0.25	0/449	0.54	0/605
44	z	0.35	0/591	0.57	0/795
All	All	0.30	0/67125	0.54	5/90985 (0.0%)

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

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	H	90	PRO	CA-C-N	-7.08	114.73	122.59
9	H	90	PRO	C-N-CA	-7.08	114.73	122.59
3	3	338	VAL	N-CA-C	-6.92	105.60	112.17
3	3	366	THR	CA-C-N	6.42	133.79	121.54
3	3	366	THR	C-N-CA	6.42	133.79	121.54

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3312	0	3269	45	0
2	2	1655	0	1668	24	0
3	3	5275	0	5300	72	0
4	4	3390	0	3333	54	0
5	5	1726	0	1676	22	0
6	6	1247	0	1259	16	0
7	9	1414	0	1371	29	0
8	A	880	0	920	19	0
9	H	2498	0	2609	45	0
10	J	1294	0	1317	24	0
11	K	749	0	793	22	0
12	L	4806	0	4945	73	0
13	M	3647	0	3849	62	0
14	N	2723	0	2930	33	0
15	V	1028	0	1036	16	0
16	W	1155	0	1177	13	0
17	X	701	0	692	6	0
17	j	660	0	663	5	0
18	Y	1403	0	1392	17	0
19	Z	1441	0	1419	19	0
20	a	371	0	344	5	0
21	b	737	0	710	7	0
22	c	1024	0	1023	12	0
23	d	2372	0	2407	18	0
24	e	691	0	706	8	0
25	f	917	0	958	6	0
26	g	969	0	980	8	0
27	h	769	0	780	8	0
28	i	1209	0	1182	13	0
29	k	2596	0	2559	17	0
30	l	874	0	869	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	m	626	0	635	6	0
32	n	634	0	616	3	0
33	o	1004	0	995	16	0
34	p	1059	0	1062	10	0
35	q	1142	0	1137	16	0
36	r	846	0	864	9	0
37	s	1047	0	1015	14	0
38	t	1520	0	1477	21	0
39	u	563	0	509	7	0
40	v	1307	0	1207	21	0
41	w	846	0	792	9	0
42	x	412	0	411	3	0
43	y	436	0	437	4	0
44	z	576	0	570	5	0
45	1	8	0	0	1	0
45	3	16	0	0	0	0
45	6	8	0	0	1	0
45	9	16	0	0	0	0
46	1	31	0	19	1	0
47	1	44	0	27	6	0
48	2	4	0	0	1	0
48	3	4	0	0	0	0
49	3	1	0	0	0	0
50	4	40	0	54	1	0
50	A	51	0	82	2	0
50	H	51	0	82	2	0
50	K	40	0	54	4	0
50	L	82	0	118	2	0
50	M	44	0	65	3	0
50	N	82	0	118	1	0
50	V	72	0	92	5	0
50	i	102	0	164	2	0
50	p	27	0	27	0	0
51	9	54	0	88	4	0
51	A	83	0	117	3	0
51	L	54	0	88	7	0
51	M	54	0	88	5	0
51	w	54	0	88	7	0
52	H	23	0	30	2	0
53	L	100	0	156	6	0
53	V	179	0	261	4	0
53	W	100	0	156	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	Y	100	0	156	9	0
53	o	165	0	230	10	0
53	z	58	0	60	0	0
54	X	31	0	34	1	0
54	g	34	0	40	1	0
55	b	1	0	0	0	0
56	d	48	0	26	0	0
57	k	23	0	12	0	0
58	s	15	0	27	0	0
All	All	67450	0	68422	720	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 5.

The worst 5 of 720 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)
37:s:57:TYR:HH	40:v:155:HIS:HD1	1.32	0.74
4:4:152:MET:HE2	4:4:174:ARG:HH12	1.58	0.69
9:H:97:ASN:H	35:q:143:THR:HG22	1.58	0.68
44:z:34:ARG:NH2	44:z:61:TYR:O	2.28	0.66
31:m:83:LEU:HD13	35:q:54:ARG:HD3	1.78	0.65

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	428/464 (92%)	405 (95%)	23 (5%)	0	100 100
2	2	211/246 (86%)	196 (93%)	15 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	3	686/727 (94%)	660 (96%)	26 (4%)	0	100	100
4	4	414/463 (89%)	397 (96%)	17 (4%)	0	100	100
5	5	206/266 (77%)	199 (97%)	7 (3%)	0	100	100
6	6	154/223 (69%)	150 (97%)	4 (3%)	0	100	100
7	9	174/217 (80%)	167 (96%)	7 (4%)	0	100	100
8	A	106/115 (92%)	94 (89%)	12 (11%)	0	100	100
9	H	310/318 (98%)	304 (98%)	6 (2%)	0	100	100
10	J	165/175 (94%)	159 (96%)	6 (4%)	0	100	100
11	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
12	L	604/606 (100%)	578 (96%)	26 (4%)	0	100	100
13	M	457/459 (100%)	452 (99%)	5 (1%)	0	100	100
14	N	345/347 (99%)	336 (97%)	9 (3%)	0	100	100
15	V	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
16	W	137/189 (72%)	136 (99%)	1 (1%)	0	100	100
17	X	85/157 (54%)	82 (96%)	3 (4%)	0	100	100
17	j	80/157 (51%)	78 (98%)	2 (2%)	0	100	100
18	Y	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
19	Z	169/175 (97%)	166 (98%)	3 (2%)	0	100	100
20	a	42/109 (38%)	41 (98%)	1 (2%)	0	100	100
21	b	93/124 (75%)	92 (99%)	1 (1%)	0	100	100
22	c	124/170 (73%)	121 (98%)	3 (2%)	0	100	100
23	d	289/380 (76%)	285 (99%)	4 (1%)	0	100	100
24	e	84/99 (85%)	81 (96%)	3 (4%)	0	100	100
25	f	111/116 (96%)	110 (99%)	1 (1%)	0	100	100
26	g	112/140 (80%)	108 (96%)	4 (4%)	0	100	100
27	h	92/114 (81%)	87 (95%)	5 (5%)	0	100	100
28	i	143/145 (99%)	142 (99%)	1 (1%)	0	100	100
29	k	317/355 (89%)	302 (95%)	15 (5%)	0	100	100
30	l	103/106 (97%)	99 (96%)	4 (4%)	0	100	100
31	m	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
32	n	77/98 (79%)	75 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	o	118/122 (97%)	116 (98%)	2 (2%)	0	100	100
34	p	126/130 (97%)	122 (97%)	4 (3%)	0	100	100
35	q	137/144 (95%)	134 (98%)	3 (2%)	0	100	100
36	r	95/128 (74%)	89 (94%)	6 (6%)	0	100	100
37	s	120/137 (88%)	113 (94%)	7 (6%)	0	100	100
38	t	175/179 (98%)	172 (98%)	3 (2%)	0	100	100
39	u	63/108 (58%)	60 (95%)	3 (5%)	0	100	100
40	v	153/186 (82%)	145 (95%)	8 (5%)	0	100	100
41	w	99/154 (64%)	94 (95%)	5 (5%)	0	100	100
42	x	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
43	y	48/58 (83%)	47 (98%)	1 (2%)	0	100	100
44	z	68/70 (97%)	68 (100%)	0	0	100	100
All	All	8048/9247 (87%)	7775 (97%)	273 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	344/368 (94%)	344 (100%)	0	100	100
2	2	183/210 (87%)	183 (100%)	0	100	100
3	3	578/608 (95%)	578 (100%)	0	100	100
4	4	363/391 (93%)	363 (100%)	0	100	100
5	5	189/230 (82%)	189 (100%)	0	100	100
6	6	132/181 (73%)	131 (99%)	1 (1%)	73	88
7	9	151/179 (84%)	150 (99%)	1 (1%)	76	90
8	A	99/103 (96%)	98 (99%)	1 (1%)	68	86
9	H	274/278 (99%)	274 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	138/144 (96%)	138 (100%)	0	100	100
11	K	86/86 (100%)	86 (100%)	0	100	100
12	L	538/538 (100%)	538 (100%)	0	100	100
13	M	411/411 (100%)	410 (100%)	1 (0%)	87	95
14	N	315/315 (100%)	315 (100%)	0	100	100
15	V	101/102 (99%)	101 (100%)	0	100	100
16	W	122/160 (76%)	122 (100%)	0	100	100
17	X	80/141 (57%)	80 (100%)	0	100	100
17	j	76/141 (54%)	76 (100%)	0	100	100
18	Y	154/155 (99%)	154 (100%)	0	100	100
19	Z	155/157 (99%)	155 (100%)	0	100	100
20	a	43/93 (46%)	43 (100%)	0	100	100
21	b	79/97 (81%)	79 (100%)	0	100	100
22	c	113/150 (75%)	113 (100%)	0	100	100
23	d	255/326 (78%)	255 (100%)	0	100	100
24	e	76/82 (93%)	76 (100%)	0	100	100
25	f	101/102 (99%)	101 (100%)	0	100	100
26	g	107/124 (86%)	107 (100%)	0	100	100
27	h	84/96 (88%)	84 (100%)	0	100	100
28	i	131/131 (100%)	131 (100%)	0	100	100
29	k	283/309 (92%)	283 (100%)	0	100	100
30	l	94/95 (99%)	94 (100%)	0	100	100
31	m	69/72 (96%)	69 (100%)	0	100	100
32	n	61/76 (80%)	61 (100%)	0	100	100
33	o	107/109 (98%)	107 (100%)	0	100	100
34	p	114/116 (98%)	114 (100%)	0	100	100
35	q	119/122 (98%)	119 (100%)	0	100	100
36	r	95/122 (78%)	95 (100%)	0	100	100
37	s	110/120 (92%)	110 (100%)	0	100	100
38	t	159/161 (99%)	159 (100%)	0	100	100
39	u	59/84 (70%)	59 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	v	140/160 (88%)	140 (100%)	0	100	100
41	w	92/130 (71%)	92 (100%)	0	100	100
42	x	44/67 (66%)	44 (100%)	0	100	100
43	y	46/54 (85%)	46 (100%)	0	100	100
44	z	59/59 (100%)	59 (100%)	0	100	100
All	All	7129/7955 (90%)	7125 (100%)	4 (0%)	87	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	6	54	CYS
7	9	78	ILE
8	A	29	VAL
13	M	144	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
25	f	49	GLN
33	o	12	GLN
26	g	25	ASN
29	k	107	GLN
37	s	3	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
27	AYA	h	1	27	6,7,8	1.25	1 (16%)	5,8,10	1.14	1 (20%)
4	2MR	4	85	4	10,12,13	2.33	3 (30%)	5,13,15	1.75	2 (40%)
29	SEP	k	36	29	8,9,10	1.55	1 (12%)	8,12,14	1.51	2 (25%)
11	FME	K	1	11	8,9,10	0.95	0	7,9,11	0.76	0
13	FME	M	1	13	8,9,10	0.96	0	7,9,11	1.03	0
15	AYA	V	1	15	6,7,8	1.22	1 (16%)	5,8,10	1.78	2 (40%)
12	FME	L	1	12	8,9,10	0.92	0	7,9,11	1.08	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	AYA	h	1	27	-	0/4/6/8	-
4	2MR	4	85	4	-	1/10/13/15	-
29	SEP	k	36	29	-	5/5/8/10	-
11	FME	K	1	11	-	3/7/9/11	-
13	FME	M	1	13	-	2/7/9/11	-
15	AYA	V	1	15	-	2/4/6/8	-
12	FME	L	1	12	-	2/7/9/11	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	85	2MR	CZ-NH2	4.53	1.43	1.33
4	4	85	2MR	CZ-NE	4.50	1.43	1.34
29	k	36	SEP	P-O1P	3.38	1.61	1.50
4	4	85	2MR	CQ1-NH1	-2.56	1.41	1.46
27	h	1	AYA	CA-N	-2.52	1.43	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	k	36	SEP	P-OG-CB	-3.28	109.26	118.30
4	4	85	2MR	NE-CZ-NH2	-2.74	116.97	119.48
15	V	1	AYA	CA-N-CT	2.56	125.24	121.52
15	V	1	AYA	CB-CA-N	2.50	112.39	109.61
27	h	1	AYA	CB-CA-N	2.30	112.17	109.61

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	K	1	FME	O1-CN-N-CA
12	L	1	FME	CA-CB-CG-SD
29	k	36	SEP	N-CA-CB-OG
29	k	36	SEP	CB-OG-P-O2P
29	k	36	SEP	CB-OG-P-O3P

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	1	FME	1	0
15	V	1	AYA	3	0
12	L	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 46 ligands modelled in this entry, 2 are monoatomic - leaving 44 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	$\#\|Z\| > 2$
48	FES	3	803	3	0,4,4	-	-	-		
50	3PE	i	501	-	50,50,50	0.30	0	53,55,55	0.34	0
57	AMP	k	501	-	25,25,25	1.37	4 (16%)	38,38,38	2.01	7 (18%)
56	NDP	d	401	-	49,52,52	0.45	0	66,80,80	0.39	0
50	3PE	N	402	-	30,30,50	0.38	0	33,35,55	0.35	0
51	PC1	M	502	-	53,53,53	0.30	0	59,61,61	0.35	0
50	3PE	V	202	-	36,36,50	0.34	0	39,41,55	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
53	CDL	o	202	-	89,89,99	0.31	0	95,101,111	0.40	0
48	FES	2	300	2	0,4,4	-	-	-		
45	SF4	3	802	3	0,12,12	-	-	-		
45	SF4	3	801	3	0,12,12	-	-	-		
50	3PE	p	201	-	26,26,50	0.48	0	30,31,55	0.52	1 (3%)
47	NAI	1	503	-	45,48,48	0.39	0	60,73,73	1.69	3 (5%)
51	PC1	A	402	-	36,36,53	0.36	0	42,44,61	0.59	1 (2%)
51	PC1	9	401	-	53,53,53	0.32	0	59,61,61	0.50	1 (1%)
52	DCQ	H	501	-	23,23,23	0.18	0	26,29,29	0.52	0
54	ZMP	g	201	-	27,33,36	0.78	1 (3%)	32,40,45	1.34	4 (12%)
50	3PE	L	1001	-	50,50,50	0.30	0	53,55,55	0.36	0
45	SF4	9	403	7	0,12,12	-	-	-		
45	SF4	6	300	6	0,12,12	-	-	-		
53	CDL	W	201	-	99,99,99	0.28	0	105,111,111	0.30	0
58	MYR	s	201	37	14,14,15	0.20	0	13,13,15	0.17	0
50	3PE	i	502	-	50,50,50	0.30	0	53,55,55	0.30	0
53	CDL	L	1003	-	99,99,99	0.26	0	105,111,111	0.32	0
51	PC1	L	1002	-	53,53,53	0.31	0	59,61,61	0.60	1 (1%)
50	3PE	L	1004	-	30,30,50	0.41	0	33,35,55	0.77	1 (3%)
53	CDL	o	201	-	74,74,99	0.30	0	80,86,111	0.46	1 (1%)
45	SF4	1	501	1	0,12,12	-	-	-		
51	PC1	w	801	-	53,53,53	0.30	0	59,61,61	0.38	0
53	CDL	Y	201	-	99,99,99	0.26	0	105,111,111	0.33	0
53	CDL	z	101	-	57,57,99	0.34	0	63,69,111	0.34	0
53	CDL	V	203	-	93,93,99	0.26	0	99,105,111	0.25	0
50	3PE	A	403	-	50,50,50	0.31	0	53,55,55	0.35	0
50	3PE	M	501	-	43,43,50	0.32	0	46,48,55	0.43	0
51	PC1	A	401	-	45,45,53	0.32	0	51,53,61	0.29	0
50	3PE	N	401	-	50,50,50	0.32	0	53,55,55	0.56	2 (3%)
46	FMN	1	502	-	33,33,33	1.10	3 (9%)	48,50,50	1.38	9 (18%)
50	3PE	V	201	-	34,34,50	0.37	0	37,39,55	0.34	0
53	CDL	V	204	-	84,84,99	0.29	0	90,96,111	0.25	0
50	3PE	H	502	-	50,50,50	0.31	0	53,55,55	0.47	1 (1%)
54	ZMP	X	101	17	24,30,36	0.74	1 (4%)	29,37,45	1.06	2 (6%)
50	3PE	K	101	-	39,39,50	0.34	0	42,44,55	0.39	0
50	3PE	4	501	-	39,39,50	0.34	0	42,44,55	0.35	0
45	SF4	9	402	7	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	3PE	i	501	-	-	10/54/54/54	-
57	AMP	k	501	-	-	6/10/26/26	0/3/3/3
48	FES	3	803	3	-	-	0/1/1/1
56	NDP	d	401	-	-	5/34/77/77	0/5/5/5
50	3PE	N	402	-	-	2/34/34/54	-
51	PC1	M	502	-	-	22/57/57/57	-
50	3PE	V	202	-	-	16/40/40/54	-
53	CDL	o	202	-	-	42/100/100/110	-
48	FES	2	300	2	-	-	0/1/1/1
45	SF4	3	802	3	-	-	0/6/5/5
45	SF4	3	801	3	-	-	0/6/5/5
50	3PE	p	201	-	-	5/27/27/54	-
47	NAI	1	503	-	-	5/29/72/72	0/5/5/5
51	PC1	A	402	-	-	5/40/40/57	-
51	PC1	9	401	-	-	18/57/57/57	-
52	DCQ	H	501	-	-	2/14/38/38	0/1/1/1
54	ZMP	g	201	-	-	3/38/40/43	-
50	3PE	L	1001	-	-	12/54/54/54	-
45	SF4	9	403	7	-	-	0/6/5/5
45	SF4	6	300	6	-	-	0/6/5/5
53	CDL	W	201	-	-	28/110/110/110	-
58	MYR	s	201	37	-	2/11/12/13	-
50	3PE	i	502	-	-	12/54/54/54	-
53	CDL	L	1003	-	1/1/9/9	35/110/110/110	-
51	PC1	L	1002	-	-	21/57/57/57	-
50	3PE	L	1004	-	-	8/34/34/54	-
53	CDL	o	201	-	2/2/9/9	22/85/85/110	-
51	PC1	w	801	-	-	10/57/57/57	-
53	CDL	Y	201	-	1/1/9/9	29/110/110/110	-
53	CDL	z	101	-	-	23/68/68/110	-
45	SF4	1	501	1	-	-	0/6/5/5
53	CDL	V	203	-	-	35/104/104/110	-
50	3PE	A	403	-	-	18/54/54/54	-
50	3PE	M	501	-	-	14/47/47/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	PC1	A	401	-	-	17/49/49/57	-
50	3PE	N	401	-	-	14/54/54/54	-
46	FMN	1	502	-	-	9/18/18/18	0/3/3/3
50	3PE	V	201	-	-	5/38/38/54	-
53	CDL	V	204	-	1/1/9/9	28/95/95/110	-
50	3PE	H	502	-	-	19/54/54/54	-
54	ZMP	X	101	17	-	12/35/37/43	-
50	3PE	K	101	-	-	7/43/43/54	-
50	3PE	4	501	-	-	9/43/43/54	-
45	SF4	9	402	7	-	-	0/6/5/5

