wwPDB EM Validation Summary Report (i)

Sep 8, 2026 – 05:12 pm BST

PDB ID	:	8RGQ / pdb_00008rgq
EMDB ID	:	EMD-19146
Title	:	Open Complex I from murine liver
Authors	:	Vercellino, I.; Sazanov, L.A.
Deposited on	:	2023-12-14
Resolution	:	3.00 Å(reported)
Based on initial model	:	6g2j

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

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

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

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

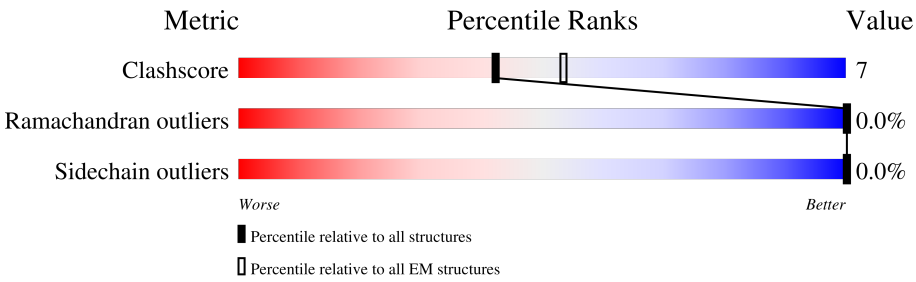
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

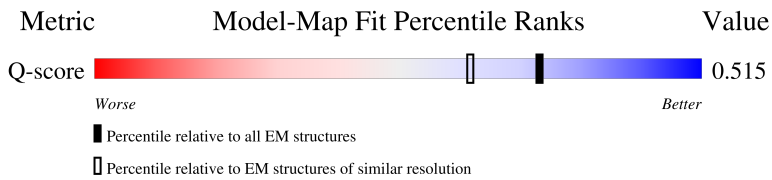
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	6	224	56% 14% 30%
2	C	263	62% 17% 21%
3	D	463	5% 72% 18% 10%
4	2	248	74% 12% 14%

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Mol	Chain	Length	Quality of chain
5	1	464	78% 15% 7%
6	3	727	80% 15% 5%
7	9	212	65% 19% 16%
8	P	377	6% 69% 14% 17%
9	Q	175	58% 14% 28%
10	7	116	72% 10% 17%
11	S	99	75% 10% 15%
12	T	156	41% 10% 49%
12	U	156	44% 13% 44%
13	V	116	87% 10%
14	W	131	72% 15% 13%
15	q	145	89% 11%
16	r	113	72% 14% 14%
17	s	104	36% 5% 60%
18	A	115	66% 15% 19%
19	H	318	72% 24%
20	J	172	11% 77% 19%
21	K	98	81% 18%
22	L	607	79% 21%
23	M	459	77% 23%
24	N	345	79% 21%
25	O	355	74% 16% 10%
26	X	172	81% 18%
27	Y	141	82% 17%
28	Z	144	83% 15%

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Mol	Chain	Length	Quality of chain
29	a	70	71% 29%
30	b	84	92% 6%
31	c	76	55% 8% 37%
32	d	120	91% 9%
33	e	106	85% 14%
34	f	57	7% 84% 9% 7%
35	g	151	7% 56% 11% 33%
36	h	189	63% 11% 26%
37	i	128	10% 73% 10% 17%
38	j	105	56% 6% 38%
39	k	104	68% 6% 26%
40	l	186	67% 18% 16%
41	m	129	5% 78% 19%
42	n	179	84% 15%
43	o	137	74% 12% 14%
44	p	176	82% 14%

2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 67118 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] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	6	157	1258	802	227	215	14	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	208	1730	1116	297	314	3	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	418	3371	2156	577	614	24	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	2	214	1660	1056	279	314	11	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	1	430	3321	2092	596	611	22	0	0

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	3	690	5305	3326	921	1017	41	0	0

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	9	178	1431	898	245	276	12	0	0

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	P	314	2513	1611	453	442	7	0	0

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	Q	126	1022	646	180	192	4	0	0

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	7	96	758	470	141	144	3	0	0

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	S	84	671	421	127	120	3	0	0

- Molecule 12 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	T	79	637	410	95	127	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	U	88	706	453	104	144	5	0	0

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	V	113	923	602	153	165	3	0	0

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

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

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	q	145	1209	777	215	212	5	0	0

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	r	97	781	493	146	139	3	0	0

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	s	42	351	219	62	70	0	0

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	A	93	760	527	104	124	5	0	0

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	H	306	2452	1652	371	407	22	0	0

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	J	165	1246	837	178	216	15	0	0

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

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

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase chain 5.

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

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	N	345	2703	1795	417	454	37	0	0

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

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

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	a	70	572	370	101	97	4	0	0

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	b	82	643	422	104	113	4	0	0

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

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

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

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	g	101	850	549	136	161	4	0	0

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	h	139	1166	764	195	204	3	0	0

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	i	106	897	584	157	152	4	0	0

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	j	65	562	370	93	98	1	0	0

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	k	77	626	414	106	104	2	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	l	157	1323	855	220	237	11	0	0

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	n	178	1541	985	276	269	11	0	0

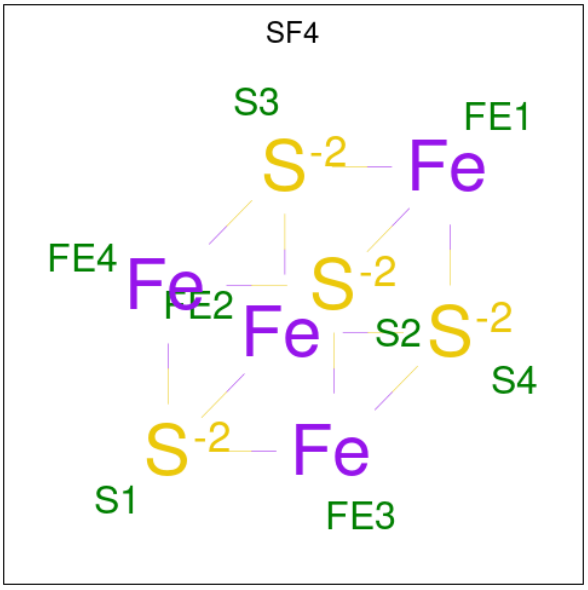
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	o	118	1014	639	190	177	8	0	0

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

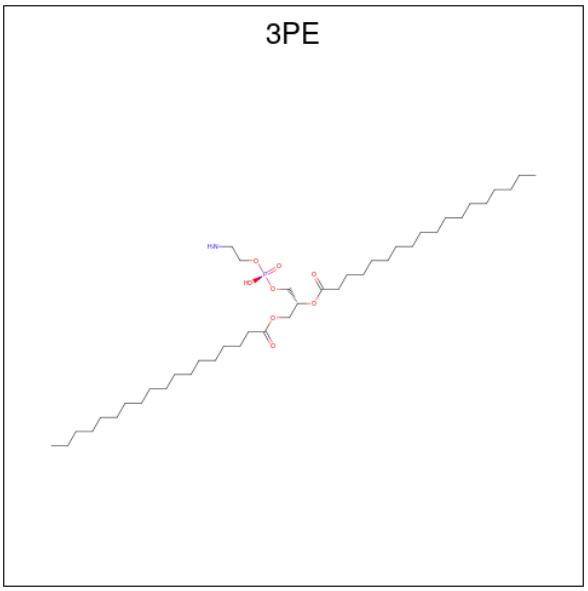
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	p	169	1430	899	257	266	8	0	0

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



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	6	1	8	4	4	0
45	1	1	8	4	4	0
45	3	1	8	4	4	0
45	3	1	8	4	4	0
45	9	1	8	4	4	0
45	9	1	8	4	4	0

- Molecule 46 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	
46	6	1	32	22	1	8	1	0
			Total	C	N	O	P	
46	r	1	46	36	1	8	1	0
			Total	C	N	O	P	
46	A	1	43	33	1	8	1	0
			Total	C	N	O	P	
46	H	1	51	41	1	8	1	0
			Total	C	N	O	P	
46	K	1	41	31	1	8	1	0
			Total	C	N	O	P	
46	L	1	51	41	1	8	1	0
			Total	C	N	O	P	
46	L	1	51	41	1	8	1	0
			Total	C	N	O	P	
46	M	1	51	41	1	8	1	0
			Total	C	N	O	P	
46	M	1	51	41	1	8	1	0
			Total	C	N	O	P	
46	M	1	36	26	1	8	1	0
			Total	C	N	O	P	
46	N	1	38	28	1	8	1	0
			Total	C	N	O	P	
46	Y	1	28	18	1	8	1	0
			Total	C	N	O	P	
46	Y	1	42	32	1	8	1	0
			Total	C	N	O	P	
46	d	1	31	21	1	8	1	0

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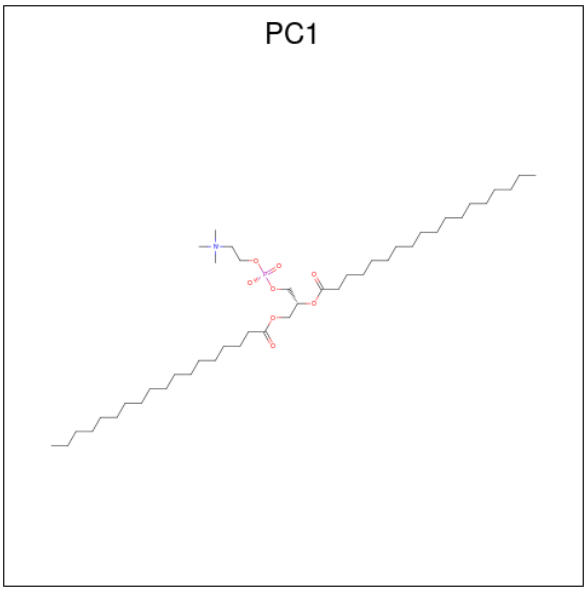
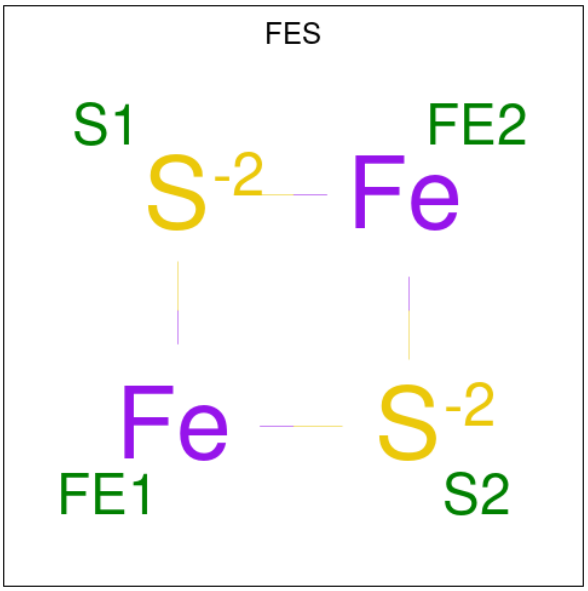
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	d	1	32	22	1	8	1	0
			Total	C	N	O	P	
46	i	1	42	32	1	8	1	0
			Total	C	N	O	P	
46	m	1	30	20	1	8	1	0