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	k	501	AMP	C5-C4	4.58	1.47	1.39
46	1	502	FMN	C4A-N5	3.15	1.36	1.30
54	g	201	ZMP	C10-S1	-3.04	1.68	1.76
57	k	501	AMP	C5-C6	2.59	1.48	1.41
57	k	501	AMP	C5-N7	-2.36	1.34	1.39

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	1	503	NAI	O5B-PA-O1A	-9.69	71.19	109.07
47	1	503	NAI	O2A-PA-O1A	-8.11	72.13	112.24
57	k	501	AMP	C5-C4-N3	-6.85	117.81	126.75
57	k	501	AMP	N3-C4-N9	5.62	136.33	127.08
57	k	501	AMP	C2-N3-C4	4.15	121.54	111.75

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
53	L	1003	CDL	CB4
53	V	204	CDL	CB4
53	Y	201	CDL	CB4
53	o	201	CDL	CA4
53	o	201	CDL	CB4

5 of 530 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	1	502	FMN	N10-C1'-C2'-O2'
46	1	502	FMN	N10-C1'-C2'-C3'
46	1	502	FMN	C5'-O5'-P-O2P
46	1	502	FMN	C5'-O5'-P-O3P
47	1	503	NAI	C5B-O5B-PA-O1A

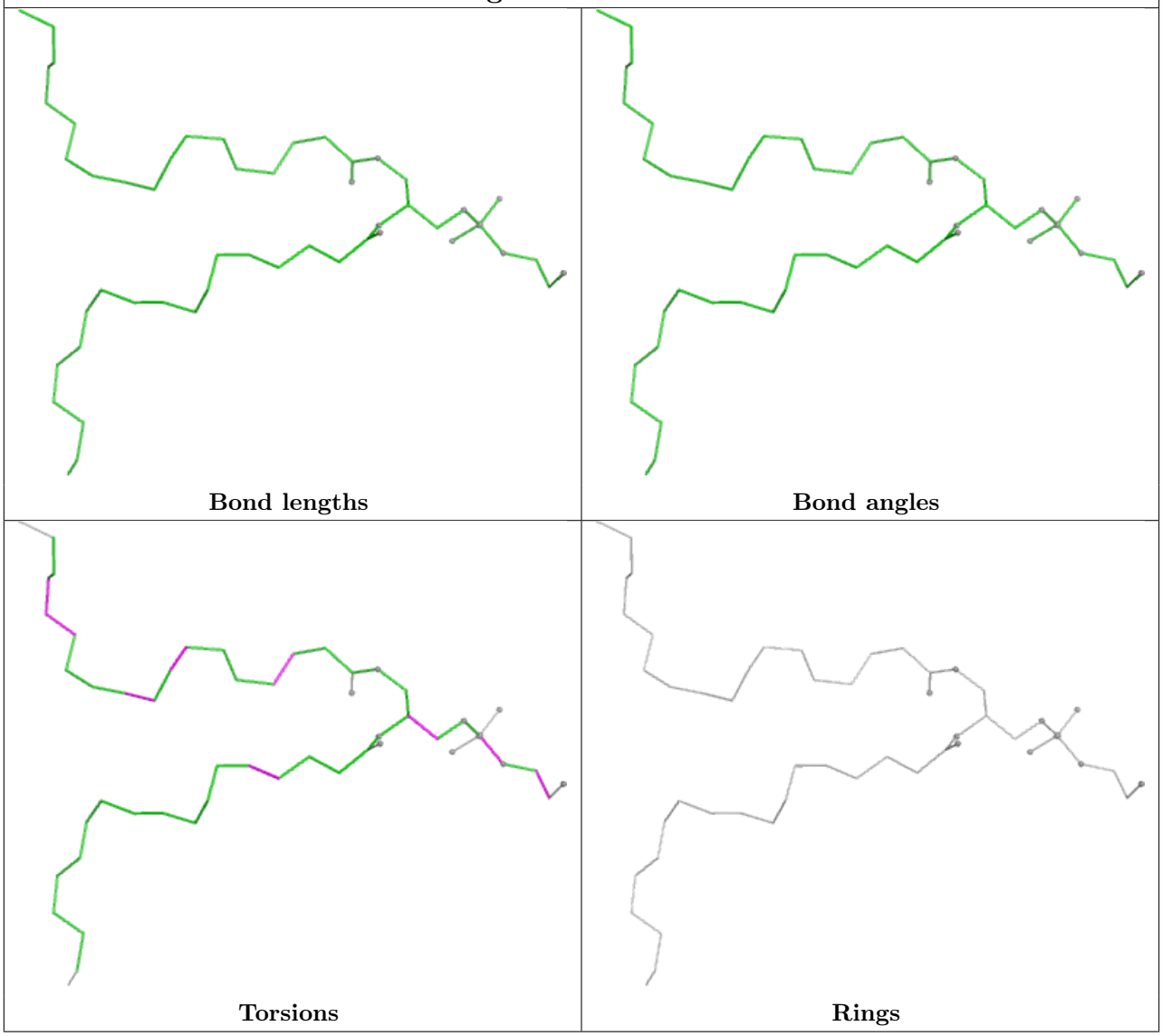
There are no ring outliers.

32 monomers are involved in 90 short contacts:

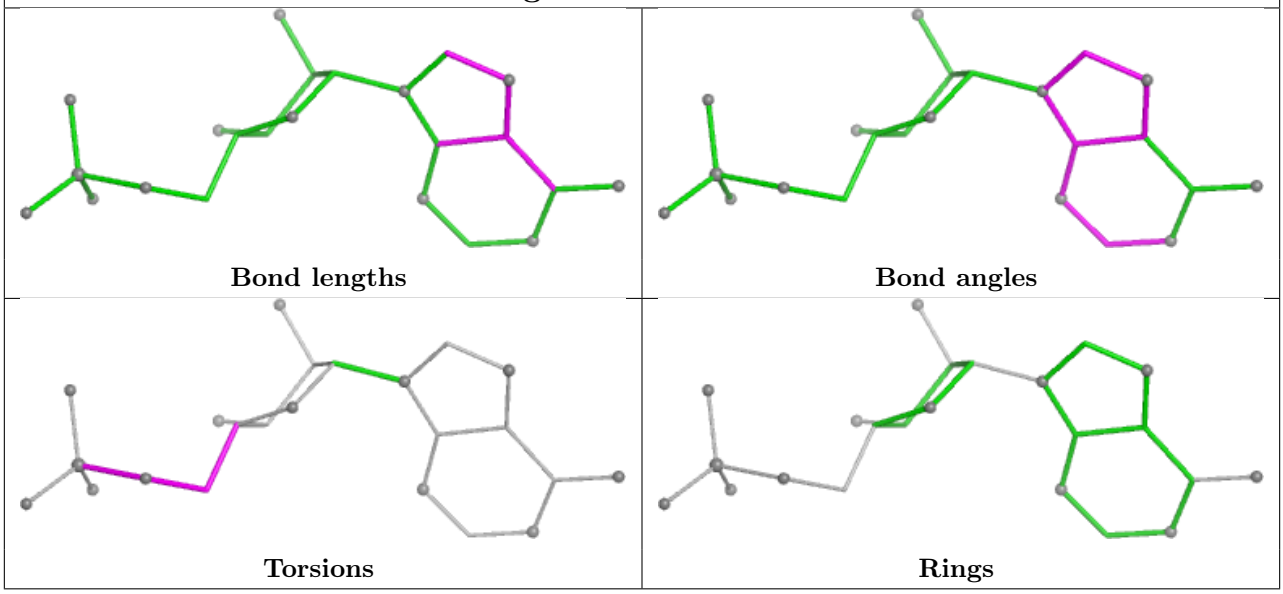
Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	i	501	3PE	2	0
51	M	502	PC1	5	0
50	V	202	3PE	2	0
53	o	202	CDL	6	0
48	2	300	FES	1	0
47	1	503	NAI	6	0
51	A	402	PC1	2	0
51	9	401	PC1	4	0
52	H	501	DCQ	2	0
54	g	201	ZMP	1	0
50	L	1001	3PE	2	0
45	6	300	SF4	1	0
53	W	201	CDL	6	0
50	i	502	3PE	1	0
53	L	1003	CDL	6	0
51	L	1002	PC1	7	0
53	o	201	CDL	4	0
45	1	501	SF4	1	0
51	w	801	PC1	7	0
53	Y	201	CDL	9	0
53	V	203	CDL	4	0
50	A	403	3PE	2	0
50	M	501	3PE	3	0
51	A	401	PC1	1	0
50	N	401	3PE	1	0
46	1	502	FMN	1	0
50	V	201	3PE	3	0
53	V	204	CDL	1	0
50	H	502	3PE	2	0
54	X	101	ZMP	1	0
50	K	101	3PE	4	0
50	4	501	3PE	1	0

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

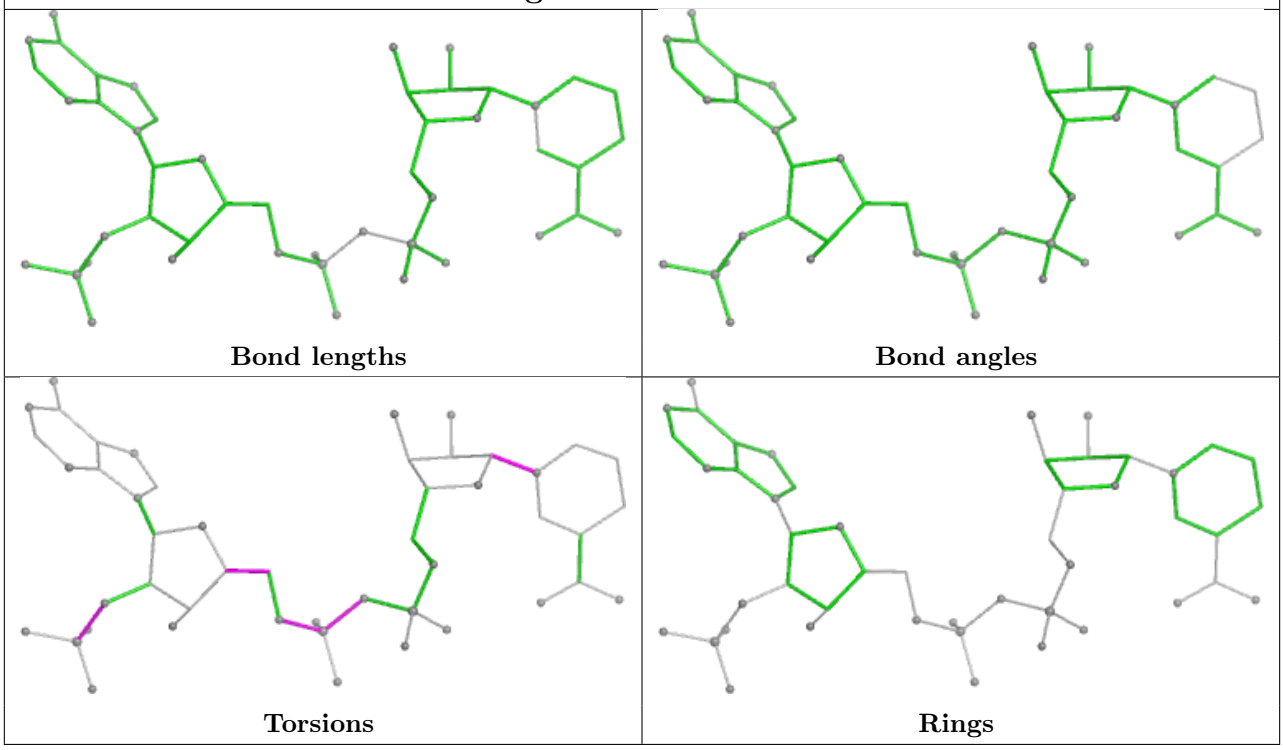
Ligand 3PE i 501



Ligand AMP k 501



Ligand NDP d 401



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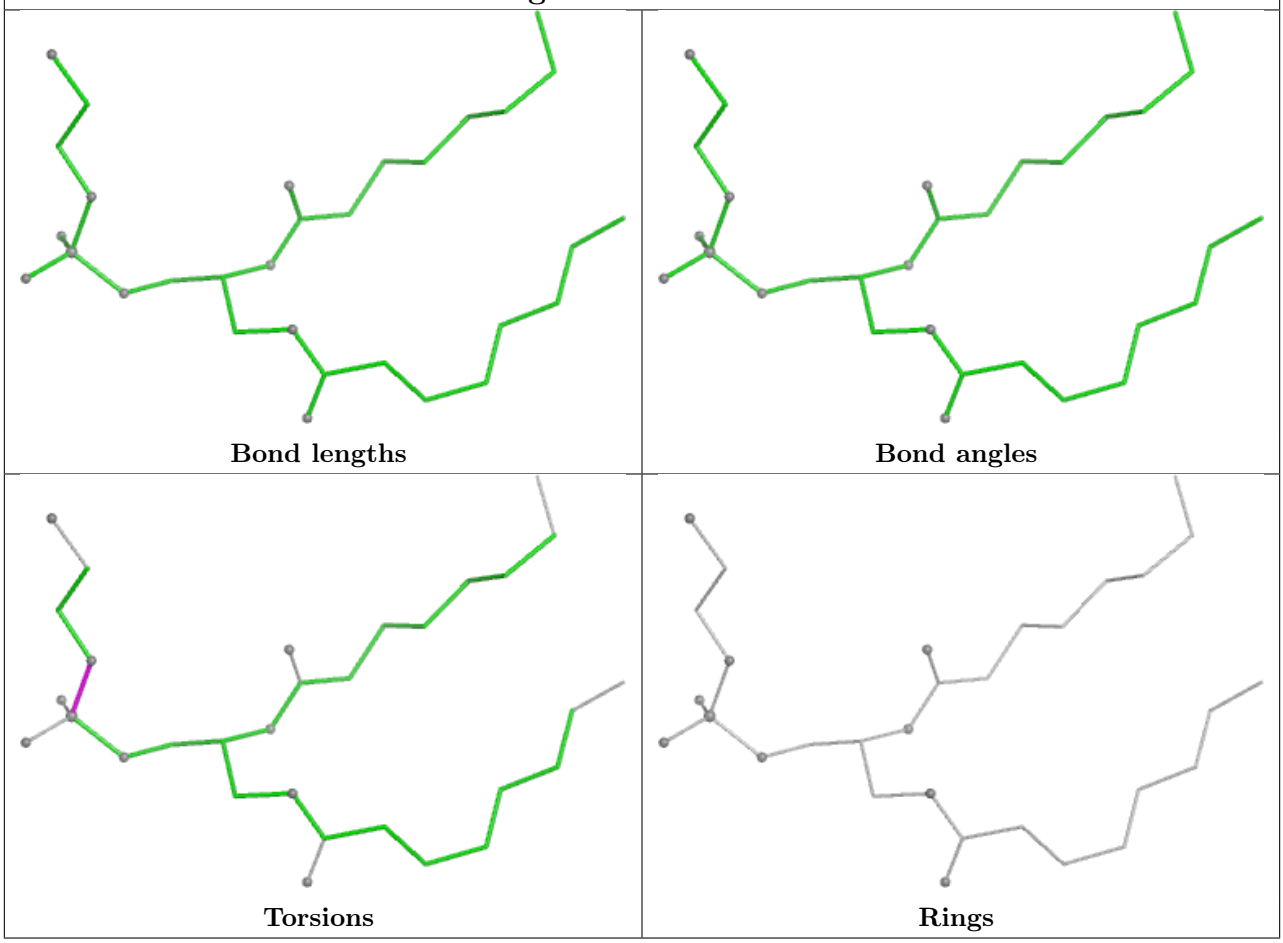
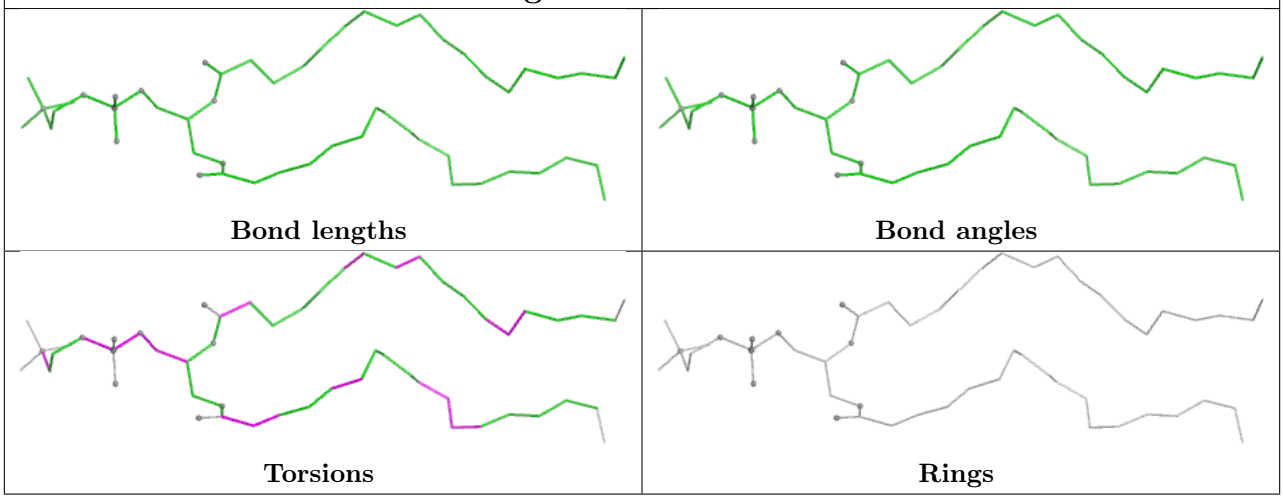


Ligand PC1 M 502



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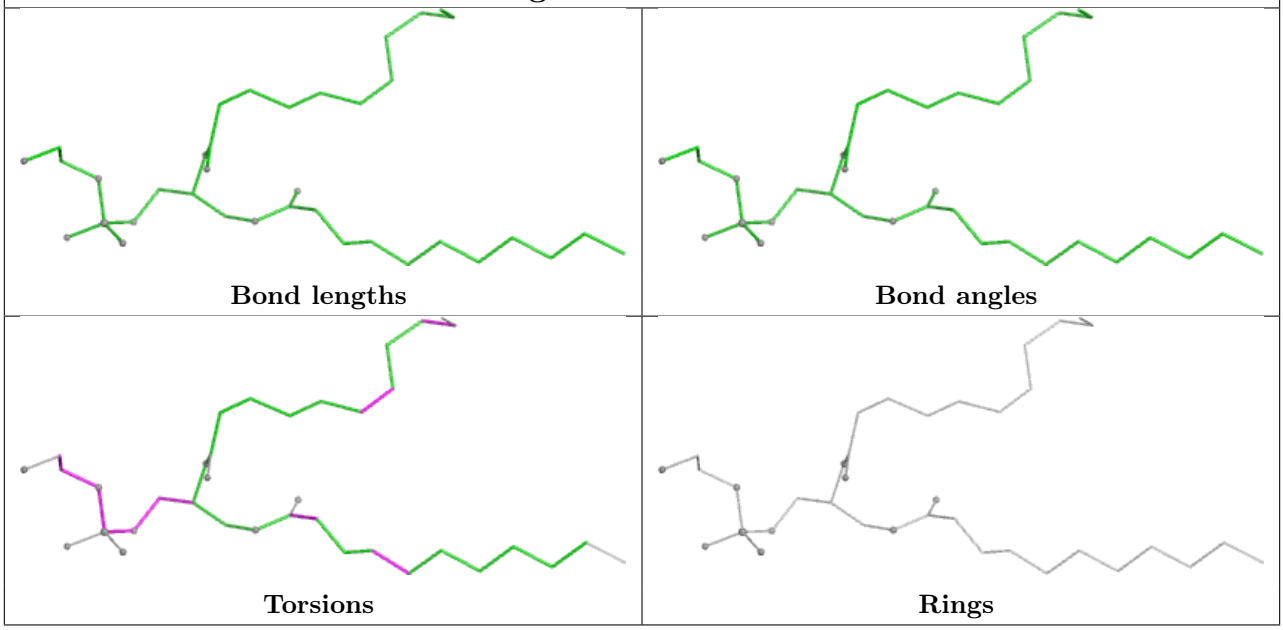

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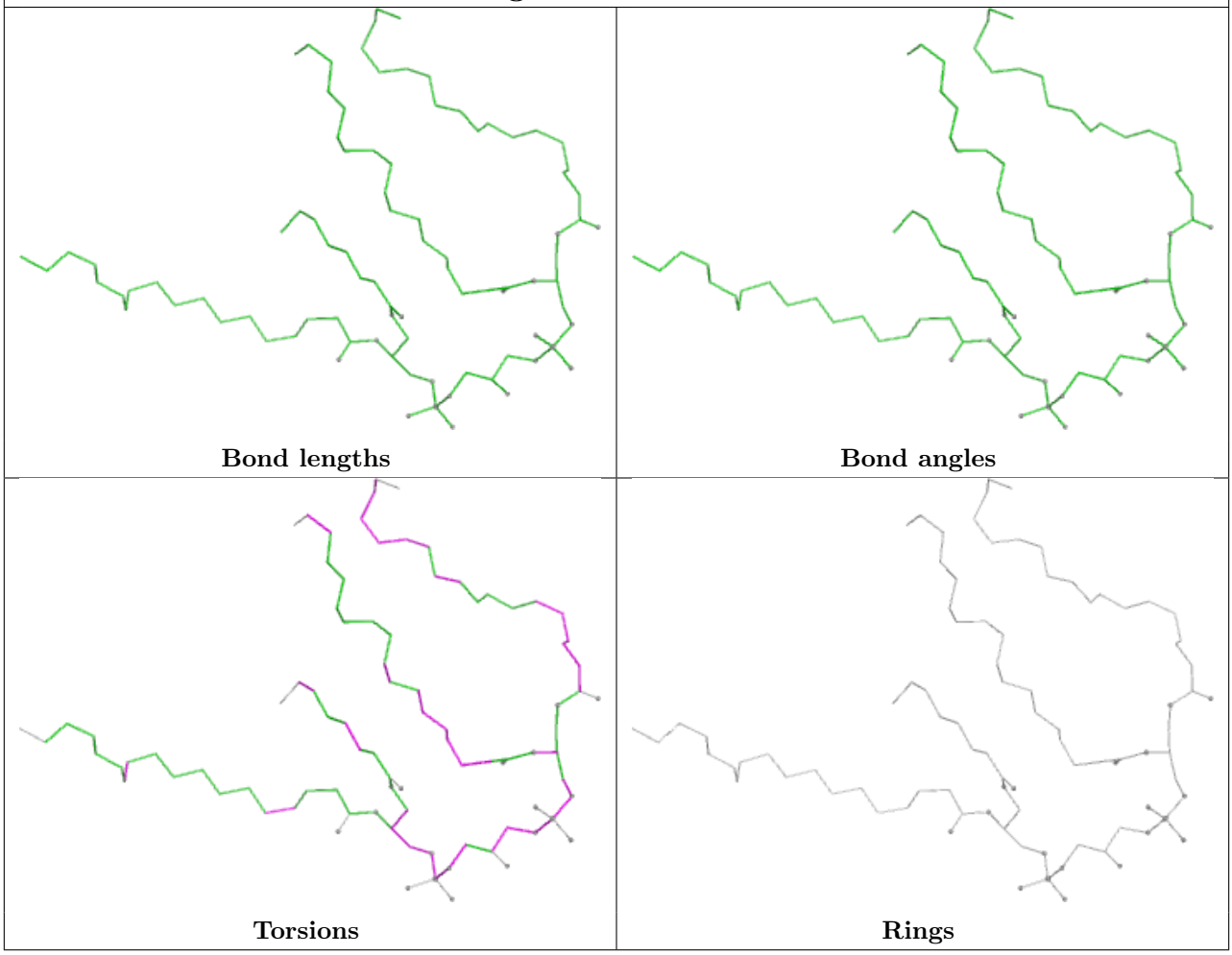

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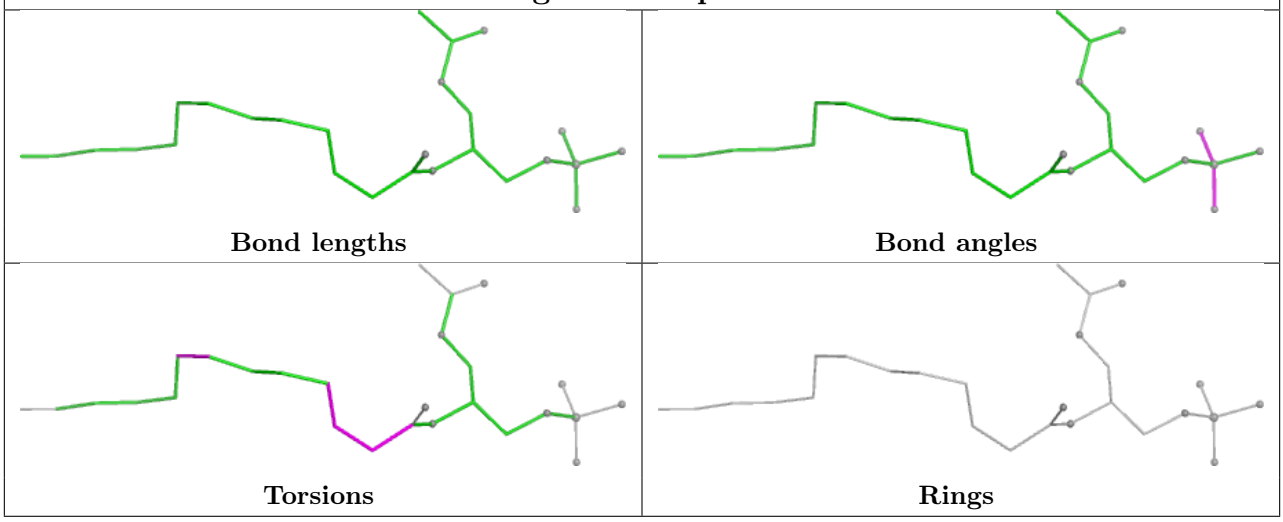

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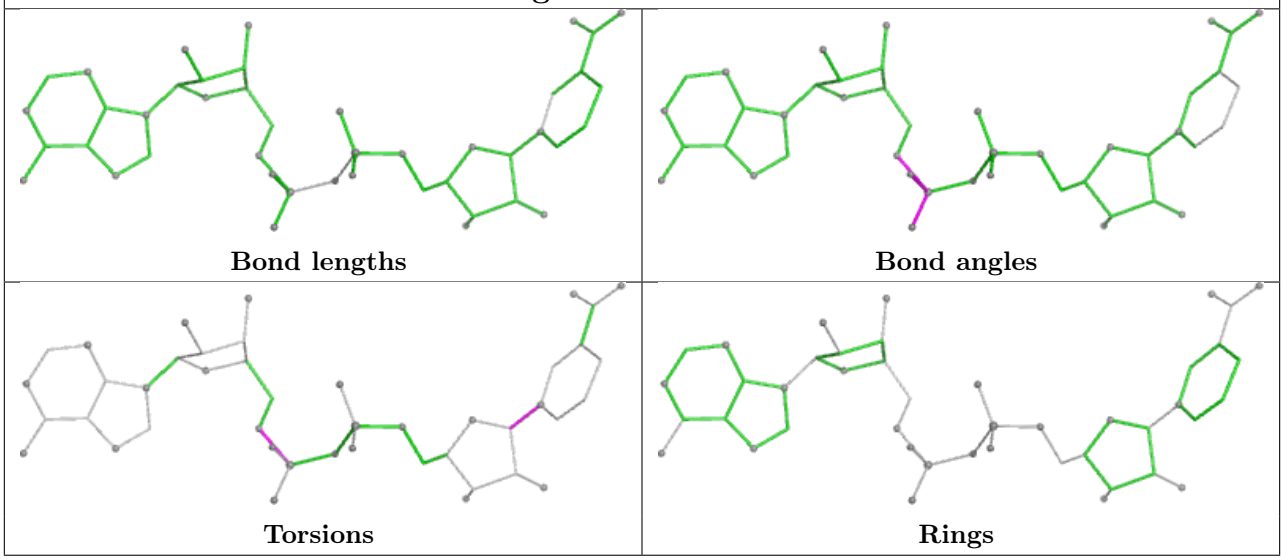

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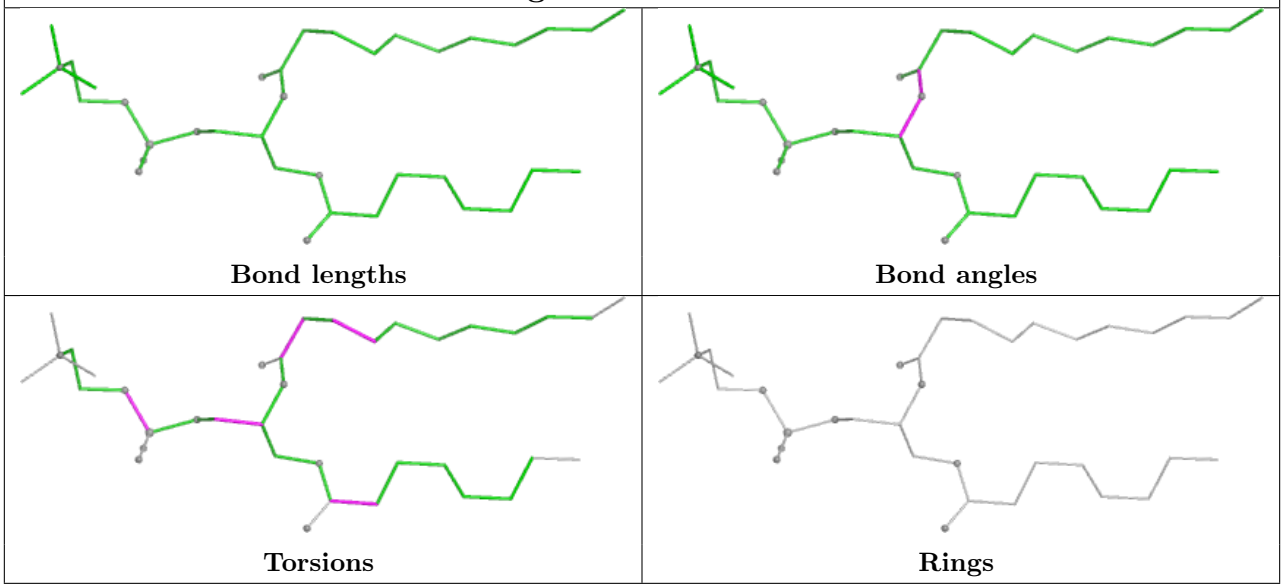
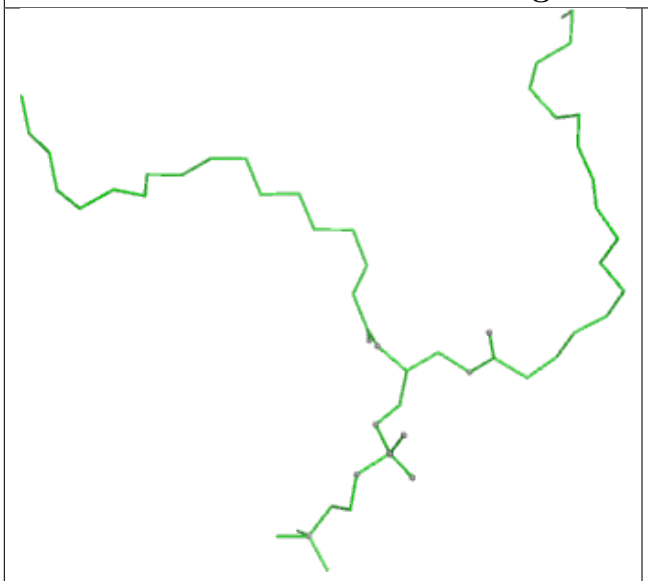
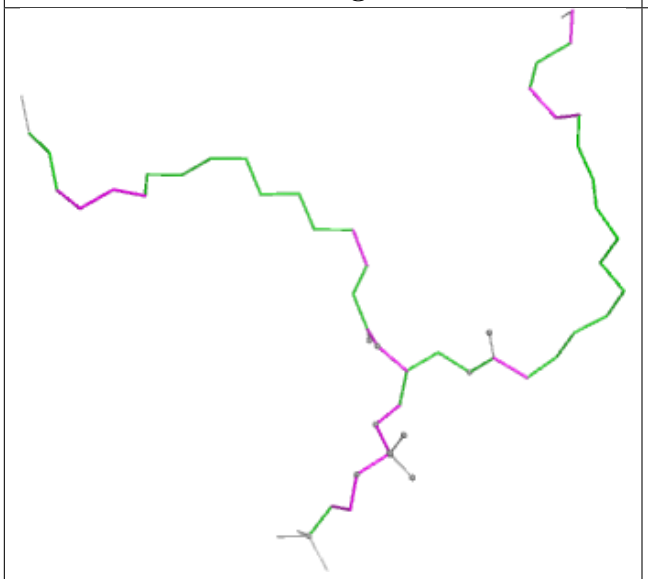


Ligand PC1 9 401



Bond lengths

Bond angles



Torsions

Rings

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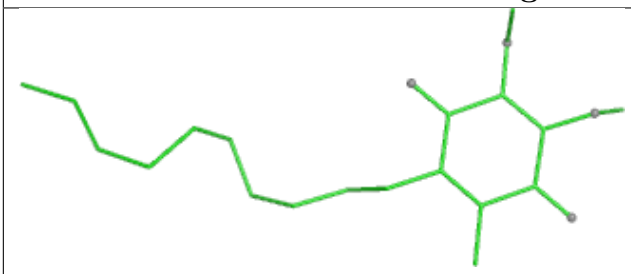
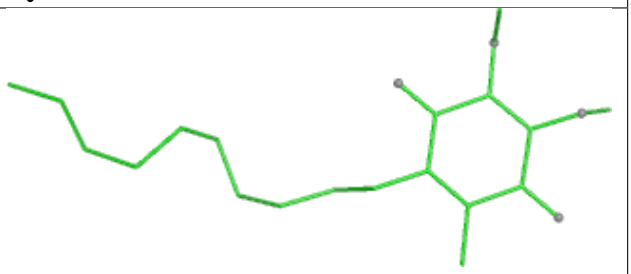
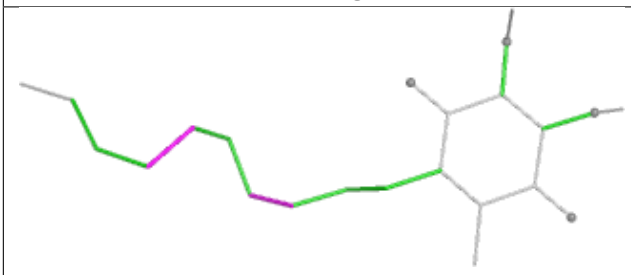
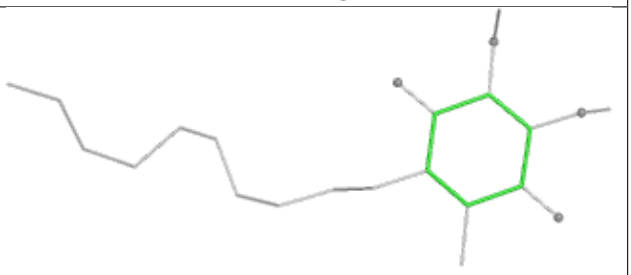
 Bond lengths	 Bond angles
 Torsions	 Rings

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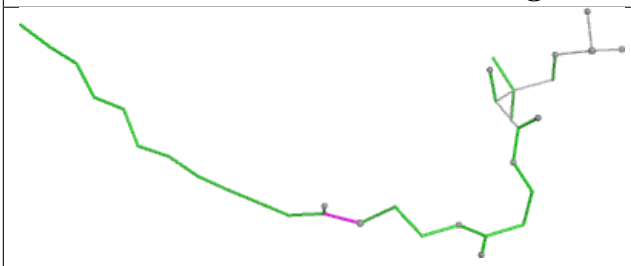
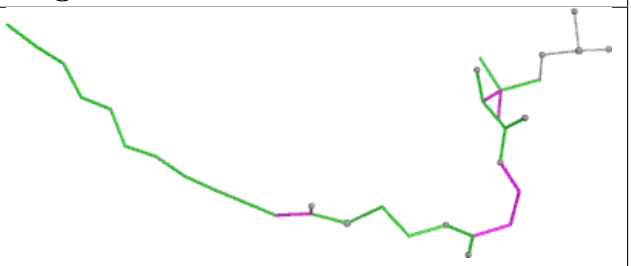
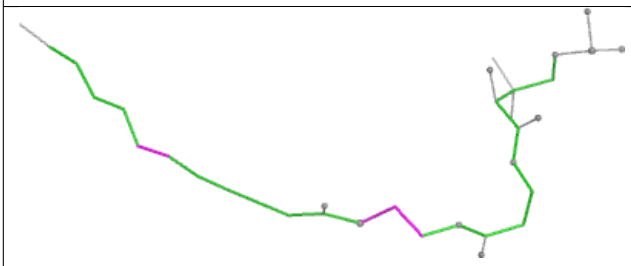
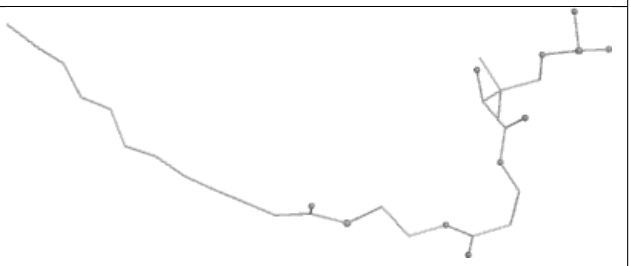
 Bond lengths	 Bond angles
 Torsions	 Rings