- Molecule 47 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



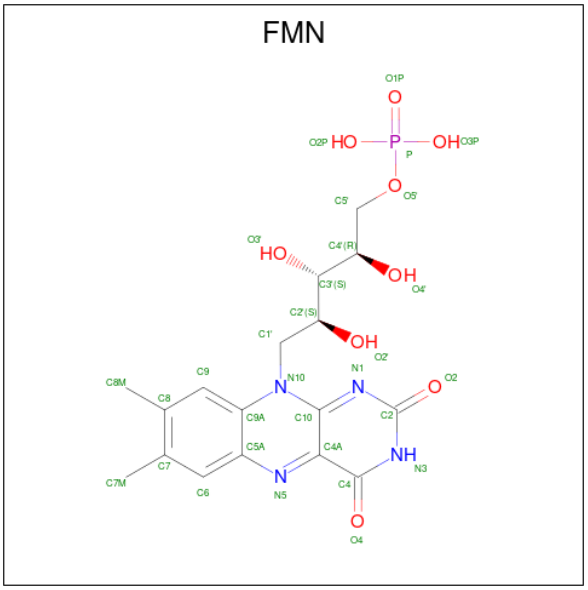
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	6	1	43	33	1	8	1	0
			Total	C	N	O	P	
47	9	1	54	44	1	8	1	0
			Total	C	N	O	P	
47	9	1	47	37	1	8	1	0
			Total	C	N	O	P	
47	M	1	54	44	1	8	1	0

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



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

- Molecule 49 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

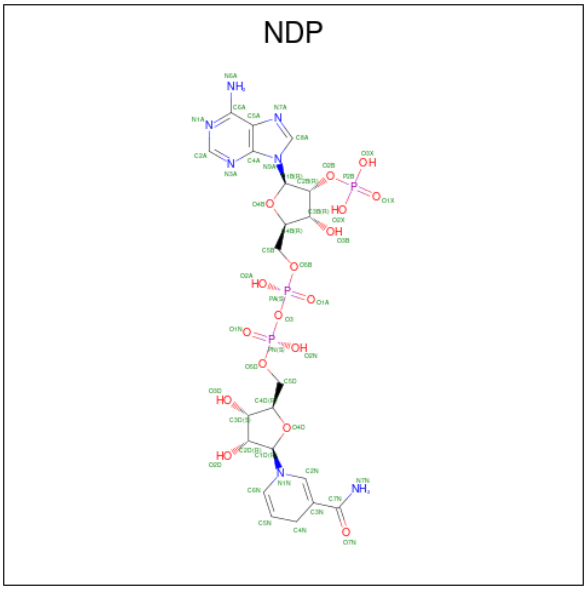


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	1	1	31	17	4	9	1	0

- Molecule 50 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
50	3	1	1	1	0

- Molecule 51 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	
51	P	1	48	21	7	17	3	0

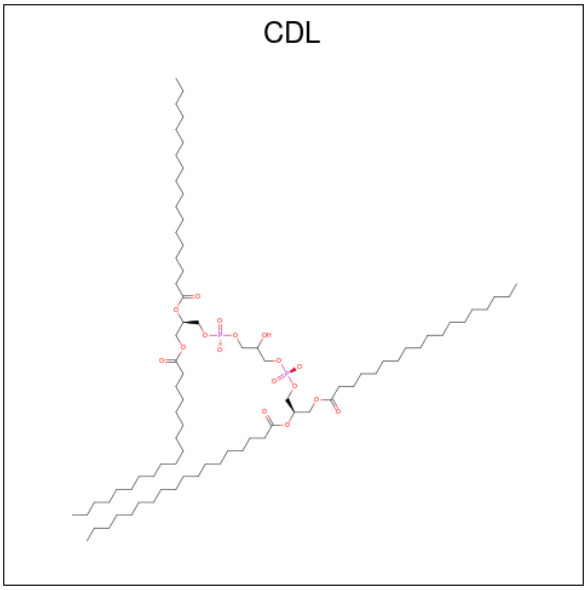
- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
52	7	1	1	1	0

- Molecule 53 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	
53	W	1	34	23	2	7	1	1	0
			Total	C	N	O	P	S	
53	n	1	32	21	2	7	1	1	0

- Molecule 54 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



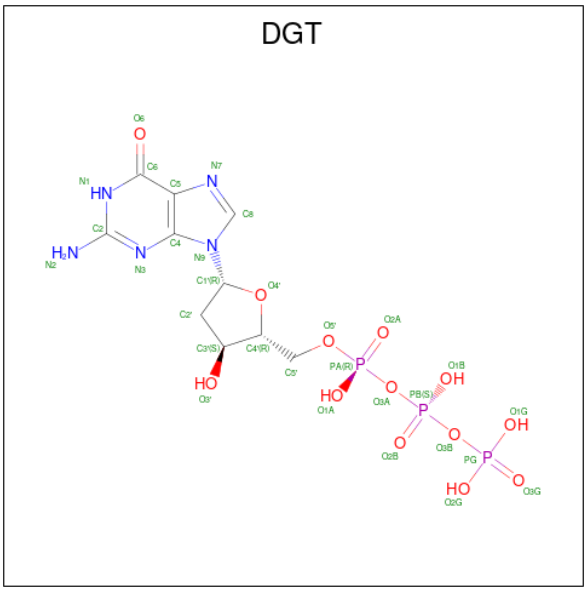
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
54	r	1	57	38	17	2	0
			Total	C	O	P	
54	L	1	78	59	17	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
54	N	1	90	71	17	2	0
			Total	C	O	P	
54	d	1	67	48	17	2	0
			Total	C	O	P	
54	h	1	70	51	17	2	0
			Total	C	O	P	
54	m	1	72	53	17	2	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).

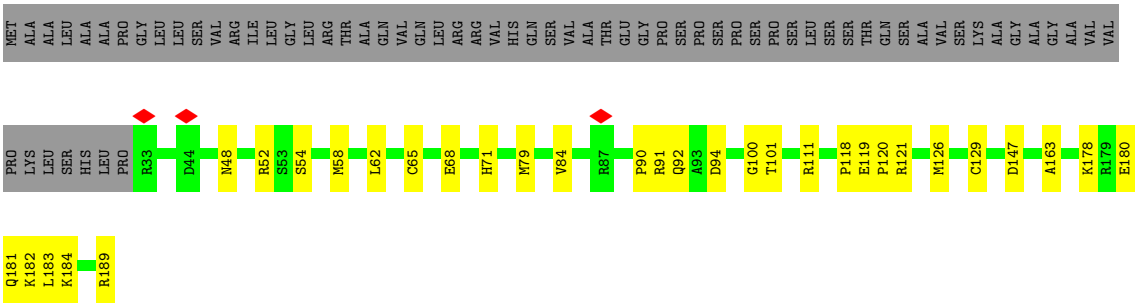
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
56	O	1	1	1	0

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.

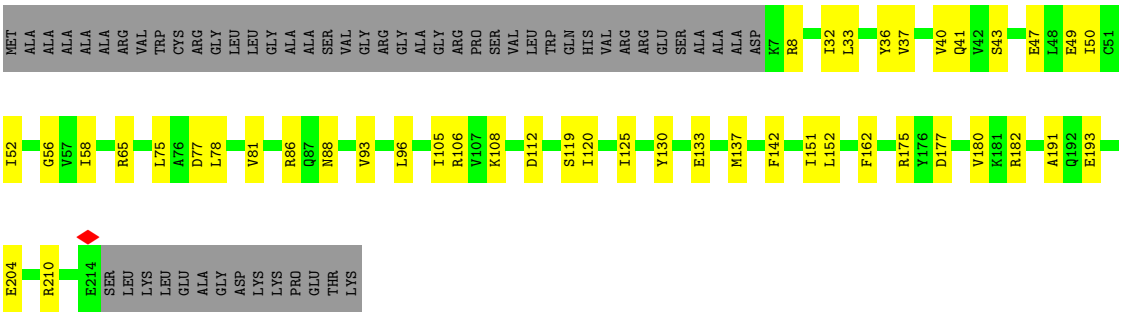
• Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain 6: 56% 14% 30%



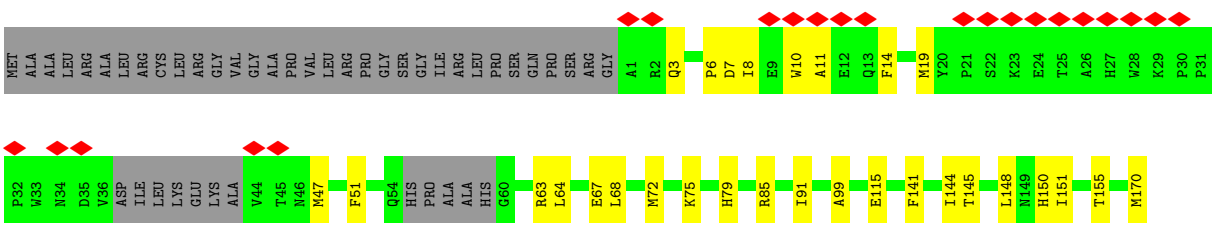
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C: 62% 17% 21%



• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D: 5% 72% 18% 10%



R174 E175 K176 M177 V184 R188 I194 R195 I211 R221 E224 V225 E226 E227 M228 L229 T230 W235 R236 N237 R238 T239 V240 D249 Y253 G257 L269 Y278 D279 Q280 V281 E282 F283 D284 V285 P286 D292 V301 E302 E303 Q313 C314 L315

I323 K324 A328 R335 K350 E354 Q357 P360 E368 A369 G372 E373 F374 S380 R388 K392 H398 K404 M410 L411 A412 D413 Q421 R430

- Molecule 4: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain 2: 74% 12% 14%

MET PHE SER LEU ALA LEU ARG ALA ARG ALA THR GLY LEU ALA ALA GLN TRP GLY ARG HIS ALA ARG ASN LEU HIS LYS THR ALA VAL HIS ASN GLY ALA GLY G4 A5 L6 N27 I31 N37 Y38 P39 V50 Q57 W60 P76 R79 E82 R92

T105 T106 P107 C108 T119 G129 I140 C144 V149 N150 A151 V154 E162 D163 L164 T165 P166 K183 P184 R190 F191 C192 C193 L217

- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1: 78% 15% 7%

MET LEU ALA ALA ARG HIS PHE LEU GLY GLY LEU VAL PRO VAL ARG VAL SER VAL ARG PHE SER SER GLY THR THR ALA PRO LYS K9 T45 L49 K61 R66 G72 L77 M82 K91 Y92 L93 V94 V95 N96 A97 D98 E99 G100 E101 C105 R112

L118 A131 R132 A133 A134 I138 R139 G140 E141 F142 E145 R154 Y171 D174 R179 G187 E188 E189 T190 A191 L192 P203 R204 G214 P219 T220 T221 V222 A223 N224 R247 N257 N263 T267 E270 S273 L276 L279 H283 A284

G285 G286 V287 L294 S303 L306 M317 T327 G328 I343 R349 D370 W371 M372 R378 A384 I399 M430 R438 ALA TRP GLN ALA ALA SER

- Molecule 6: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 3: 80% 15% 5%

MET LEU ARG ILE PRO ILE LYS ARG ALA LEU ILE GLY LEU SER ASN SER PRO LYS GLY TYR VAL ARG THR THR GLY THR ALA A5 L8 I9 E10 V11 F12 V13 M19 V20 T25 Q28 K32 V33 Q36 S47 P72 V73 A99 C105 C114 Q117

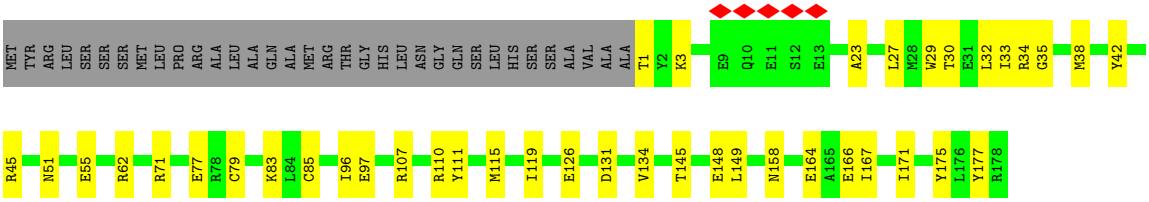
M121 D126 E132 G133 K134 I142 V146 I160 R161 F162 A163 A167 N179 V183 F191 I200 D201 S227 I228 M231 D232 R243 T244 G245 E246 P252 I263 K266 T267 R268 F269 A270 G273 L274 K275 R276 V284 E297 L300

S301 R302 A325 L328 L335 V338 F349 T356 L364 N365 T366 G370 L379 V380 G381 R396 V413 T416 Y419 E441 K444 V452 L453 A457 K488 N491 I492 L503 P509 T533 R534 L537 H549 M556 A557

D558 V559 A564 K569 S570 A571 Q582 T583 T588 G591 R601 A602 L603 D614 T615 L616 R620 Y633 E638 I668 K669 D670 F671 D675 S676 I677 A680 G694 ALA GLN ALA VAL GLU GLU PRO SER ILE CYS

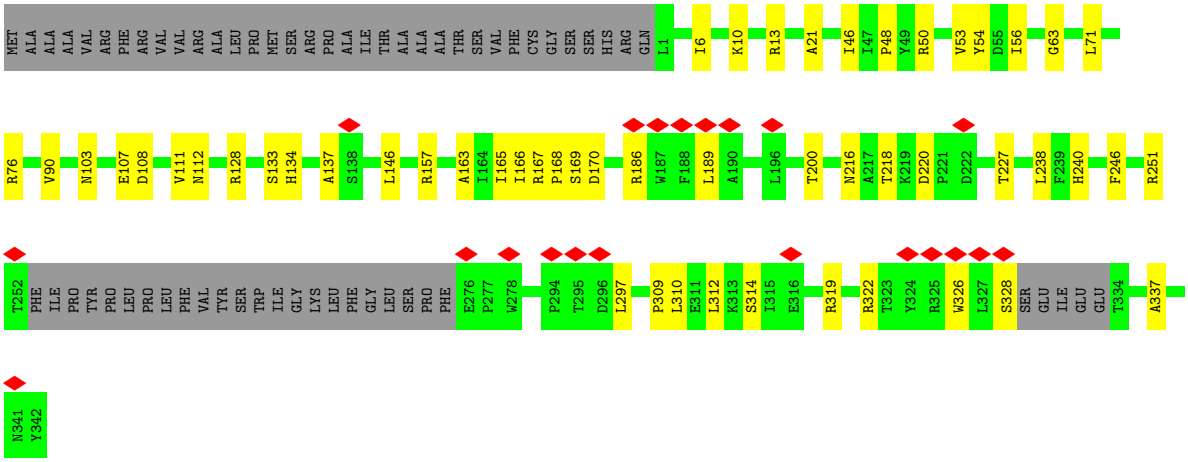
- Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 9:



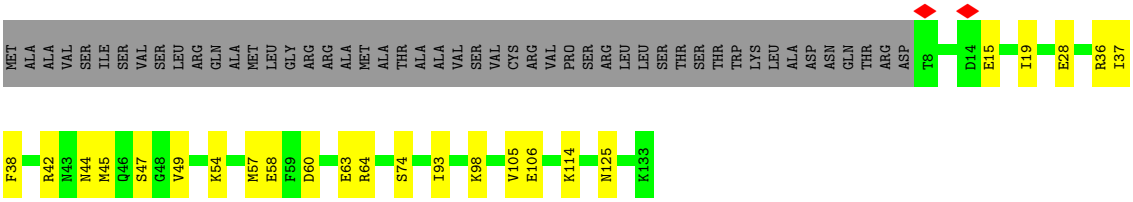
• Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:



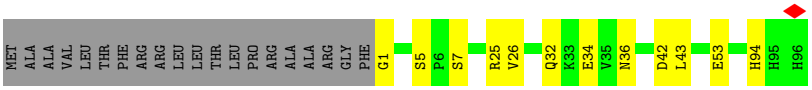
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:



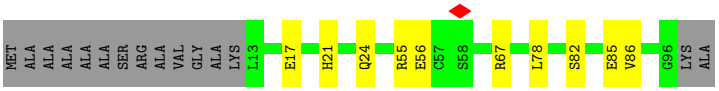
• Molecule 10: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain 7:



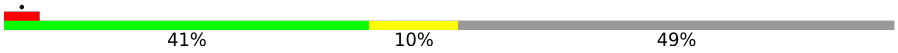
• Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

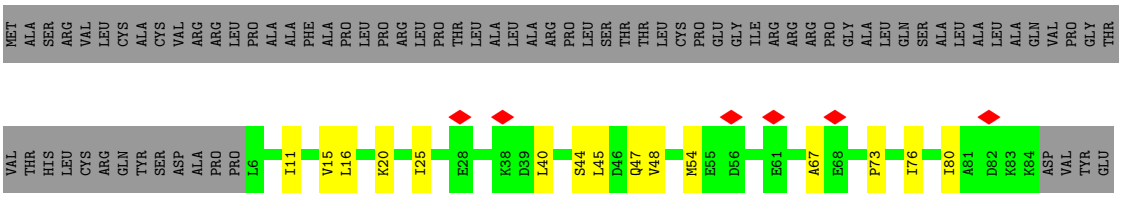
Chain S:



• Molecule 12: Acyl carrier protein, mitochondrial

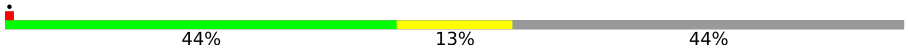
Chain T:

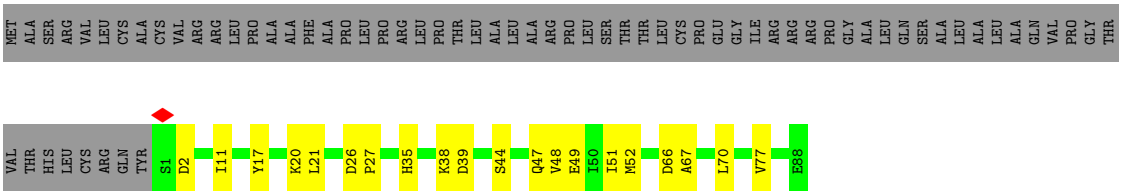




• Molecule 12: Acyl carrier protein, mitochondrial

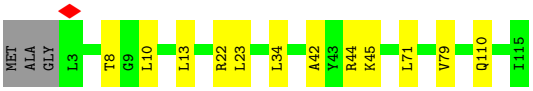
Chain U:





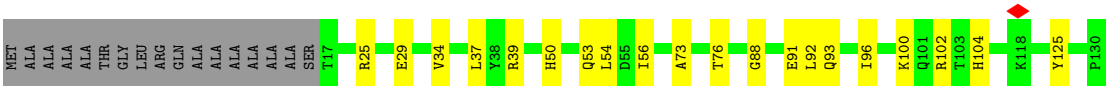
• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:



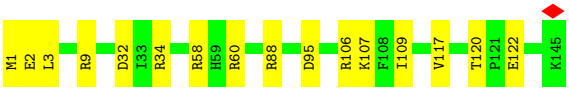
• Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:



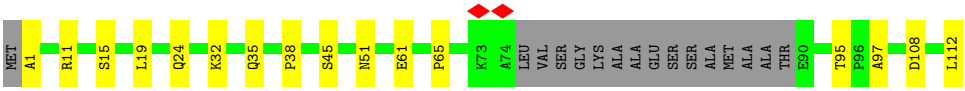
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:



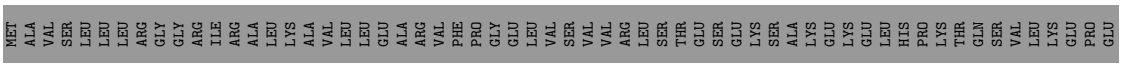
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

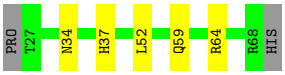
Chain r:



• Molecule 17: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

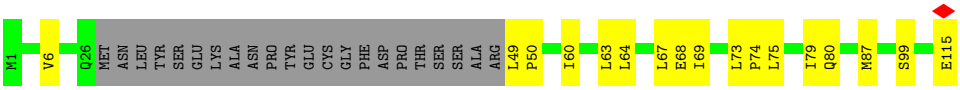
Chain s:





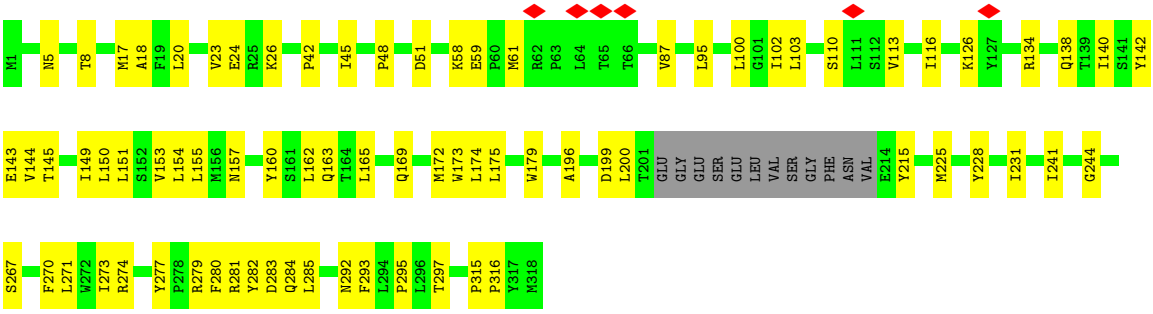
• Molecule 18: NADH-ubiquinone oxidoreductase chain 3

Chain A:



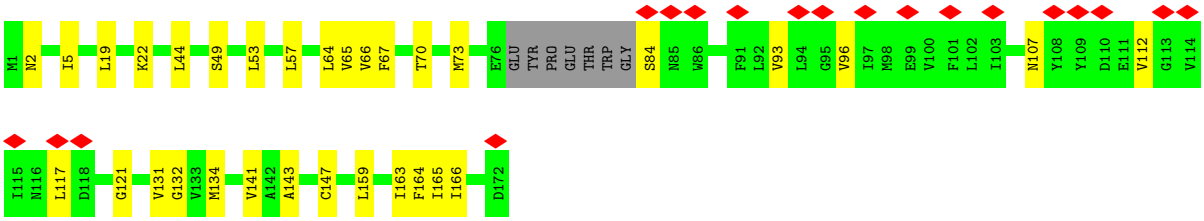
• Molecule 19: NADH-ubiquinone oxidoreductase chain 1