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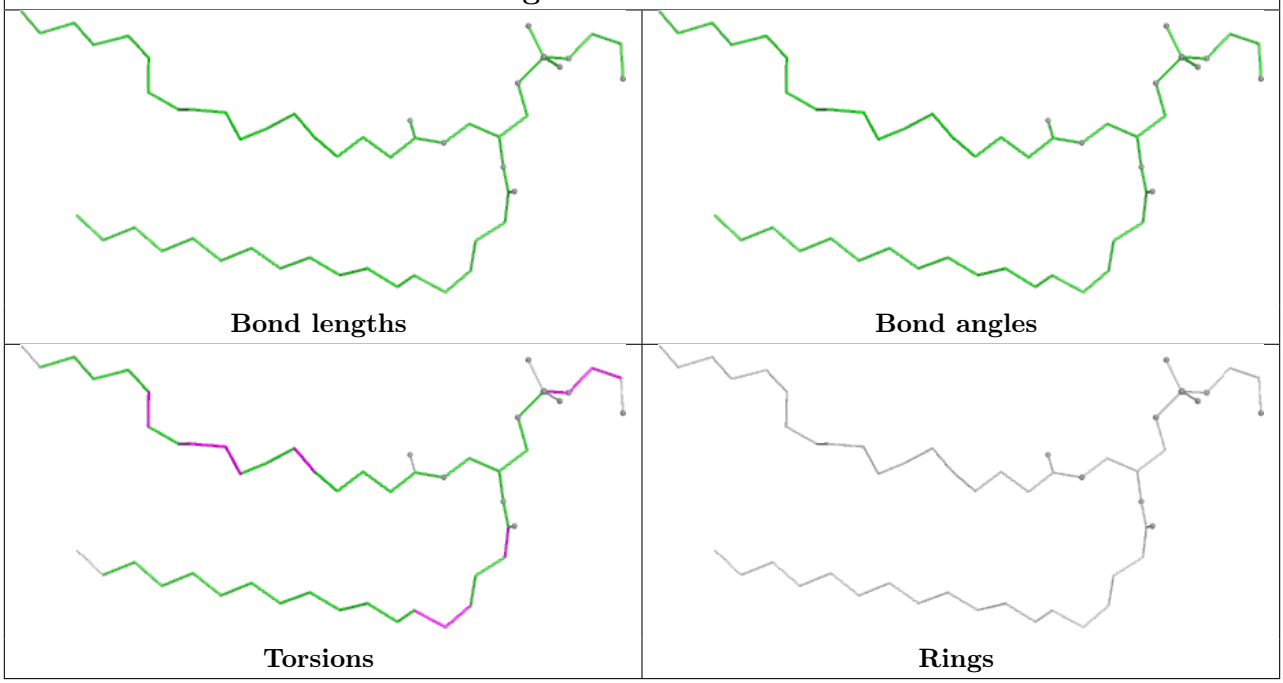
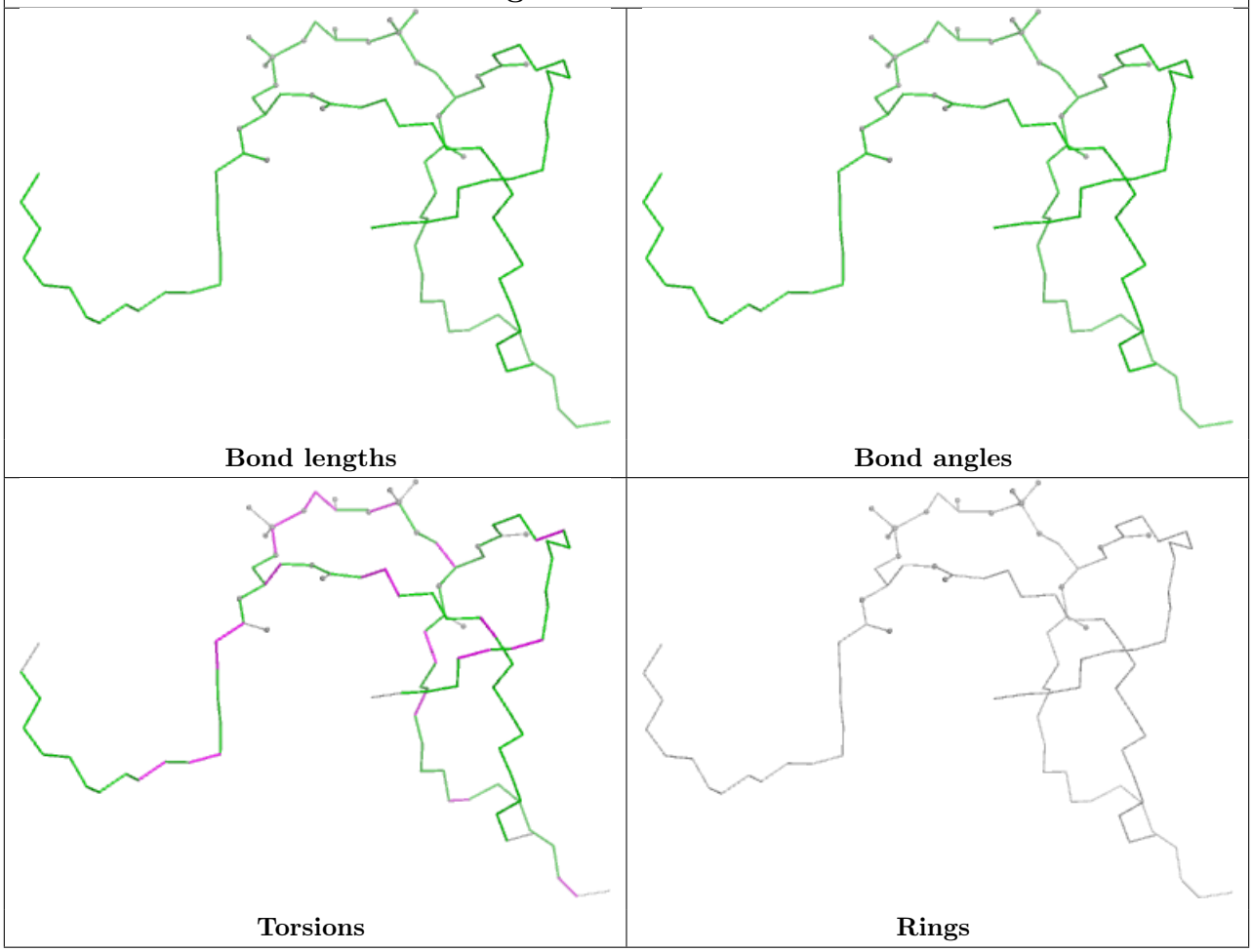
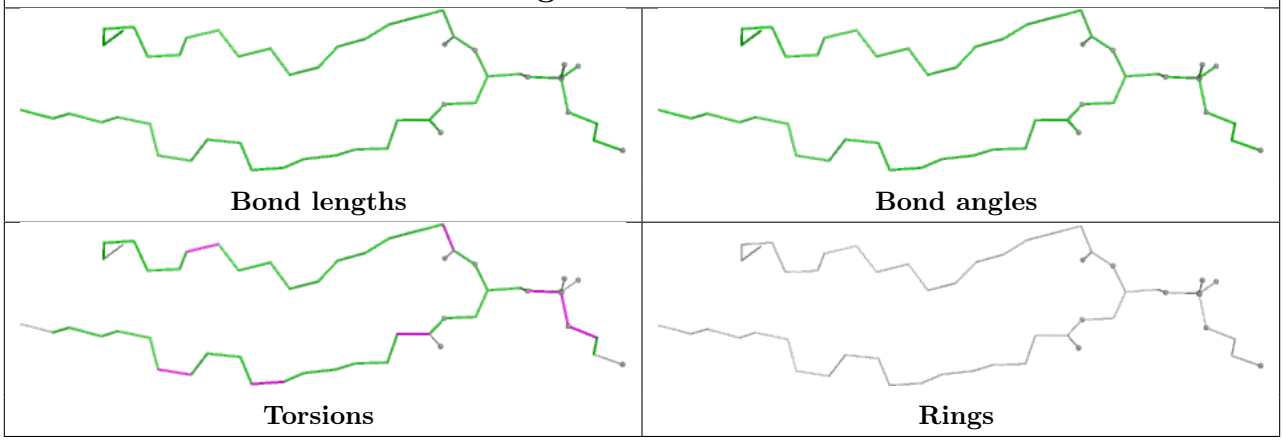


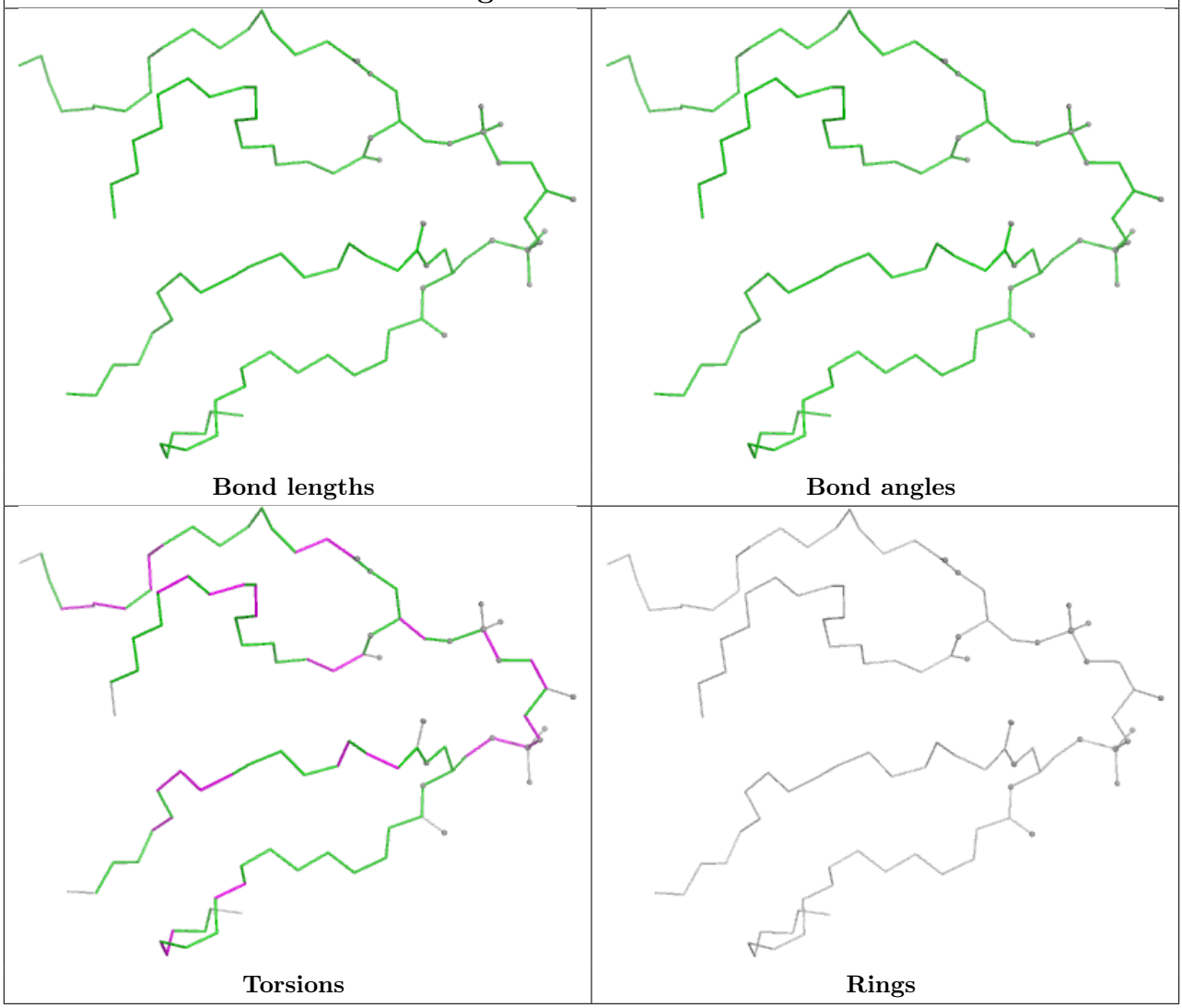
Ligand CDL W 201



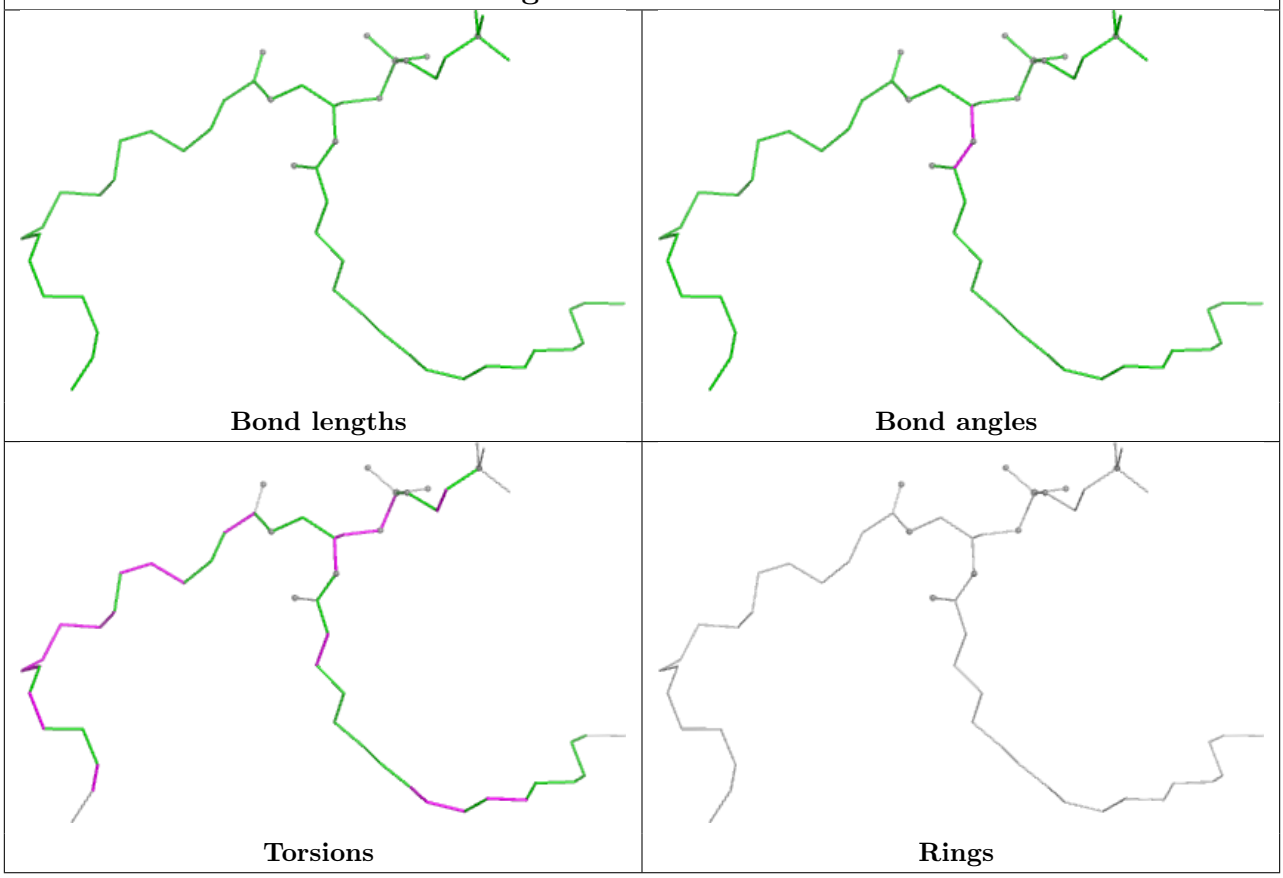
Ligand 3PE i 502



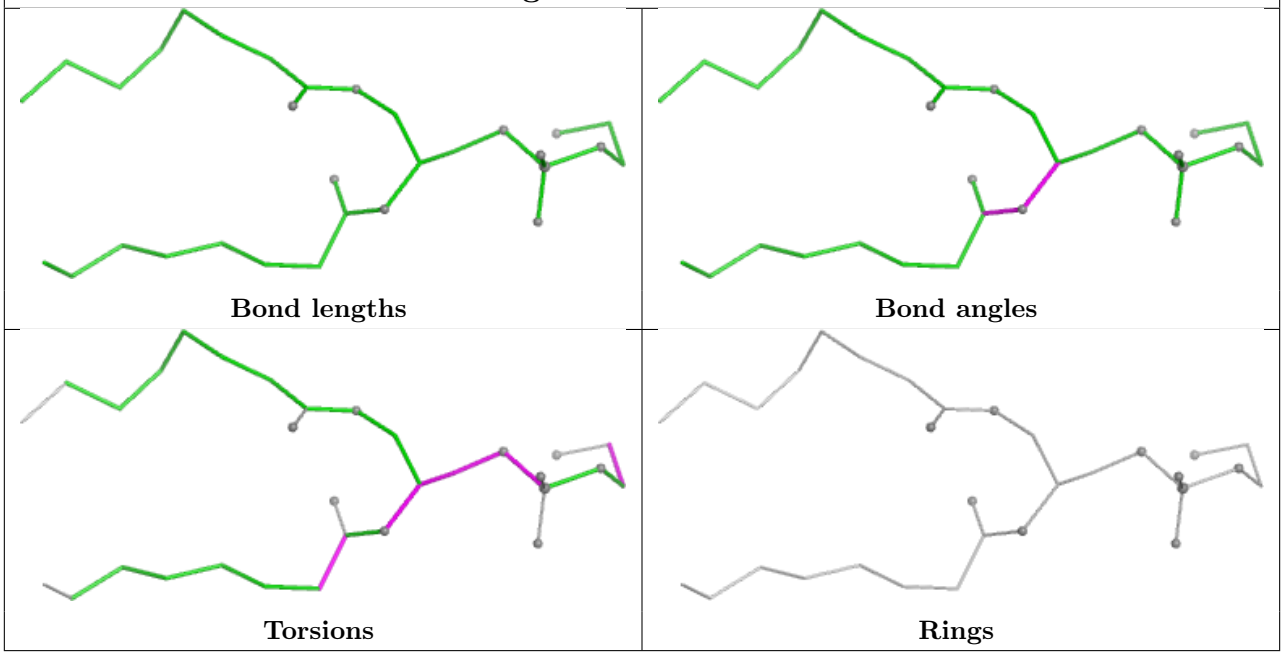
Ligand CDL L 1003

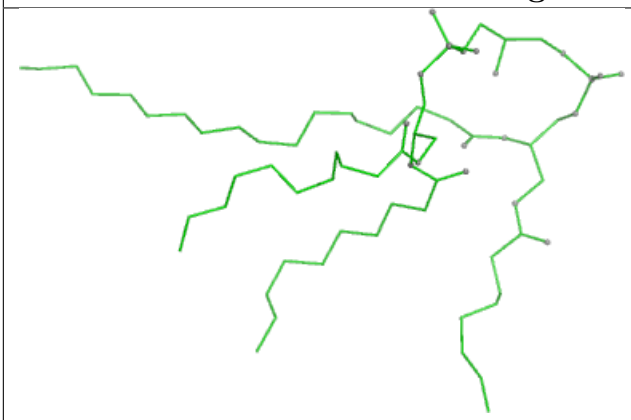
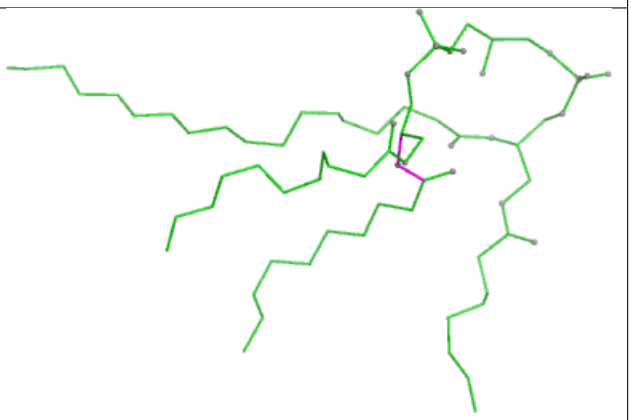
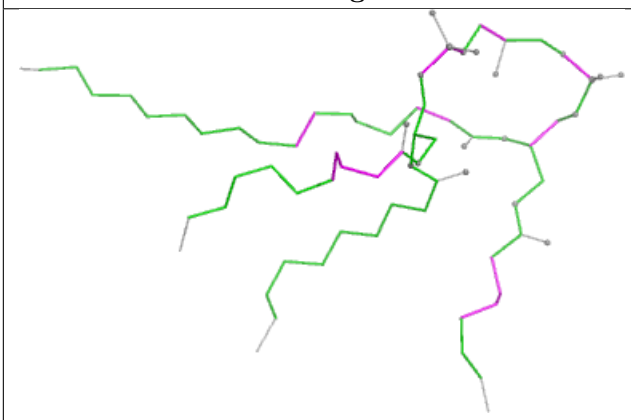