Chain H:



• Molecule 20: NADH-ubiquinone oxidoreductase chain 6

Chain J:

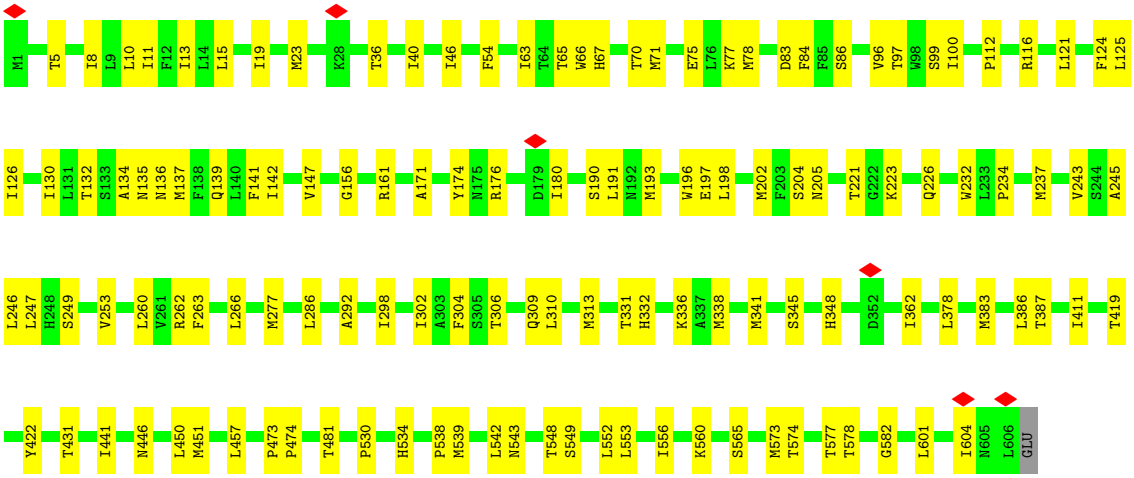


• Molecule 21: NADH-ubiquinone oxidoreductase chain 4L

Chain K:

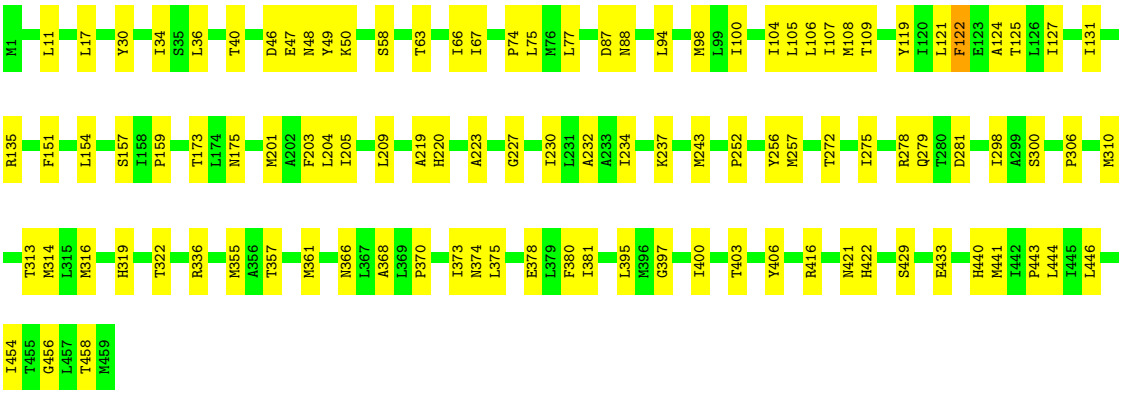
• Molecule 22: NADH-ubiquinone oxidoreductase chain 5

Chain L:



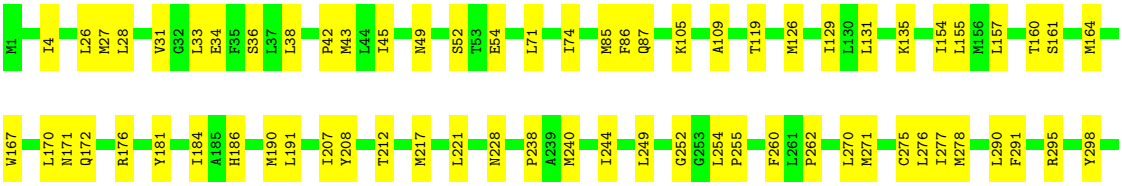
• Molecule 23: NADH-ubiquinone oxidoreductase chain 4

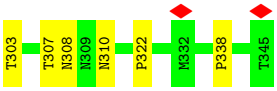
Chain M:



• Molecule 24: NADH-ubiquinone oxidoreductase chain 2

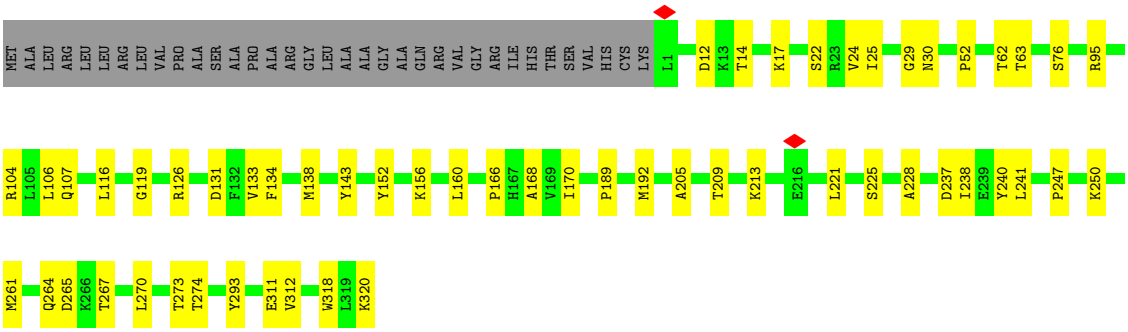
Chain N:





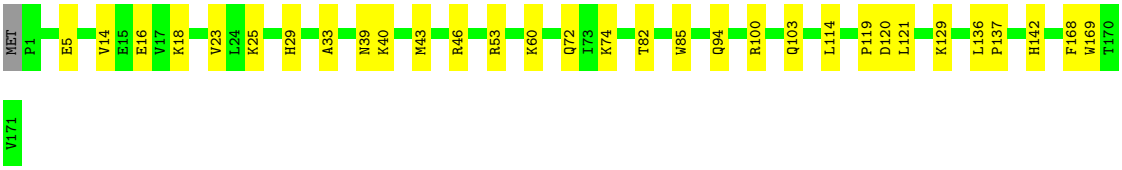
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:



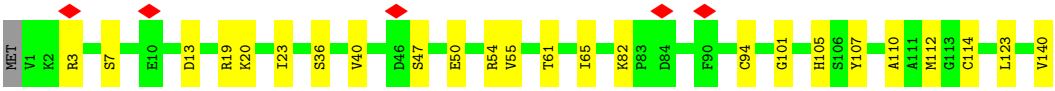
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:



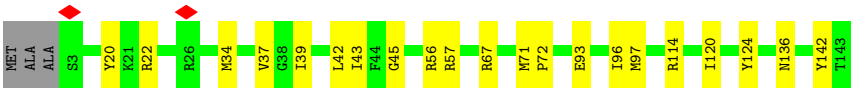
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:



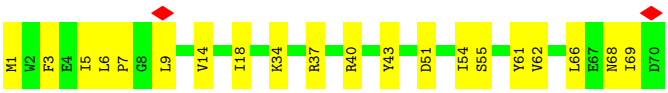
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:



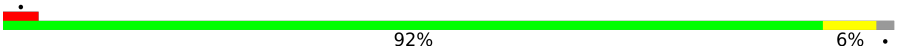
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

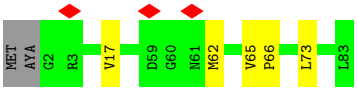
Chain a:



• Molecule 30: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

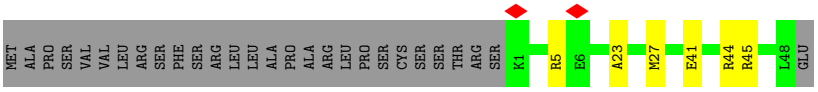
Chain b:





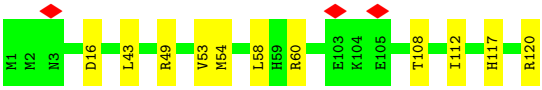
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c:



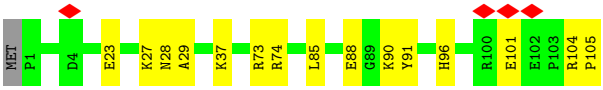
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:



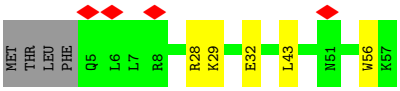
• Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:



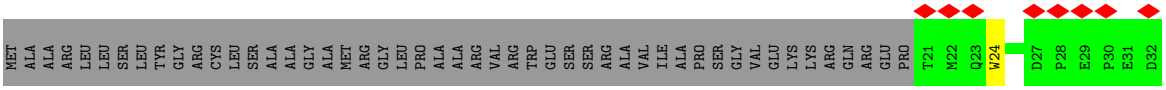
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

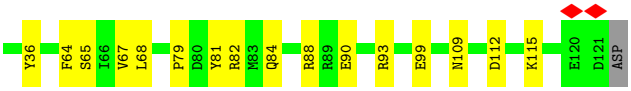
Chain f:



• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

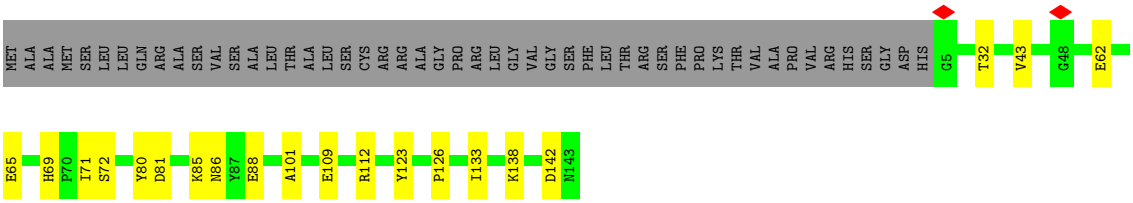
Chain g:





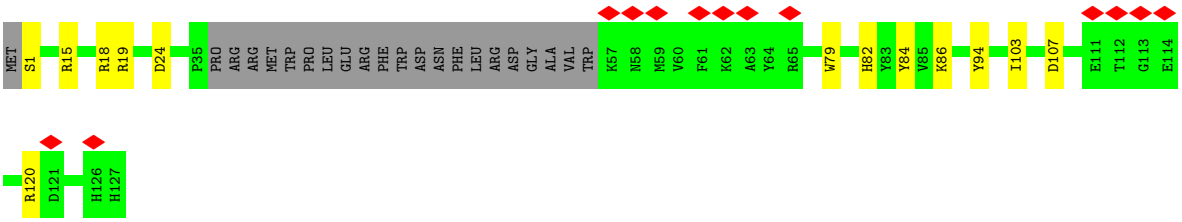
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:



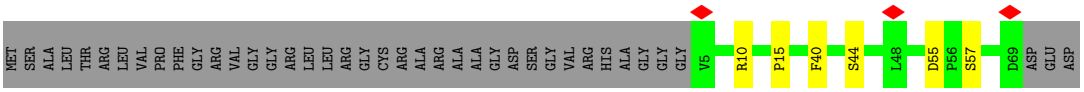
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



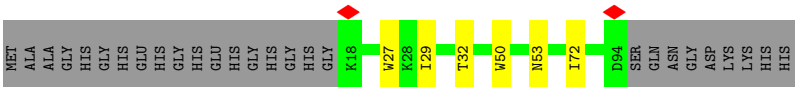
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



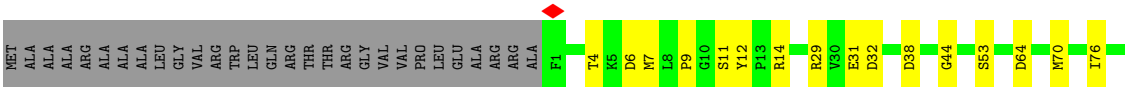
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

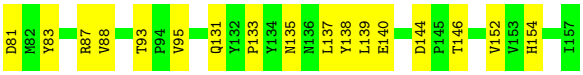
Chain k:



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

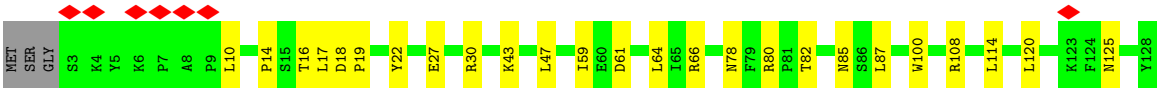
Chain l:





• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain m:



• Molecule 42: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n:

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

Chain o:

• Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	317317	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 ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.122	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	232.13998, 207.76, 207.76	wwPDB
Map dimensions	219, 196, 196	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: NDP, FMN, ZMP, AYA, SF4, DGT, PC1, MG, FES, ZN, SAC, FME, 3PE, 2MR, CDL, K

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	6	0.21	0/1289	0.51	0/1744
2	C	0.16	0/1780	0.37	0/2424
3	D	0.19	0/3442	0.43	0/4659
4	2	0.18	0/1700	0.42	0/2316
5	1	0.19	0/3396	0.44	0/4586
6	3	0.17	0/5392	0.36	0/7305
7	9	0.19	0/1461	0.45	0/1974
8	P	0.16	0/2574	0.39	0/3483
9	Q	0.17	0/1045	0.34	0/1411
10	7	0.14	0/773	0.29	0/1041
11	S	0.17	0/682	0.50	0/920
12	T	0.22	0/646	0.59	0/869
12	U	0.17	0/718	0.41	0/970
13	V	0.17	0/945	0.36	0/1281
14	W	0.18	0/993	0.42	0/1335
15	q	0.16	0/1251	0.39	0/1702
16	r	0.15	0/791	0.31	0/1069
17	s	0.13	0/360	0.36	0/489
18	A	0.23	0/770	0.50	0/1052
19	H	0.26	0/2517	0.55	0/3441
20	J	0.24	0/1263	0.59	2/1715 (0.1%)
21	K	0.23	0/738	0.52	0/1002
22	L	0.23	0/4913	0.49	0/6686
23	M	0.23	0/3709	0.52	2/5052 (0.0%)
24	N	0.24	0/2755	0.53	0/3751
25	O	0.16	0/2674	0.42	0/3626
26	X	0.16	0/1434	0.39	0/1937
27	Y	0.22	0/1061	0.52	1/1439 (0.1%)
28	Z	0.17	0/1198	0.40	0/1616
29	a	0.25	0/585	0.45	0/788
30	b	0.16	0/666	0.40	0/914
31	c	0.13	0/409	0.33	0/555

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	d	0.15	0/1028	0.37	0/1387
33	e	0.13	0/900	0.31	0/1199
34	f	0.14	0/468	0.34	0/630
35	g	0.16	0/878	0.41	0/1196
36	h	0.18	0/1201	0.38	0/1626
37	i	0.17	0/917	0.39	0/1243
38	j	0.16	0/587	0.42	0/804
39	k	0.15	0/646	0.35	0/873
40	l	0.14	0/1379	0.38	0/1882
41	m	0.18	0/1079	0.43	0/1463
42	n	0.15	0/1596	0.40	0/2162
43	o	0.16	0/1039	0.42	0/1394
44	p	0.16	0/1463	0.35	0/1977
All	All	0.19	0/67111	0.44	5/90988 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	J	84	SER	CA-C-N	5.59	132.21	121.54
20	J	84	SER	C-N-CA	5.59	132.21	121.54
23	M	122	PHE	CA-C-N	-5.29	111.26	121.58
23	M	122	PHE	C-N-CA	-5.29	111.26	121.58
27	Y	82	LYS	CB-CA-C	5.09	116.99	110.98

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	6	1258	0	1268	28	0
2	C	1730	0	1686	30	0
3	D	3371	0	3320	70	0
4	2	1660	0	1653	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	1	3321	0	3278	43	0
6	3	5305	0	5330	63	0
7	9	1431	0	1383	41	0
8	P	2513	0	2536	35	0
9	Q	1022	0	1023	19	0
10	7	758	0	731	9	0
11	S	671	0	688	5	0
12	T	637	0	640	10	0
12	U	706	0	699	17	0
13	V	923	0	965	8	0
14	W	970	0	991	15	0
15	q	1209	0	1170	12	0
16	r	781	0	811	13	0
17	s	351	0	331	5	0
18	A	760	0	811	24	0
19	H	2452	0	2547	62	0
20	J	1246	0	1270	28	0
21	K	737	0	768	16	0
22	L	4800	0	4985	94	0
23	M	3632	0	3853	77	0
24	N	2703	0	2902	58	0
25	O	2607	0	2566	39	0
26	X	1396	0	1385	26	0
27	Y	1037	0	1025	15	0
28	Z	1167	0	1166	18	0
29	a	572	0	583	16	0
30	b	643	0	644	4	0
31	c	398	0	401	5	0
32	d	996	0	1001	10	0
33	e	877	0	871	13	0
34	f	456	0	452	4	0
35	g	850	0	783	14	0
36	h	1166	0	1166	16	0
37	i	897	0	902	13	0
38	j	562	0	515	4	0
39	k	626	0	620	5	0
40	l	1323	0	1216	23	0
41	m	1050	0	1061	19	0
42	n	1541	0	1473	22	0
43	o	1014	0	1002	12	0
44	p	1430	0	1400	22	0
45	1	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	3	16	0	0	0	0
45	6	8	0	0	0	0
45	9	16	0	0	1	0
46	6	32	0	38	2	0
46	A	43	0	60	3	0
46	H	51	0	82	2	0
46	K	41	0	59	0	0
46	L	102	0	164	5	0
46	M	138	0	210	5	0
46	N	38	0	50	2	0
46	Y	70	0	88	4	0
46	d	63	0	74	0	0
46	i	42	0	61	2	0
46	m	30	0	34	2	0
46	r	46	0	66	0	0
47	6	43	0	63	2	0
47	9	101	0	159	7	0
47	M	54	0	88	5	0
48	2	4	0	0	0	0
48	3	4	0	0	0	0
49	1	31	0	19	3	0
50	3	1	0	0	0	0
51	P	48	0	26	2	0
52	7	1	0	0	0	0
53	W	34	0	40	3	0
53	n	32	0	36	4	0
54	L	78	0	100	1	0
54	N	90	0	133	7	0
54	d	67	0	81	6	0
54	h	70	0	87	7	0
54	m	72	0	91	1	0
54	r	57	0	58	3	0
55	O	31	0	12	1	0
56	O	1	0	0	0	0
All	All	67118	0	67850	904	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 7.

The worst 5 of 904 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)
18:A:49:LEU:CD1	19:H:126:LYS:HD3	1.78	1.14
18:A:49:LEU:HD13	19:H:126:LYS:HD3	1.09	1.09
3:D:228:MET:HA	3:D:228:MET:HE2	1.32	1.07
5:1:99:GLU:OE2	5:1:105:CYS:HA	1.67	0.95
18:A:49:LEU:HD13	19:H:126:LYS:CD	1.99	0.88

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	6	155/224 (69%)	145 (94%)	10 (6%)	0	100	100
2	C	206/263 (78%)	198 (96%)	8 (4%)	0	100	100
3	D	411/463 (89%)	391 (95%)	20 (5%)	0	100	100
4	2	212/248 (86%)	202 (95%)	9 (4%)	1 (0%)	24	60
5	1	428/464 (92%)	409 (96%)	19 (4%)	0	100	100
6	3	688/727 (95%)	660 (96%)	28 (4%)	0	100	100
7	9	176/212 (83%)	173 (98%)	3 (2%)	0	100	100
8	P	308/377 (82%)	296 (96%)	12 (4%)	0	100	100
9	Q	124/175 (71%)	121 (98%)	3 (2%)	0	100	100
10	7	94/116 (81%)	91 (97%)	3 (3%)	0	100	100
11	S	82/99 (83%)	78 (95%)	4 (5%)	0	100	100
12	T	77/156 (49%)	75 (97%)	2 (3%)	0	100	100
12	U	86/156 (55%)	83 (96%)	3 (4%)	0	100	100
13	V	111/116 (96%)	109 (98%)	2 (2%)	0	100	100
14	W	112/131 (86%)	107 (96%)	5 (4%)	0	100	100
15	q	143/145 (99%)	138 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	r	93/113 (82%)	91 (98%)	2 (2%)	0	100	100
17	s	40/104 (38%)	39 (98%)	1 (2%)	0	100	100
18	A	89/115 (77%)	86 (97%)	3 (3%)	0	100	100
19	H	302/318 (95%)	290 (96%)	12 (4%)	0	100	100
20	J	161/172 (94%)	151 (94%)	10 (6%)	0	100	100
21	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
22	L	604/607 (100%)	571 (94%)	33 (6%)	0	100	100
23	M	457/459 (100%)	443 (97%)	14 (3%)	0	100	100
24	N	343/345 (99%)	327 (95%)	16 (5%)	0	100	100
25	O	318/355 (90%)	305 (96%)	13 (4%)	0	100	100
26	X	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
27	Y	138/141 (98%)	138 (100%)	0	0	100	100
28	Z	139/144 (96%)	137 (99%)	2 (1%)	0	100	100
29	a	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
30	b	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
31	c	46/76 (60%)	46 (100%)	0	0	100	100
32	d	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
33	e	103/106 (97%)	99 (96%)	4 (4%)	0	100	100
34	f	51/57 (90%)	51 (100%)	0	0	100	100
35	g	99/151 (66%)	96 (97%)	3 (3%)	0	100	100
36	h	137/189 (72%)	133 (97%)	4 (3%)	0	100	100
37	i	102/128 (80%)	96 (94%)	6 (6%)	0	100	100
38	j	63/105 (60%)	59 (94%)	4 (6%)	0	100	100
39	k	75/104 (72%)	73 (97%)	2 (3%)	0	100	100
40	l	155/186 (83%)	151 (97%)	4 (3%)	0	100	100
41	m	124/129 (96%)	124 (100%)	0	0	100	100
42	n	176/179 (98%)	172 (98%)	4 (2%)	0	100	100
43	o	116/137 (85%)	108 (93%)	8 (7%)	0	100	100
44	p	167/176 (95%)	165 (99%)	2 (1%)	0	100	100
All	All	8042/9212 (87%)	7742 (96%)	299 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	2	183	LYS

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	6	133/185 (72%)	133 (100%)	0	100	100
2	C	190/227 (84%)	190 (100%)	0	100	100
3	D	361/394 (92%)	360 (100%)	1 (0%)	86	91
4	2	184/206 (89%)	184 (100%)	0	100	100
5	1	345/370 (93%)	345 (100%)	0	100	100
6	3	580/610 (95%)	580 (100%)	0	100	100
7	9	152/178 (85%)	152 (100%)	0	100	100
8	P	273/325 (84%)	273 (100%)	0	100	100
9	Q	113/153 (74%)	113 (100%)	0	100	100
10	7	81/96 (84%)	81 (100%)	0	100	100
11	S	74/80 (92%)	74 (100%)	0	100	100
12	T	73/135 (54%)	73 (100%)	0	100	100
12	U	81/135 (60%)	81 (100%)	0	100	100
13	V	101/102 (99%)	101 (100%)	0	100	100
14	W	108/114 (95%)	108 (100%)	0	100	100
15	q	131/131 (100%)	131 (100%)	0	100	100
16	r	86/96 (90%)	86 (100%)	0	100	100
17	s	41/95 (43%)	41 (100%)	0	100	100
18	A	84/103 (82%)	84 (100%)	0	100	100
19	H	269/279 (96%)	269 (100%)	0	100	100
20	J	131/137 (96%)	131 (100%)	0	100	100
21	K	87/87 (100%)	87 (100%)	0	100	100
22	L	548/549 (100%)	548 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	M	414/414 (100%)	414 (100%)	0	100	100
24	N	307/307 (100%)	307 (100%)	0	100	100
25	O	284/309 (92%)	284 (100%)	0	100	100
26	X	153/154 (99%)	153 (100%)	0	100	100
27	Y	105/106 (99%)	105 (100%)	0	100	100
28	Z	122/123 (99%)	122 (100%)	0	100	100
29	a	60/60 (100%)	60 (100%)	0	100	100
30	b	72/73 (99%)	72 (100%)	0	100	100
31	c	42/67 (63%)	42 (100%)	0	100	100
32	d	107/107 (100%)	107 (100%)	0	100	100
33	e	93/94 (99%)	93 (100%)	0	100	100
34	f	49/53 (92%)	49 (100%)	0	100	100
35	g	92/129 (71%)	92 (100%)	0	100	100
36	h	123/162 (76%)	123 (100%)	0	100	100
37	i	99/119 (83%)	99 (100%)	0	100	100
38	j	61/87 (70%)	61 (100%)	0	100	100
39	k	60/78 (77%)	60 (100%)	0	100	100
40	l	142/161 (88%)	142 (100%)	0	100	100
41	m	112/114 (98%)	112 (100%)	0	100	100
42	n	163/164 (99%)	163 (100%)	0	100	100
43	o	109/121 (90%)	109 (100%)	0	100	100
44	p	154/158 (98%)	154 (100%)	0	100	100
All	All	7149/7947 (90%)	7148 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	228	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
26	X	142	HIS

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Mol	Chain	Res	Type
42	n	140	GLN
32	d	3	ASN
40	l	54	GLN
44	p	103	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	FME	A	1	18	8,9,10	0.92	0	7,9,11	0.88	0
24	FME	N	1	24	8,9,10	0.94	0	7,9,11	0.93	0
23	FME	M	1	23	8,9,10	0.97	0	7,9,11	0.72	0
37	SAC	i	1	37	7,8,9	1.00	0	8,9,11	0.87	1 (12%)
3	2MR	D	85	3	10,12,13	2.61	2 (20%)	5,13,15	3.03	2 (40%)
20	FME	J	1	20	8,9,10	0.94	0	7,9,11	0.95	0
22	FME	L	1	22	8,9,10	0.92	0	7,9,11	0.93	0
16	AYA	r	1	16	6,7,8	1.27	1 (16%)	5,8,10	1.27	1 (20%)
21	FME	K	1	21	8,9,10	0.91	0	7,9,11	2.05	2 (28%)
19	FME	H	1	19	8,9,10	0.94	0	7,9,11	0.90	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	FME	A	1	18	-	2/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	FME	N	1	24	-	3/7/9/11	-
23	FME	M	1	23	-	1/7/9/11	-
37	SAC	i	1	37	-	0/7/8/10	-
3	2MR	D	85	3	-	3/10/13/15	-
20	FME	J	1	20	-	4/7/9/11	-
22	FME	L	1	22	-	3/7/9/11	-
16	AYA	r	1	16	-	0/4/6/8	-
21	FME	K	1	21	-	3/7/9/11	-
19	FME	H	1	19	-	3/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	85	2MR	CZ-NE	5.92	1.47	1.34
3	D	85	2MR	CZ-NH2	5.12	1.44	1.33
16	r	1	AYA	CA-N	-2.47	1.44	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	85	2MR	CD-NE-CZ	5.73	134.13	123.41
21	K	1	FME	C-CA-N	4.68	118.17	109.73
3	D	85	2MR	NE-CZ-NH2	-3.45	116.32	119.48
16	r	1	AYA	CB-CA-N	2.63	112.53	109.61
21	K	1	FME	O-C-CA	-2.20	119.02	124.78

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	85	2MR	C-CA-CB-CG
18	A	1	FME	N-CA-CB-CG
19	H	1	FME	N-CA-CB-CG
19	H	1	FME	O-C-CA-CB
20	J	1	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	K	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 43 ligands modelled in this entry, 3 are monoatomic - leaving 40 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	SF4	1	502	5	0,12,12	-	-	-		
54	CDL	m	201	-	71,71,99	0.36	0	77,83,111	0.42	1 (1%)
46	3PE	M	504	-	35,35,50	0.35	0	38,40,55	0.30	0
54	CDL	L	702	-	77,77,99	0.34	0	83,89,111	0.30	0
54	CDL	N	401	-	89,89,99	0.32	0	95,101,111	0.39	1 (1%)
46	3PE	6	202	-	31,31,50	0.37	0	34,36,55	0.30	0
46	3PE	L	703	-	50,50,50	0.31	0	53,55,55	0.31	0
54	CDL	h	201	-	69,69,99	0.35	0	75,81,111	0.42	0
54	CDL	d	201	-	66,66,99	0.36	0	72,78,111	0.31	0
46	3PE	i	201	-	41,41,50	0.33	0	44,46,55	0.31	0
47	PC1	M	501	-	53,53,53	0.29	0	59,61,61	0.38	0
46	3PE	L	701	-	50,50,50	0.31	0	53,55,55	0.46	0
46	3PE	d	203	-	31,31,50	0.37	0	34,36,55	0.33	0
46	3PE	H	401	-	50,50,50	0.31	0	53,55,55	0.47	1 (1%)
53	ZMP	W	201	-	27,33,36	0.62	1 (3%)	32,40,45	1.13	2 (6%)
45	SF4	3	801	6	0,12,12	-	-	-		
45	SF4	9	202	7	0,12,12	-	-	-		
46	3PE	A	201	-	42,42,50	0.33	0	45,47,55	0.33	0
46	3PE	Y	202	-	41,41,50	0.33	0	44,46,55	0.31	0
46	3PE	d	202	-	30,30,50	0.37	0	33,35,55	0.32	0
47	PC1	9	203	-	53,53,53	0.30	0	59,61,61	0.44	0
49	FMN	1	501	-	33,33,33	0.27	0	48,50,50	0.49	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
45	SF4	3	802	6	0,12,12	-	-	-		
45	SF4	6	201	1	0,12,12	-	-	-		
46	3PE	M	502	-	50,50,50	0.30	0	53,55,55	0.29	0
48	FES	2	301	4	0,4,4	-	-	-		
54	CDL	r	202	-	56,56,99	0.39	0	62,68,111	0.47	0
51	NDP	P	501	-	49,52,52	0.34	0	66,80,80	0.41	0
45	SF4	9	201	7	0,12,12	-	-	-		
47	PC1	9	204	-	46,46,53	0.32	0	52,54,61	0.30	0
46	3PE	K	201	-	40,40,50	0.33	0	43,45,55	0.31	0
46	3PE	M	503	-	50,50,50	0.30	0	53,55,55	0.27	0
47	PC1	6	203	-	42,42,53	0.35	0	48,50,61	0.49	1 (2%)
46	3PE	Y	201	-	27,27,50	0.40	0	30,32,55	0.36	0
48	FES	3	803	6	0,4,4	-	-	-		
46	3PE	m	202	-	29,29,50	0.38	0	32,34,55	0.33	0
46	3PE	N	402	-	37,37,50	0.35	0	40,42,55	0.32	0
53	ZMP	n	201	-	25,31,36	0.75	1 (4%)	30,38,45	0.92	1 (3%)
55	DGT	O	401	56	29,33,33	0.31	0	44,52,52	0.29	0
46	3PE	r	201	-	45,45,50	0.32	0	48,50,55	0.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	1	502	5	-	-	0/6/5/5
54	CDL	m	201	-	-	21/82/82/110	-
46	3PE	M	504	-	-	9/39/39/54	-
54	CDL	L	702	-	-	15/88/88/110	-
54	CDL	N	401	-	-	16/100/100/110	-
46	3PE	6	202	-	-	4/35/35/54	-
46	3PE	L	703	-	-	8/54/54/54	-
54	CDL	h	201	-	-	20/80/80/110	-
54	CDL	d	201	-	-	11/77/77/110	-
46	3PE	i	201	-	-	7/45/45/54	-
47	PC1	M	501	-	-	11/57/57/57	-
46	3PE	d	203	-	-	6/35/35/54	-
46	3PE	L	701	-	-	8/54/54/54	-
46	3PE	H	401	-	-	14/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	ZMP	W	201	-	-	8/38/40/43	-
45	SF4	3	801	6	-	-	0/6/5/5
45	SF4	9	202	7	-	-	0/6/5/5
46	3PE	A	201	-	-	8/46/46/54	-
46	3PE	Y	202	-	-	9/45/45/54	-
46	3PE	d	202	-	-	9/34/34/54	-
47	PC1	9	203	-	-	11/57/57/57	-
49	FMN	1	501	-	-	5/18/18/18	0/3/3/3
45	SF4	3	802	6	-	-	0/6/5/5
45	SF4	6	201	1	-	-	0/6/5/5
46	3PE	M	502	-	-	13/54/54/54	-
48	FES	2	301	4	-	-	0/1/1/1
54	CDL	r	202	-	-	15/67/67/110	-
51	NDP	P	501	-	-	6/34/77/77	0/5/5/5
45	SF4	9	201	7	-	-	0/6/5/5
47	PC1	9	204	-	-	13/50/50/57	-
46	3PE	K	201	-	-	12/44/44/54	-
46	3PE	M	503	-	-	13/54/54/54	-
47	PC1	6	203	-	-	10/46/46/57	-
46	3PE	Y	201	-	-	4/31/31/54	-
48	FES	3	803	6	-	-	0/1/1/1
46	3PE	m	202	-	-	12/33/33/54	-
46	3PE	N	402	-	-	7/41/41/54	-
53	ZMP	n	201	-	-	12/36/38/43	-
55	DGT	O	401	56	-	9/22/34/34	0/3/3/3
46	3PE	r	201	-	-	7/49/49/54	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	n	201	ZMP	C9-C10	2.60	1.53	1.50
53	W	201	ZMP	C9-C10	2.10	1.53	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	W	201	ZMP	O1-C10-C9	-3.12	120.30	123.99
53	n	201	ZMP	O1-C10-C9	-2.49	121.05	123.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	W	201	ZMP	C15-C14-C13	-2.31	108.51	112.36
49	1	501	FMN	P-O5'-C5'	2.18	124.31	118.30
47	6	203	PC1	C2-O21-C21	2.09	122.94	117.79

There are no chirality outliers.