Ligand PC1 L 1002

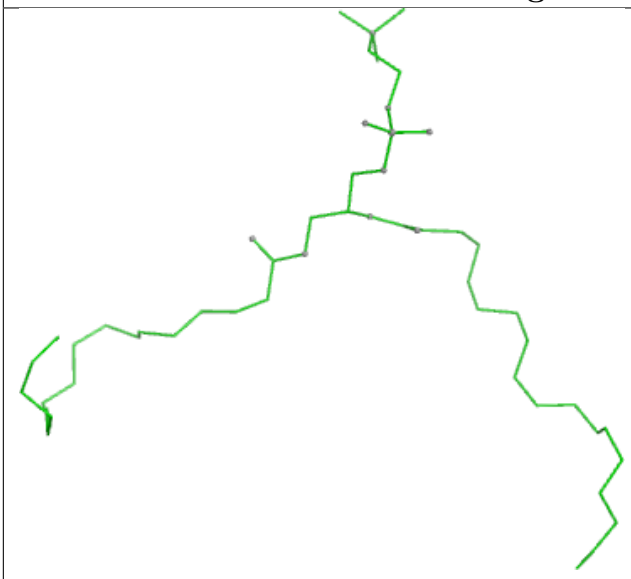


Ligand 3PE L 1004

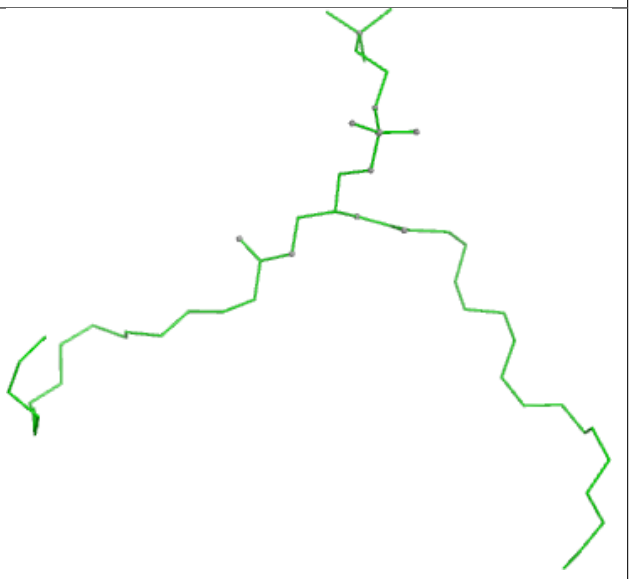


Ligand CDL o 201	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

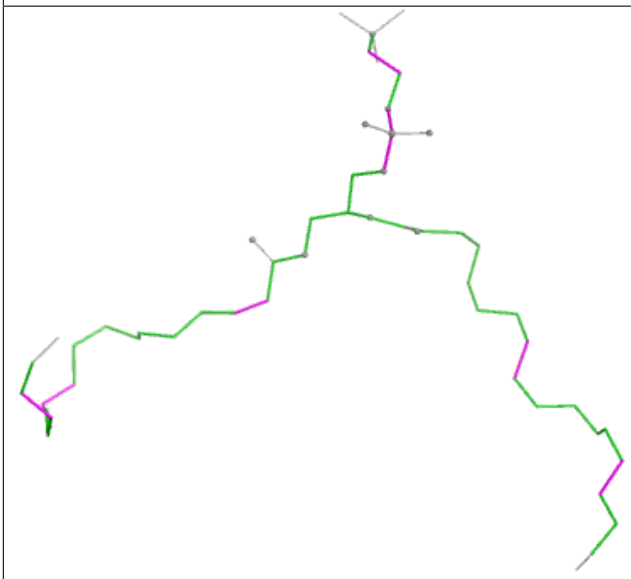
Ligand PC1 w 801



Bond lengths



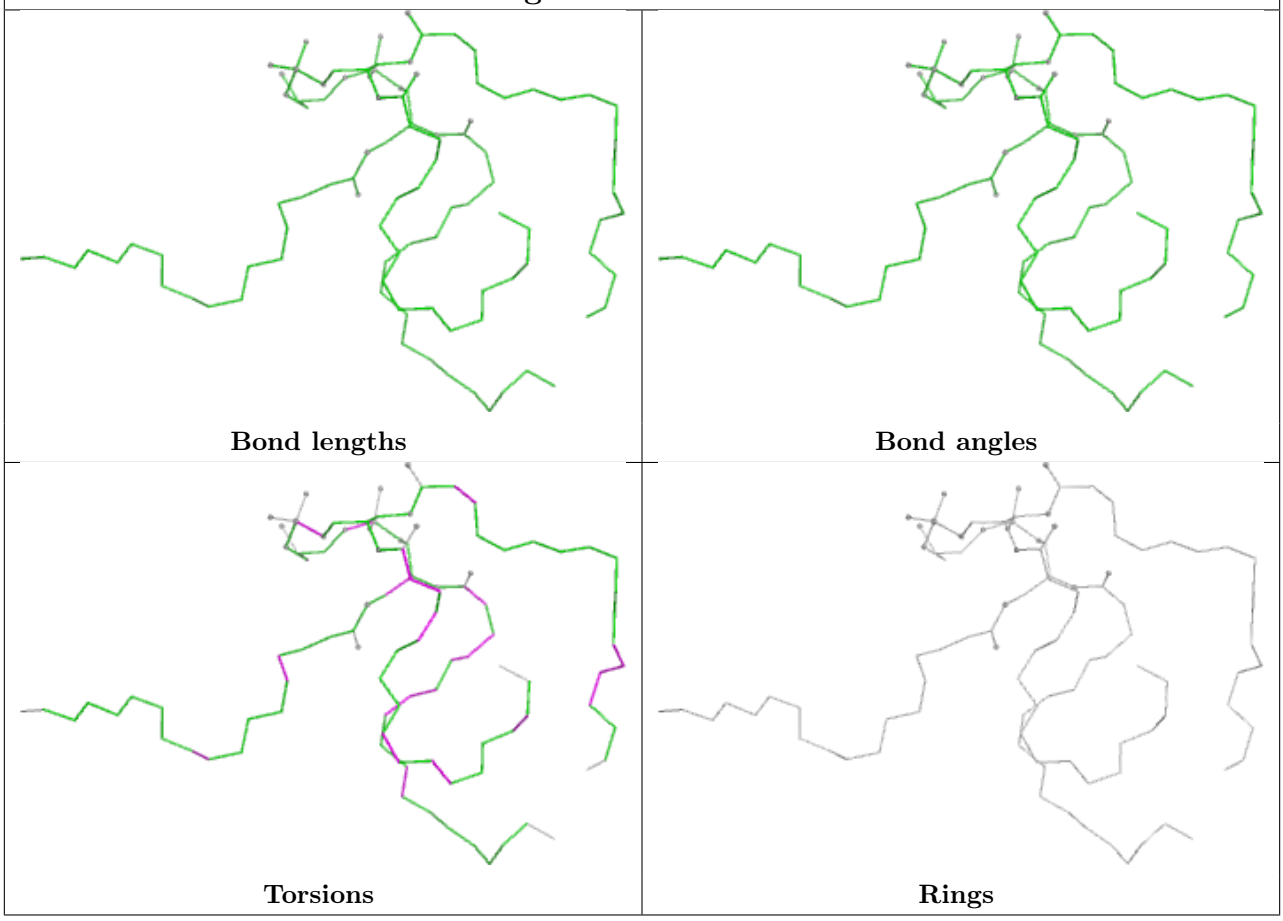
Bond angles



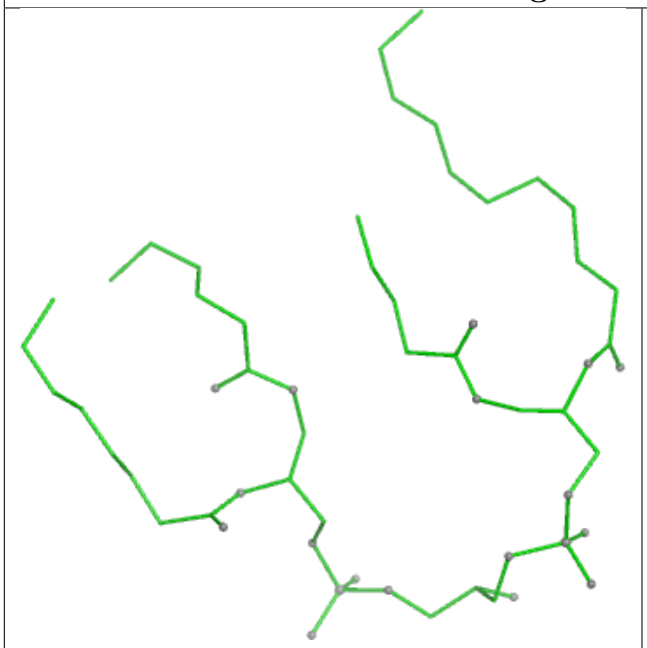
Torsions

Rings

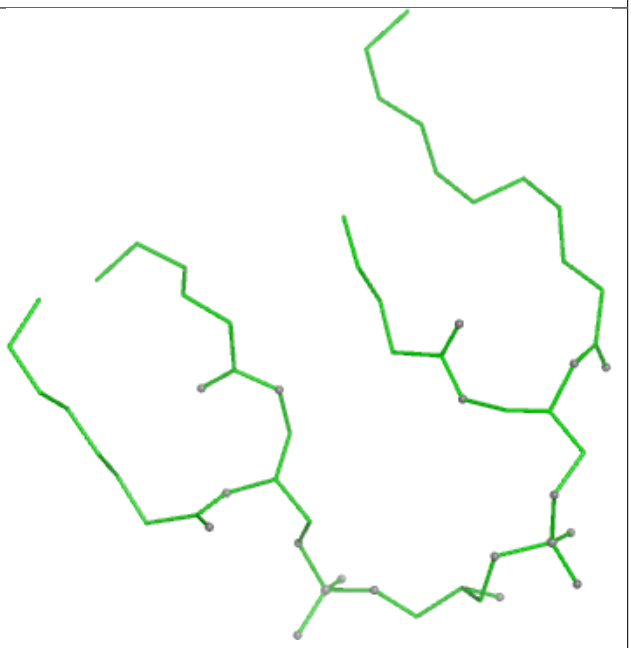
Ligand CDL Y 201



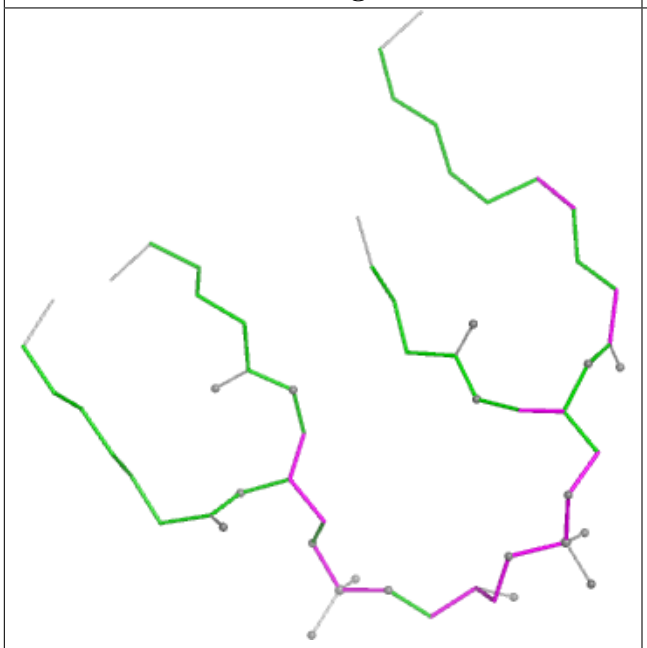
Ligand CDL z 101



Bond lengths



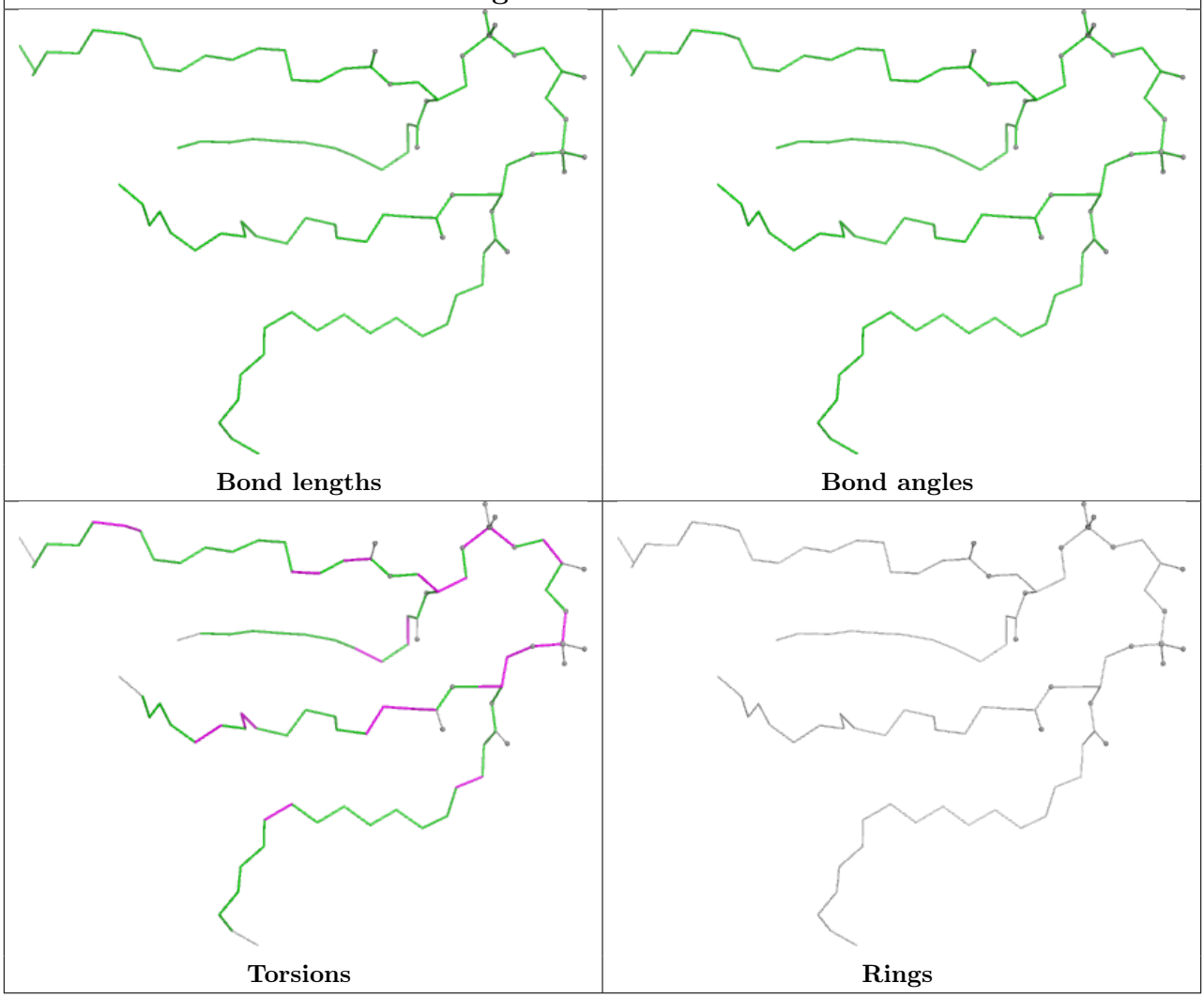
Bond angles



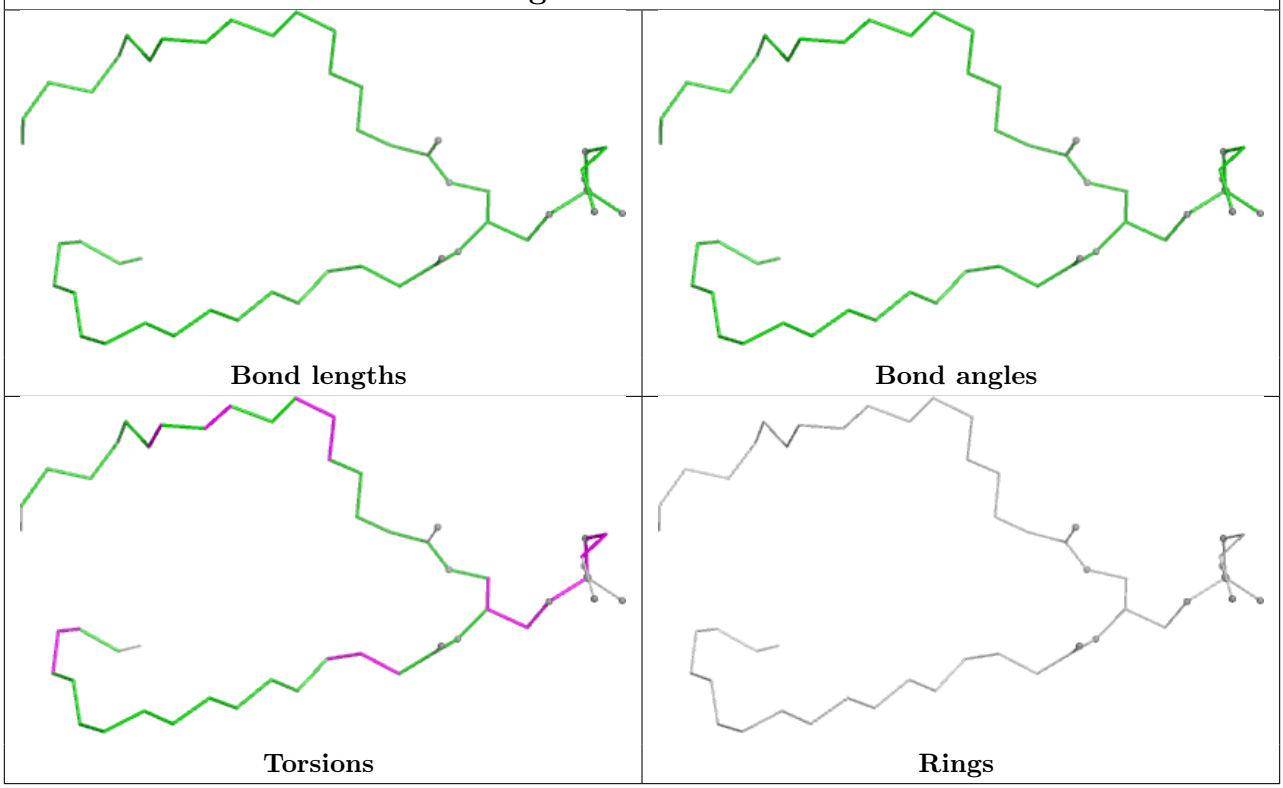
Torsions

Rings

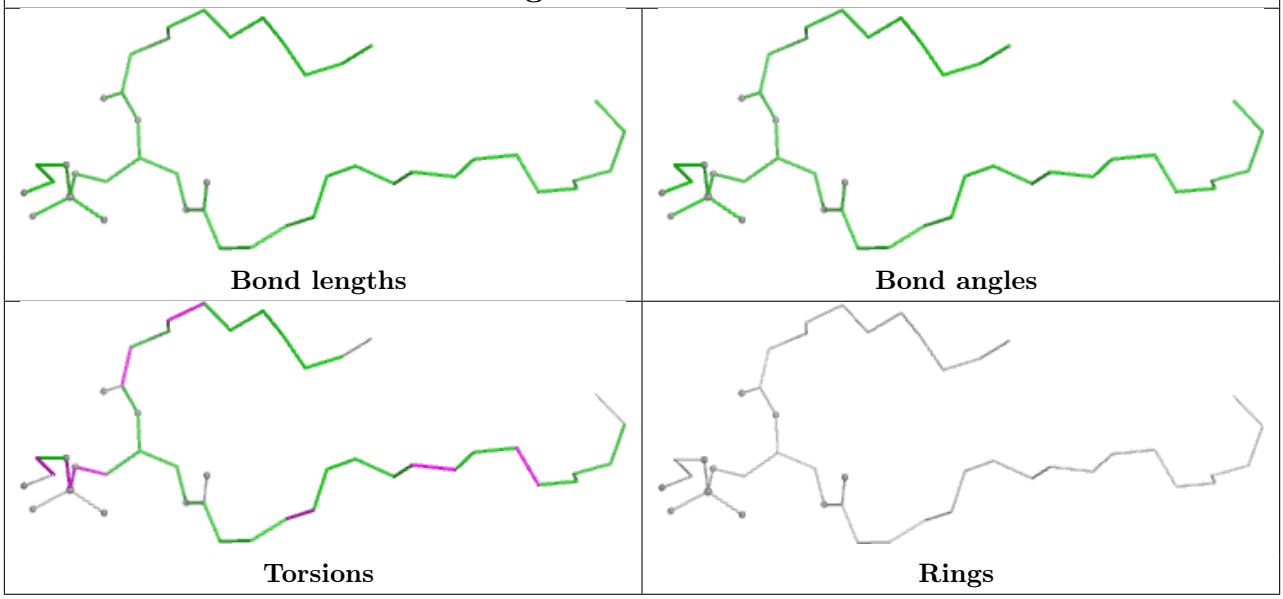
Ligand CDL V 203



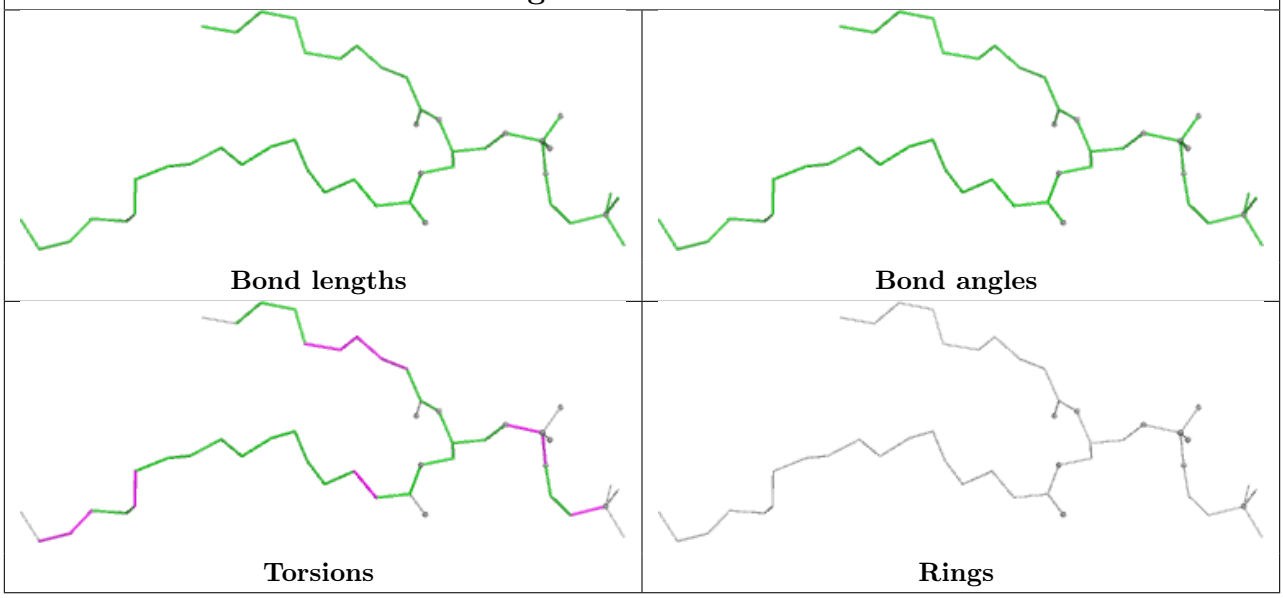
Ligand 3PE A 403



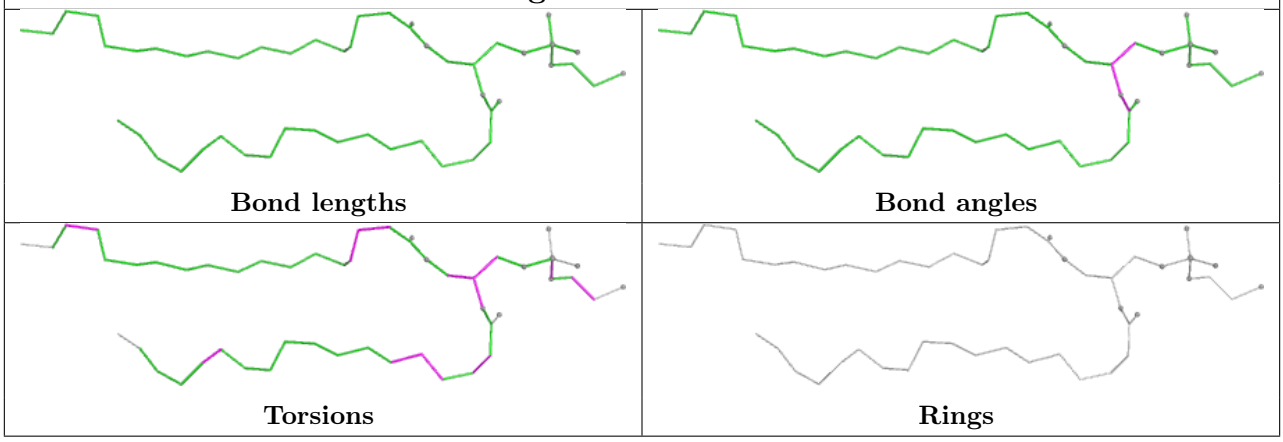
Ligand 3PE M 501



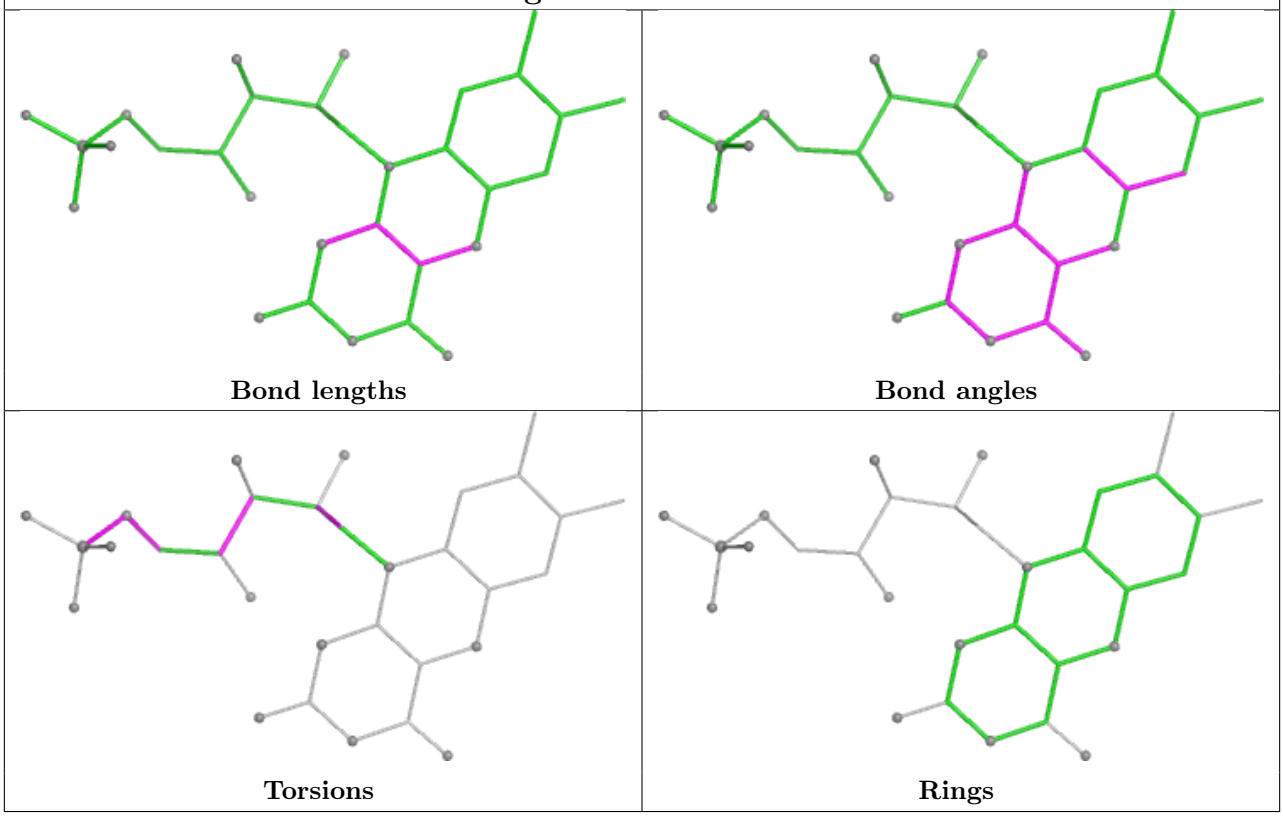
Ligand PC1 A 401



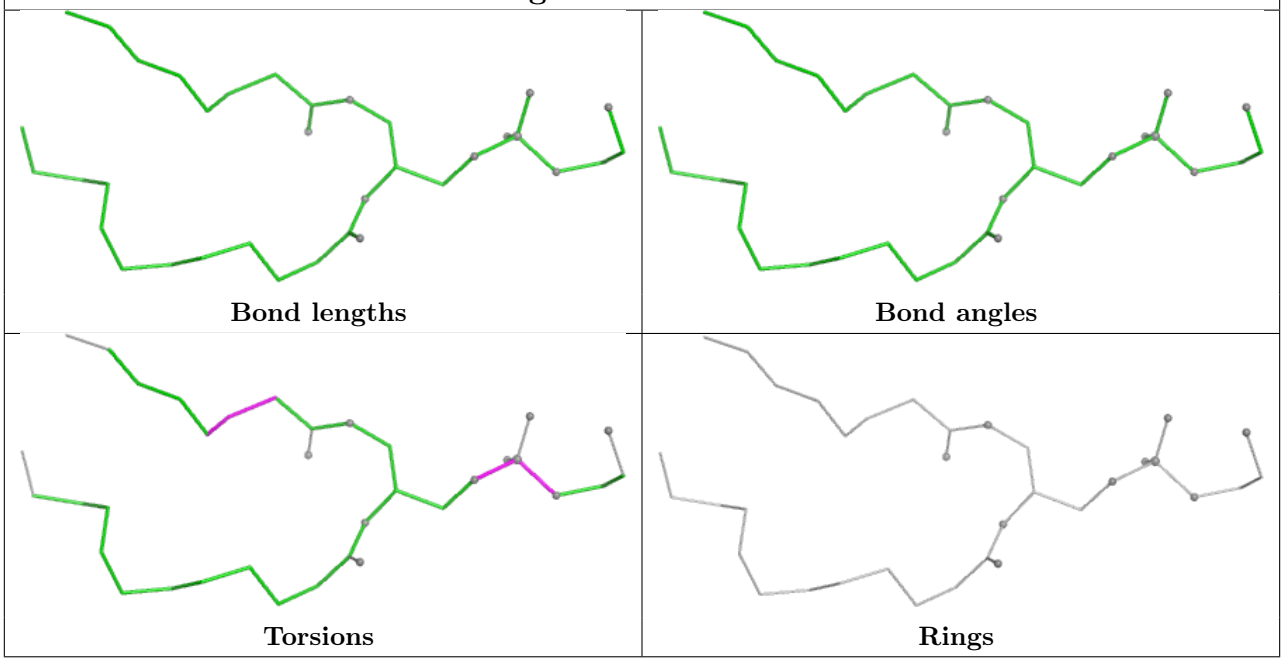
Ligand 3PE N 401

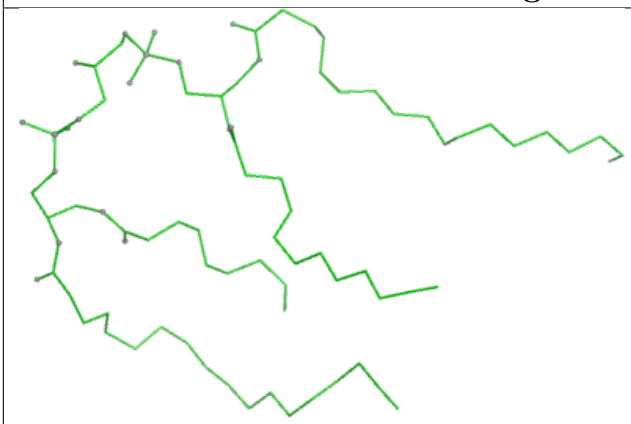
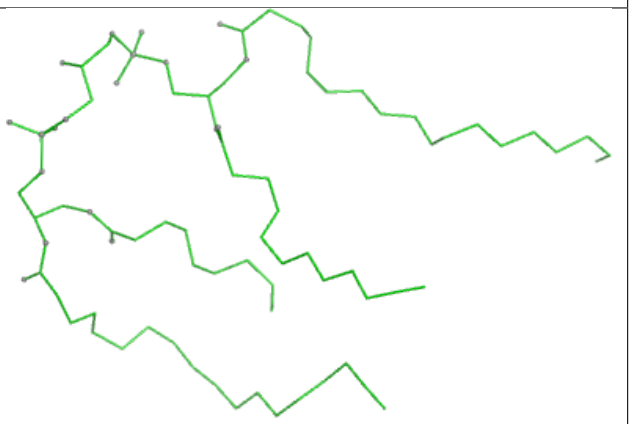
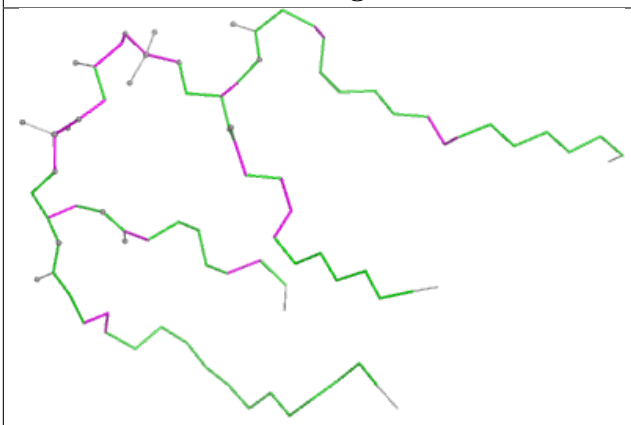
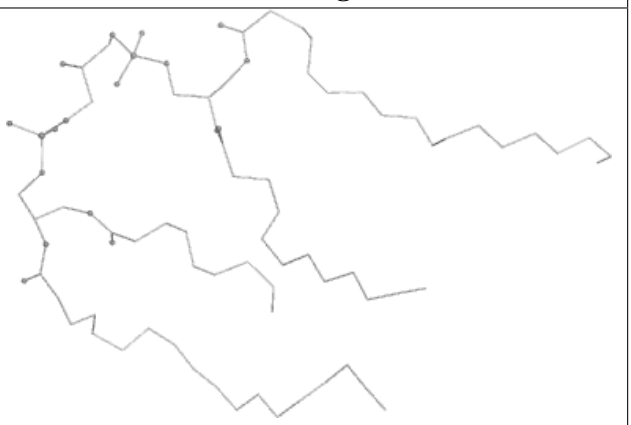