5 of 333 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	6	202	3PE	C11-O13-P-O11
46	6	202	3PE	C11-O13-P-O14
46	6	202	3PE	O13-C11-C12-N
46	r	201	3PE	O13-C11-C12-N
46	A	201	3PE	C11-O13-P-O11

There are no ring outliers.

27 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	m	201	CDL	1	0
54	L	702	CDL	1	0
54	N	401	CDL	7	0
46	6	202	3PE	2	0
46	L	703	3PE	2	0
54	h	201	CDL	7	0
54	d	201	CDL	6	0
46	i	201	3PE	2	0
47	M	501	PC1	5	0
46	L	701	3PE	3	0
46	H	401	3PE	2	0
53	W	201	ZMP	3	0
46	A	201	3PE	3	0
46	Y	202	3PE	3	0
47	9	203	PC1	1	0
49	1	501	FMN	3	0
46	M	502	3PE	5	0
54	r	202	CDL	3	0
51	P	501	NDP	2	0
45	9	201	SF4	1	0
47	9	204	PC1	6	0
47	6	203	PC1	2	0
46	Y	201	3PE	1	0

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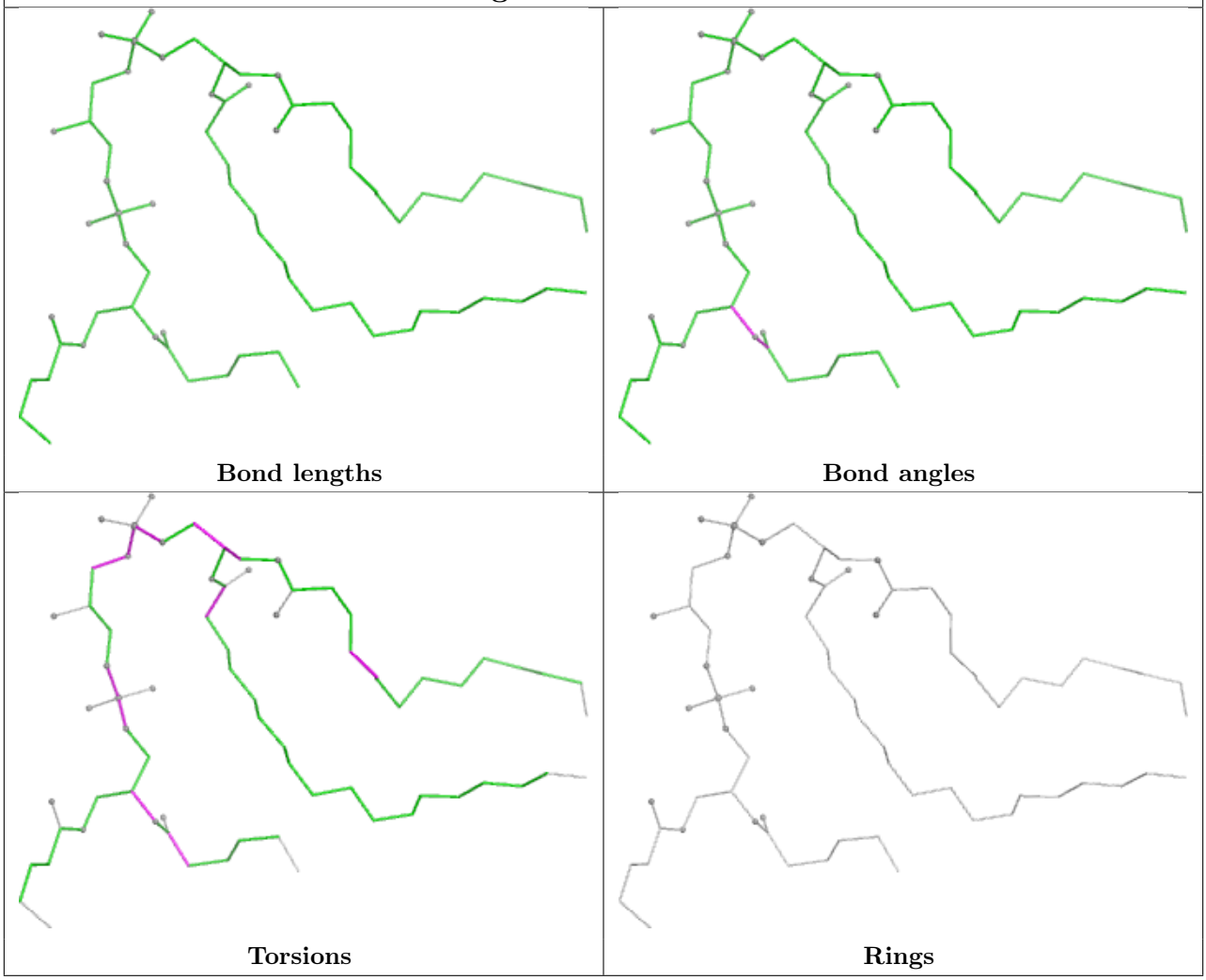
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	m	202	3PE	2	0
46	N	402	3PE	2	0
53	n	201	ZMP	4	0
55	O	401	DGT	1	0

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 CDL m 201



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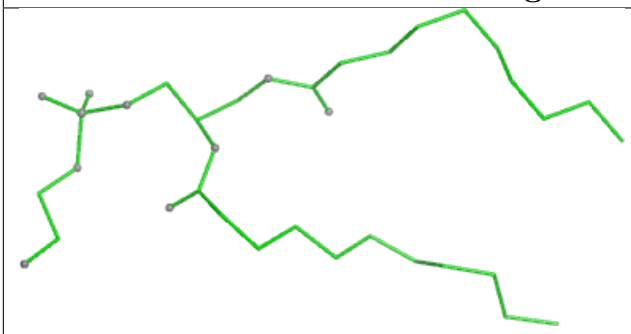
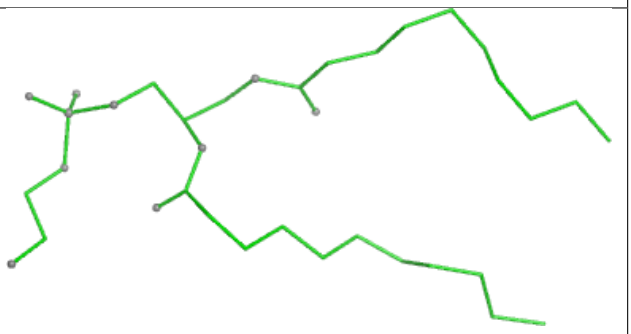
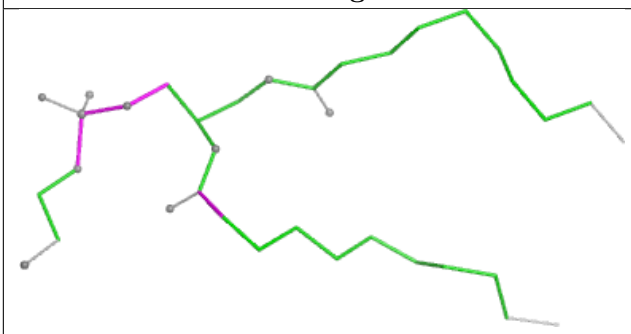
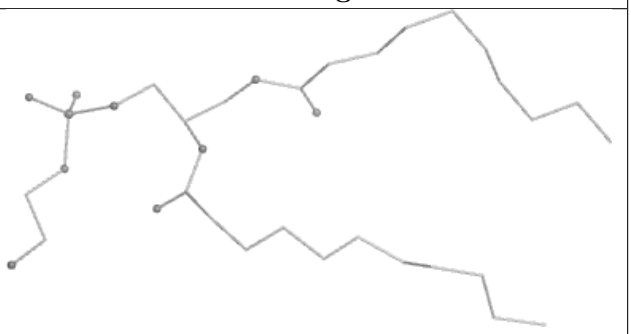
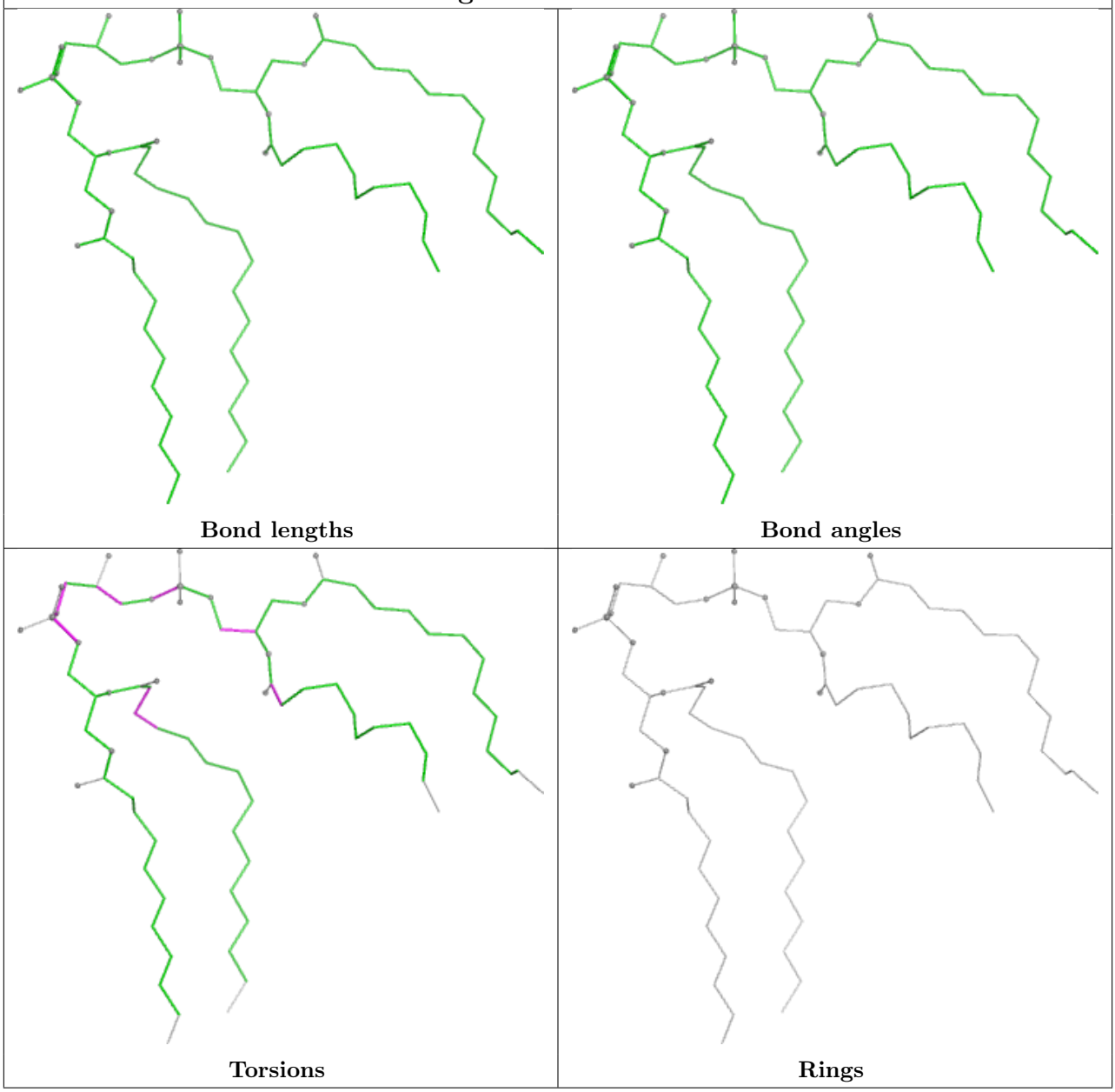
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL L 702