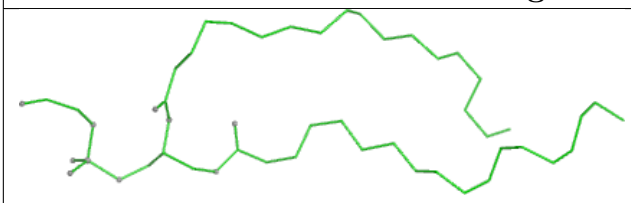
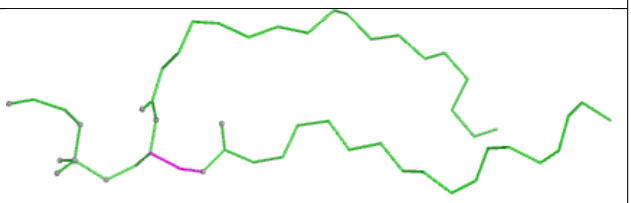
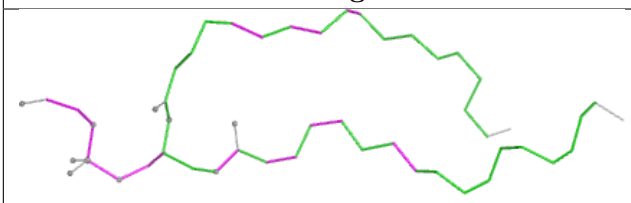
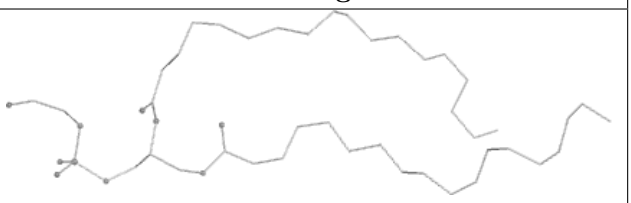
Ligand FMN 1 502

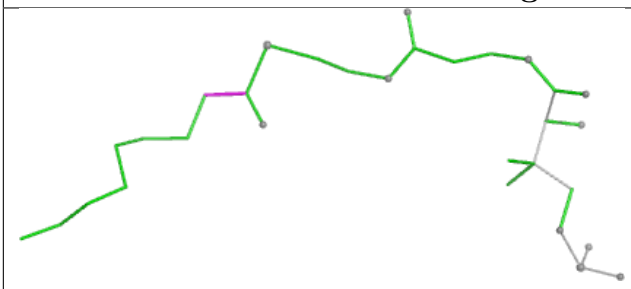
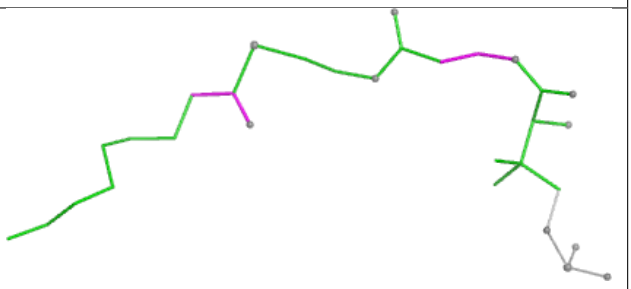
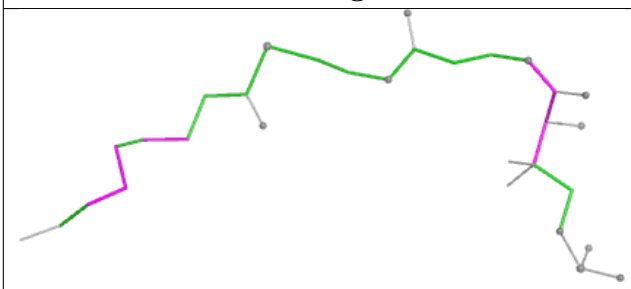
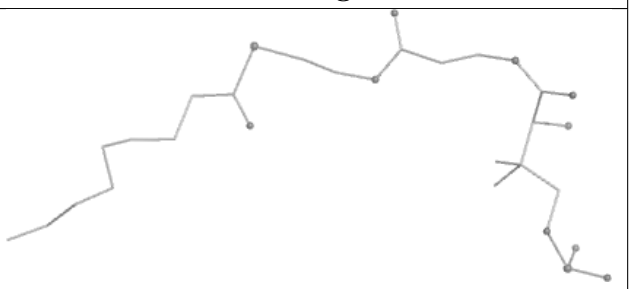


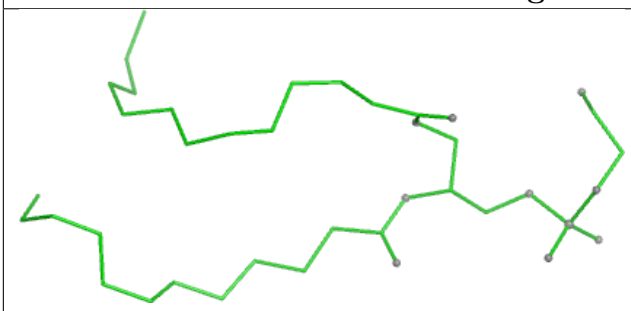
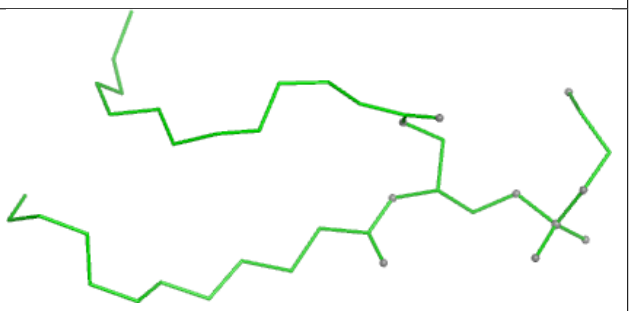
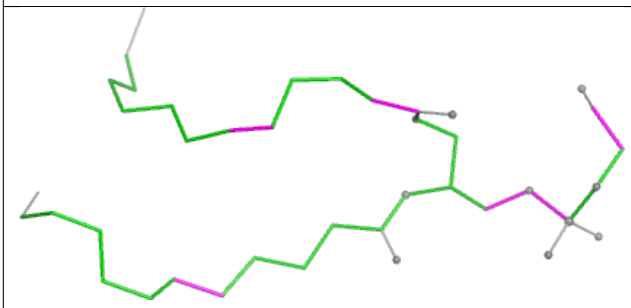
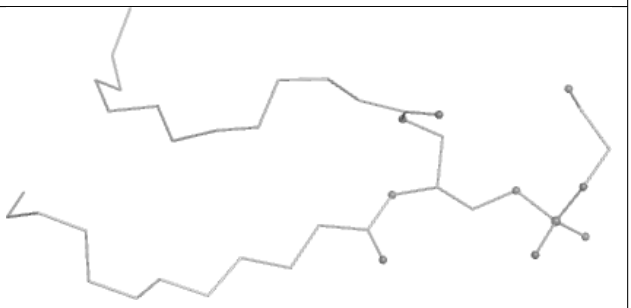
Ligand 3PE V 201

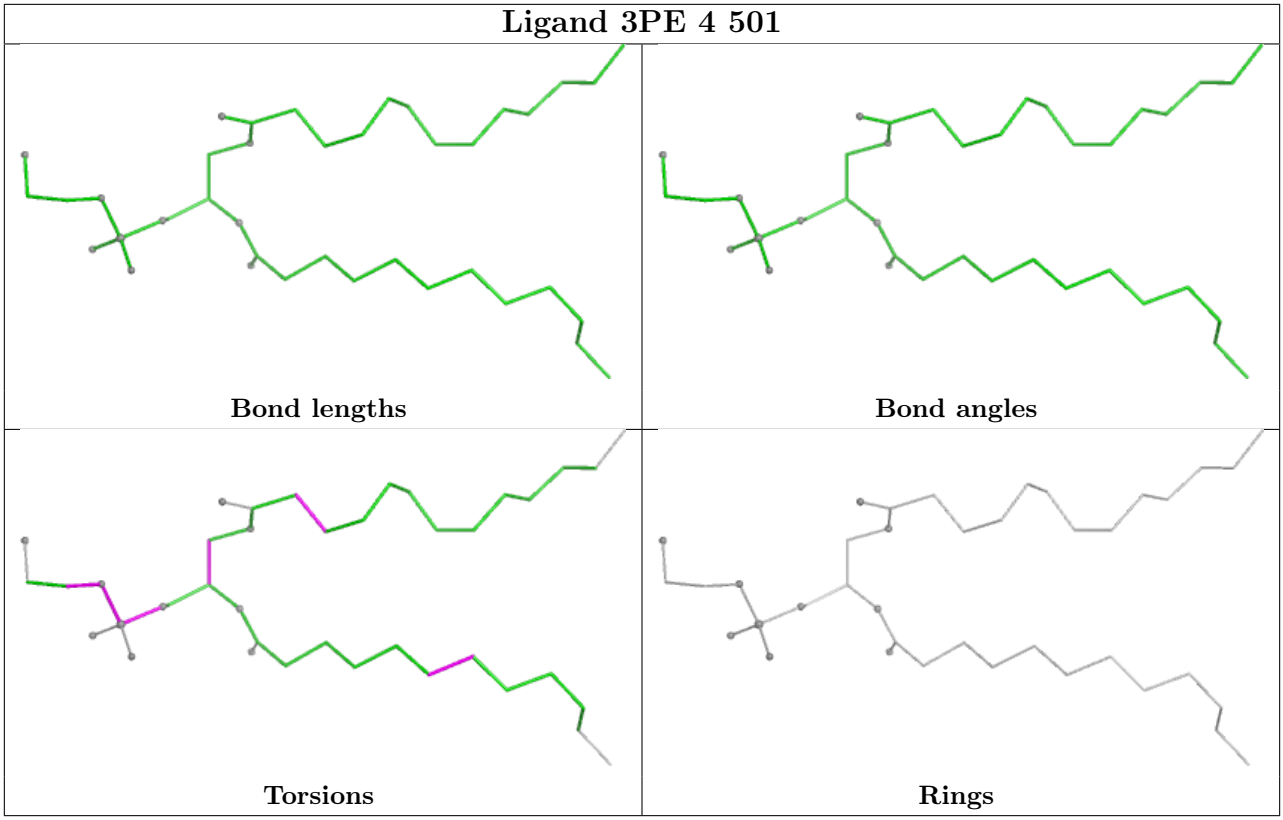


Ligand CDL V 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE H 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ZMP X 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings



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.

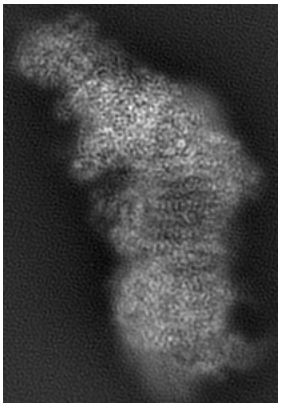
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11245. These allow visual inspection of the internal detail of the map and identification of artifacts.

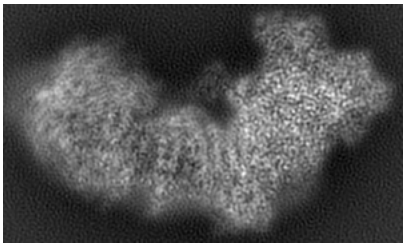
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

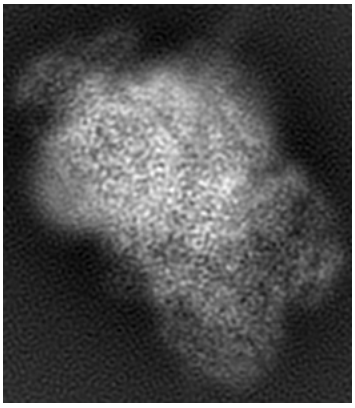
6.1.1 Primary map



X



Y

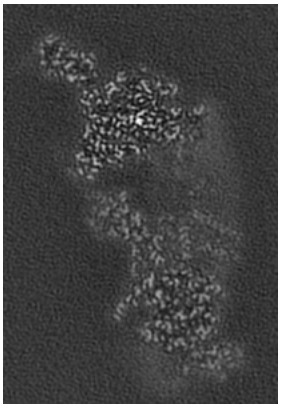


Z

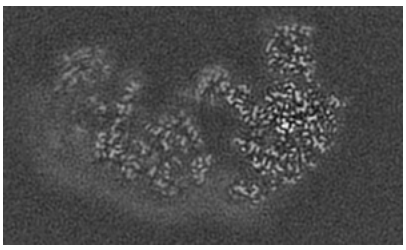
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

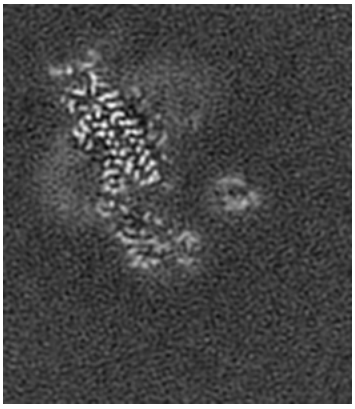
6.2.1 Primary map



X Index: 80



Y Index: 92

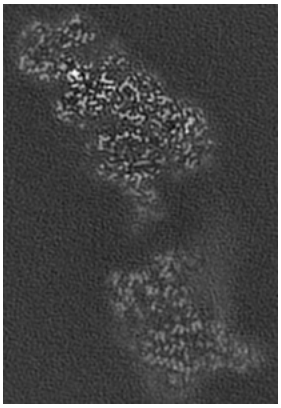


Z Index: 135

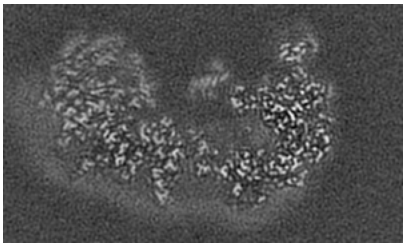
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

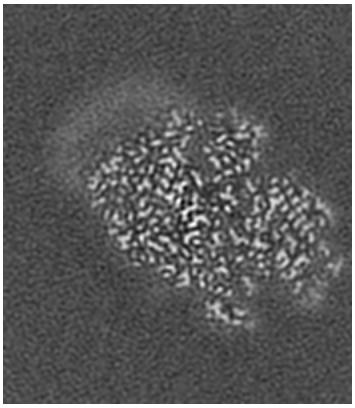
6.3.1 Primary map



X Index: 99



Y Index: 102

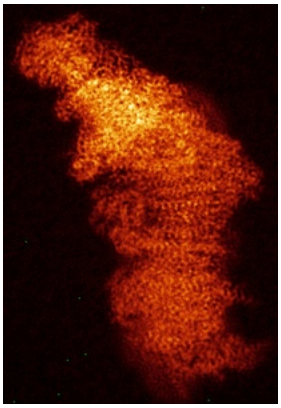


Z Index: 196

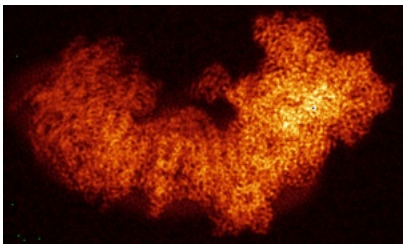
The images above show the largest variance slices of the map in three orthogonal directions.

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

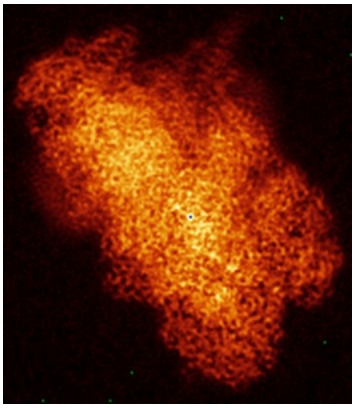
6.4.1 Primary map



X



Y

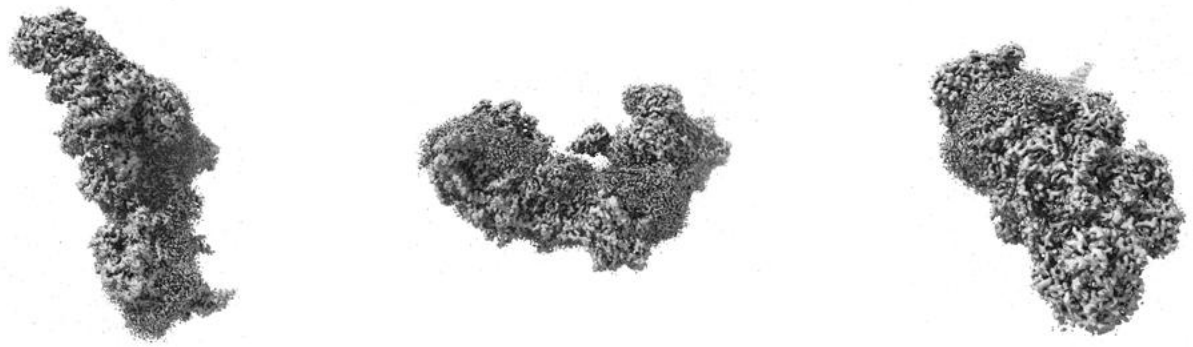


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

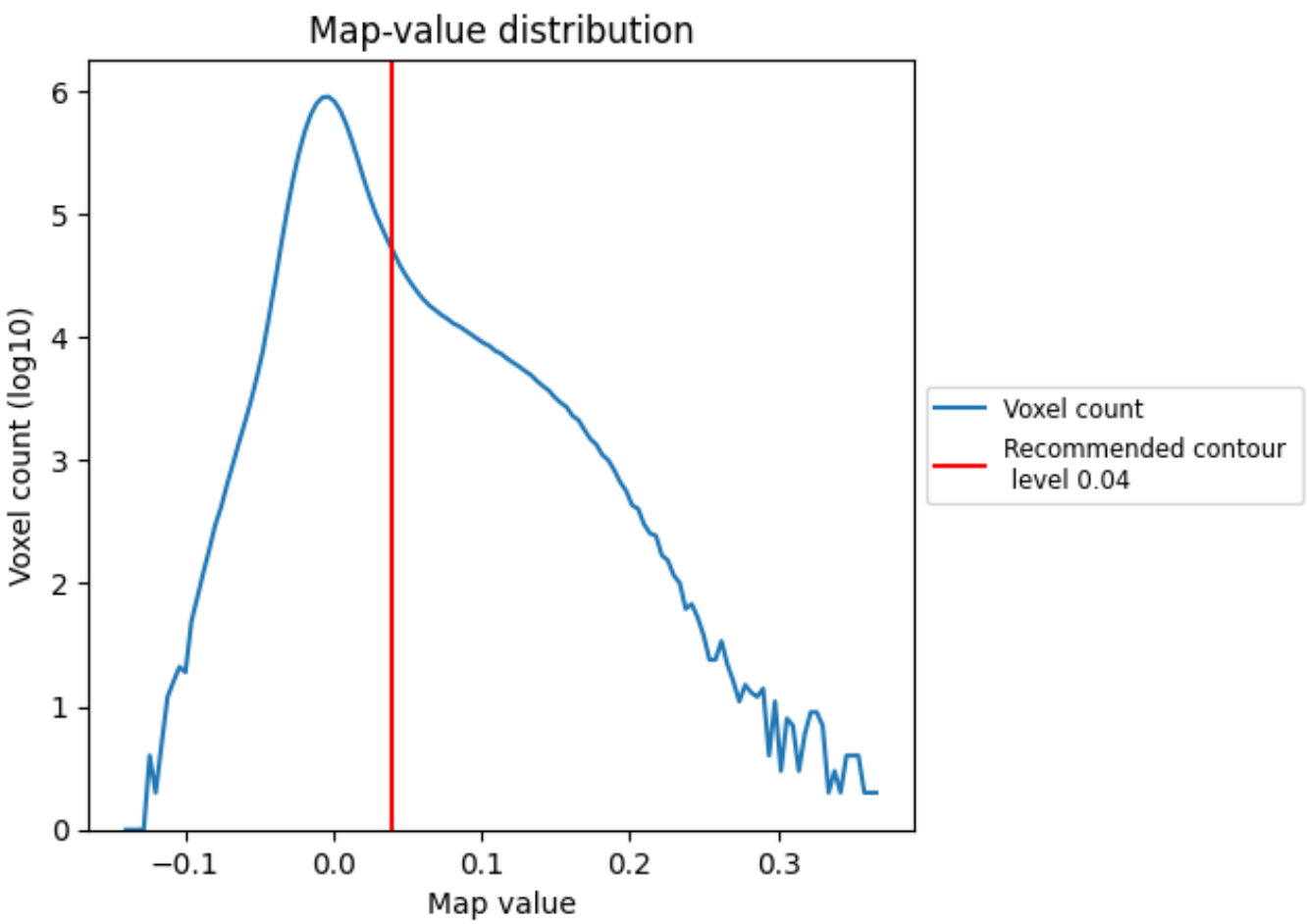
6.6 Mask visualisation (i)

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

7 Map analysis (i)

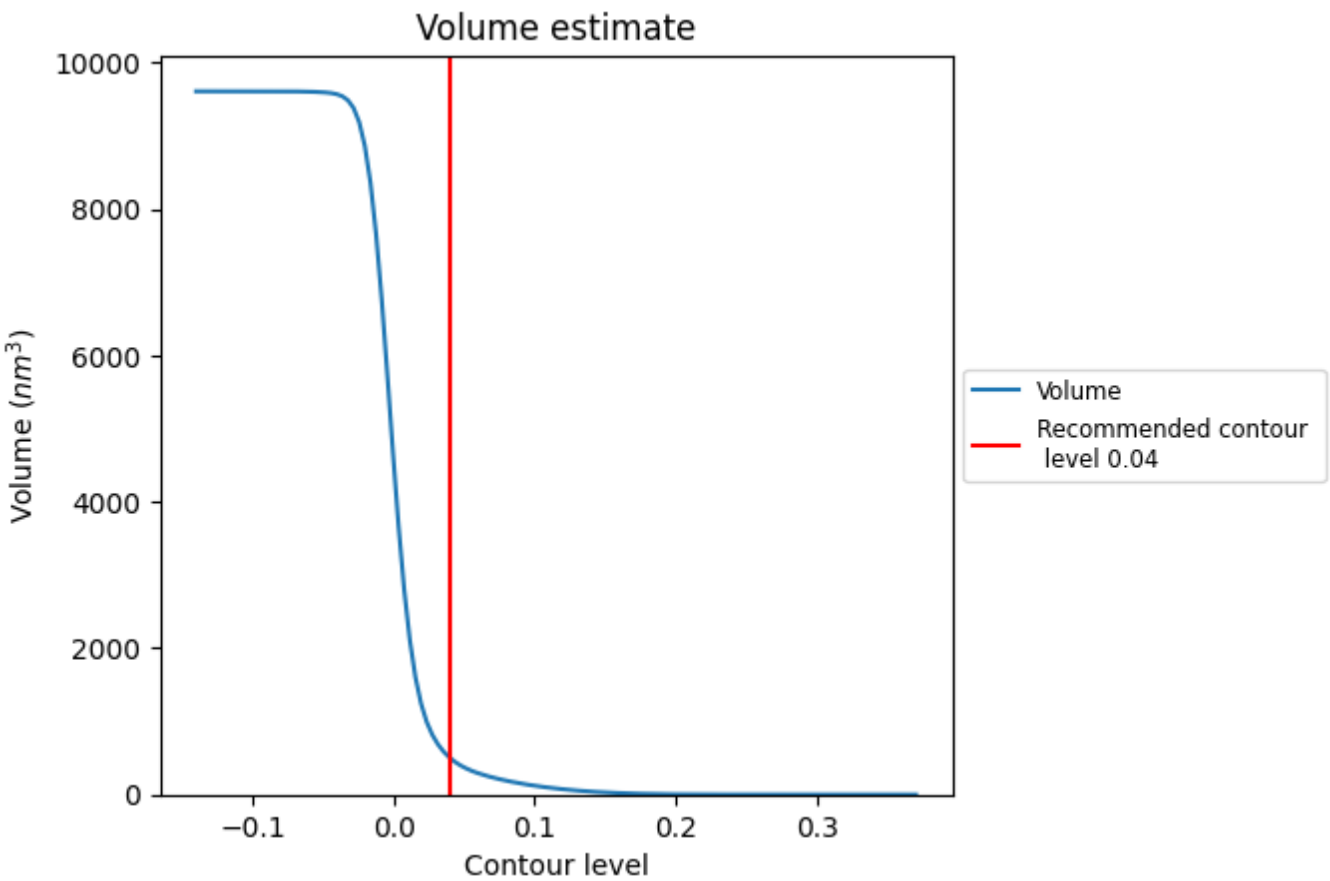
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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 500 nm^3; this corresponds to an approximate mass of 452 kDa.

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

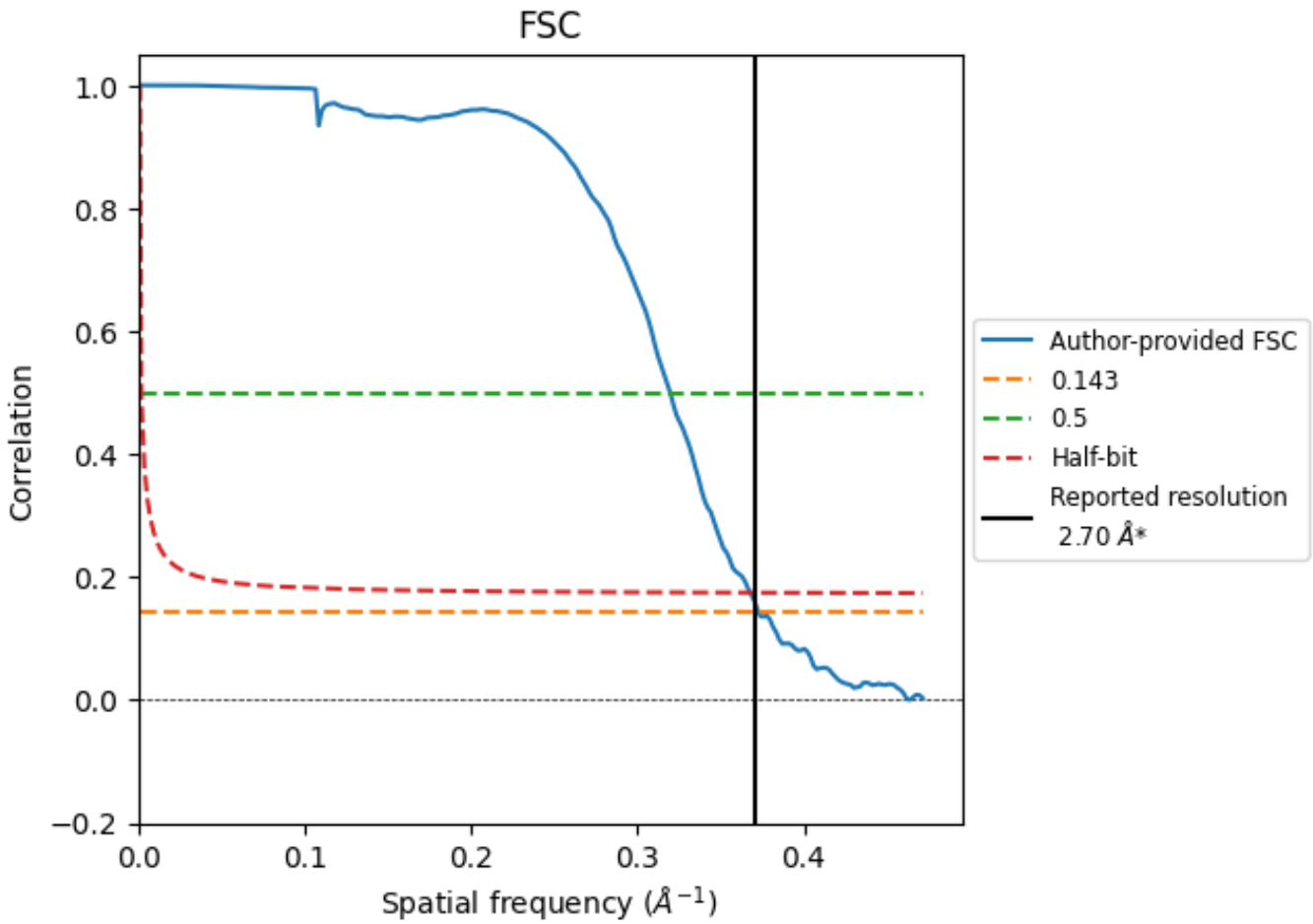
7.3 Rotationally averaged power spectrum (i)

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

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates (i)

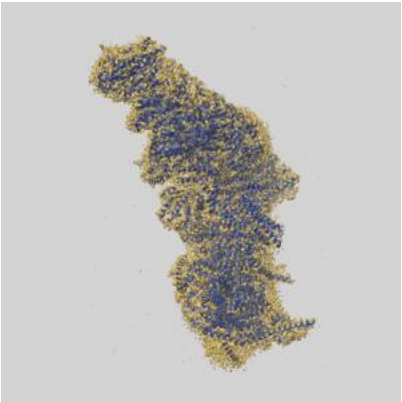
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.68	3.13	2.72
Unmasked-calculated*	-	-	-

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

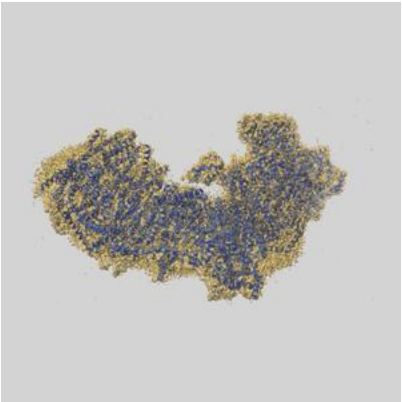
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11245 and PDB model 6ZKD. Per-residue inclusion information can be found in section 3 on page 20.

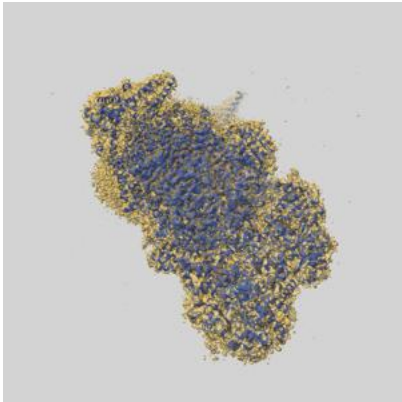
9.1 Map-model overlay (i)



X



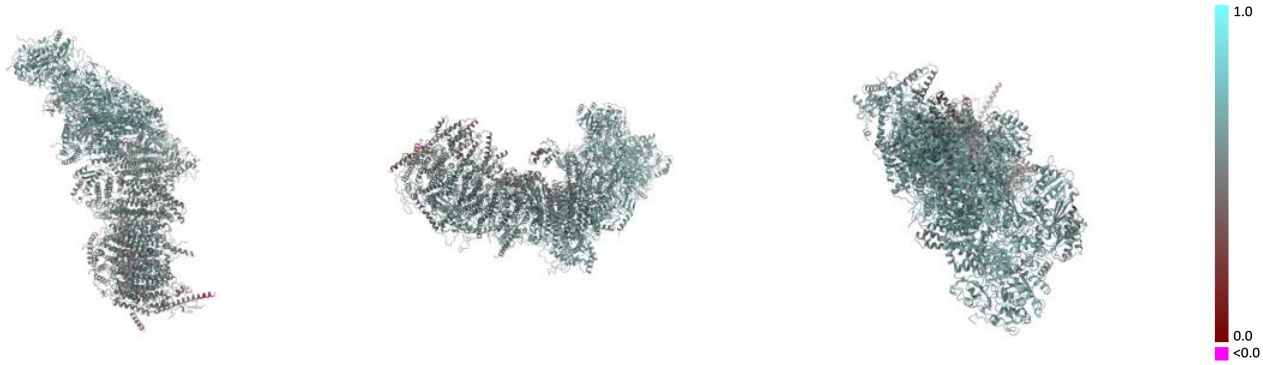
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

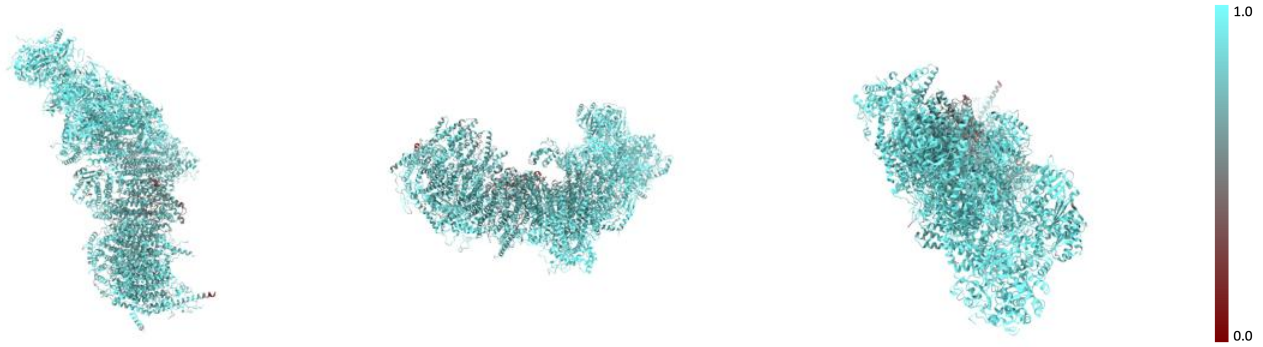
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

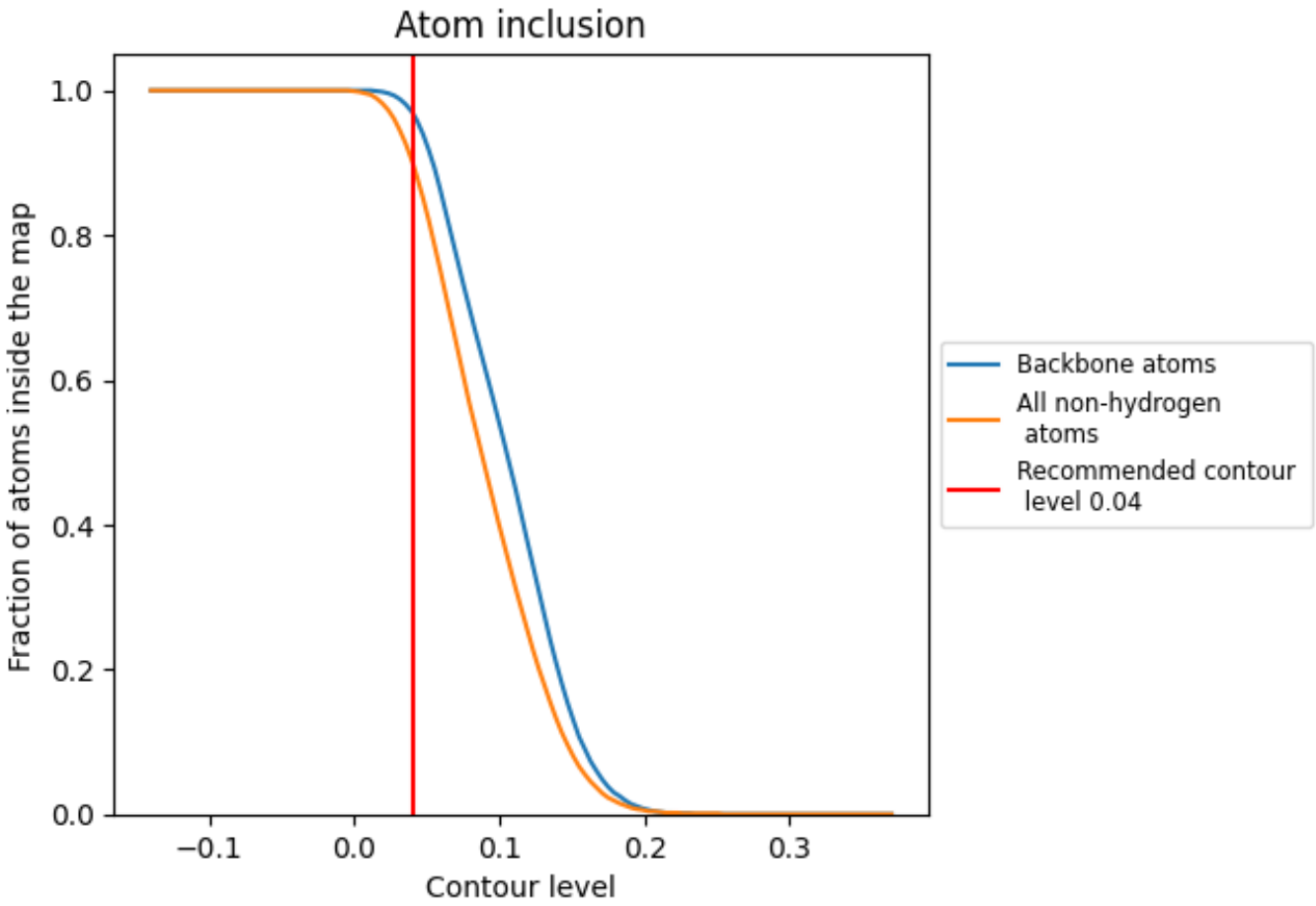
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9020	0.5790
1	0.9630	0.6050
2	0.9360	0.5960
3	0.9470	0.6130
4	0.9370	0.6240
5	0.9610	0.6370
6	0.9640	0.6290
9	0.9650	0.6400
A	0.8230	0.5560
H	0.9360	0.6110
J	0.8600	0.5580
K	0.9070	0.5940
L	0.8720	0.5570
M	0.9380	0.6060
N	0.9450	0.6120
V	0.5810	0.4830
W	0.8970	0.5820
X	0.7990	0.4760
Y	0.9050	0.5780
Z	0.8950	0.5510
a	0.9610	0.6000
b	0.9420	0.6210
c	0.9330	0.6220
d	0.9300	0.5910
e	0.9020	0.5590
f	0.9050	0.5860
g	0.9190	0.6030
h	0.9380	0.6140
i	0.9280	0.6170
j	0.7970	0.4740
k	0.8720	0.5490
l	0.9010	0.5600
m	0.9230	0.5800
n	0.7830	0.4420
o	0.8810	0.5750

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Chain	Atom inclusion	Q-score
p	0.8220	0.5130
q	0.9460	0.5930
r	0.8560	0.5050
s	0.8020	0.4510
t	0.8290	0.4980
u	0.8290	0.4680
v	0.8620	0.5110
w	0.8560	0.5480
x	0.8590	0.5380
y	0.8700	0.5460
z	0.9440	0.6020