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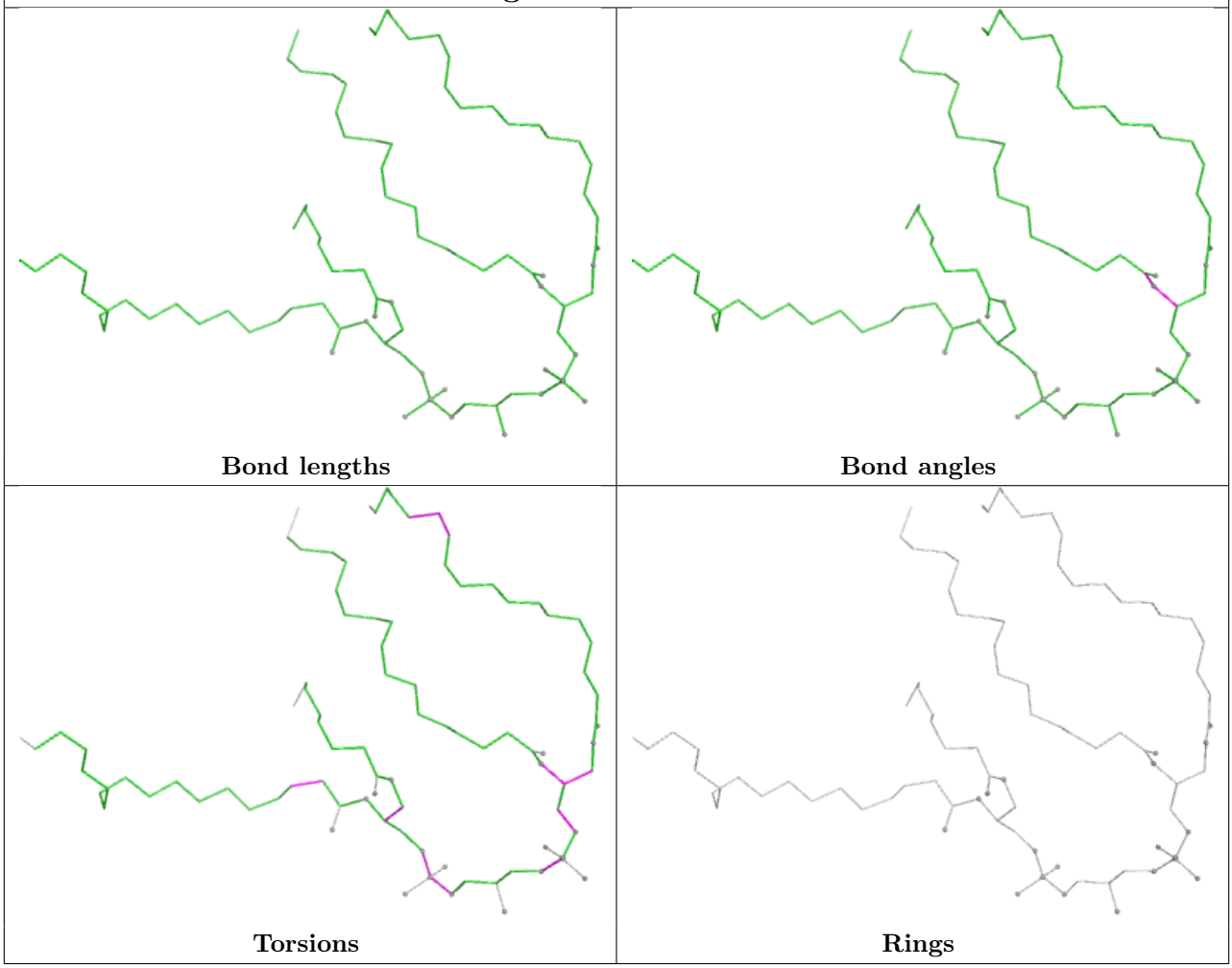

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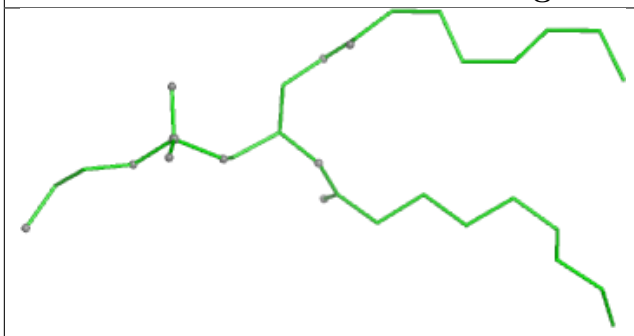

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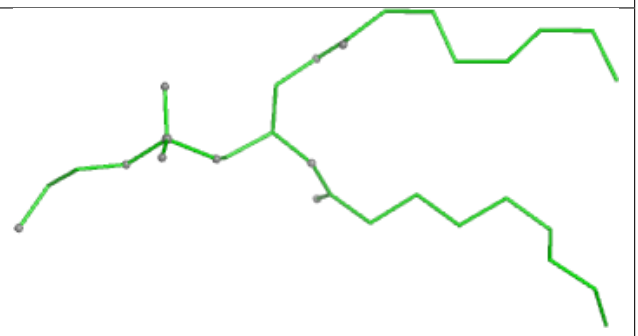
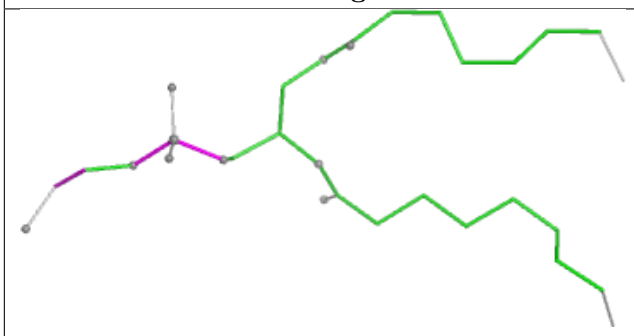
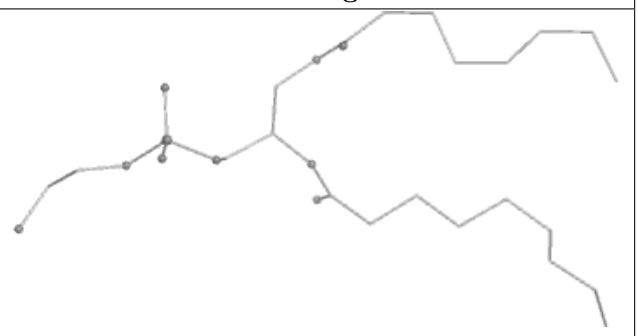


Bond angles

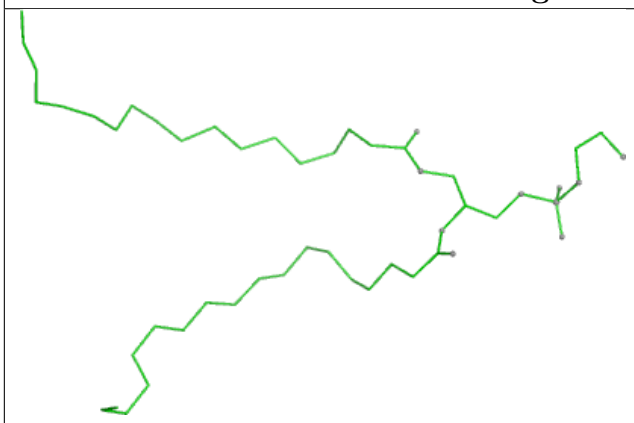


Torsions



Rings

Ligand 3PE L 703



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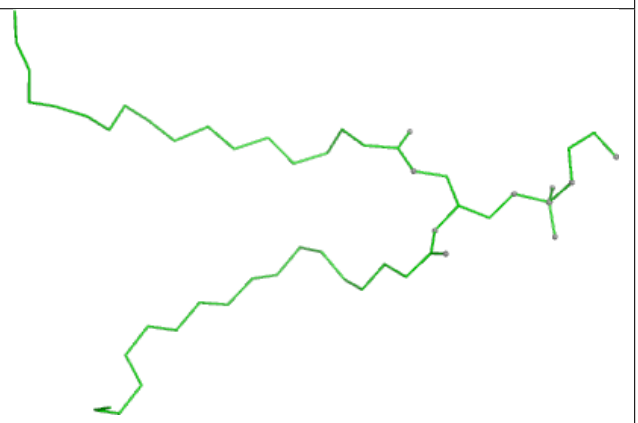

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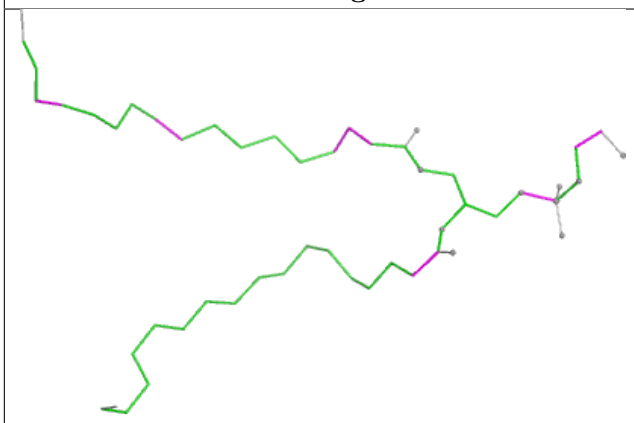

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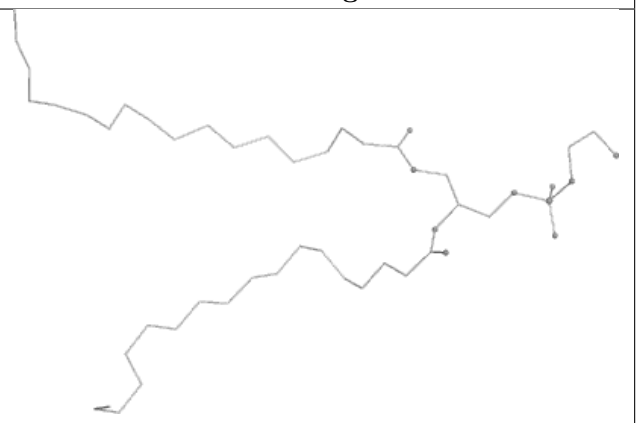
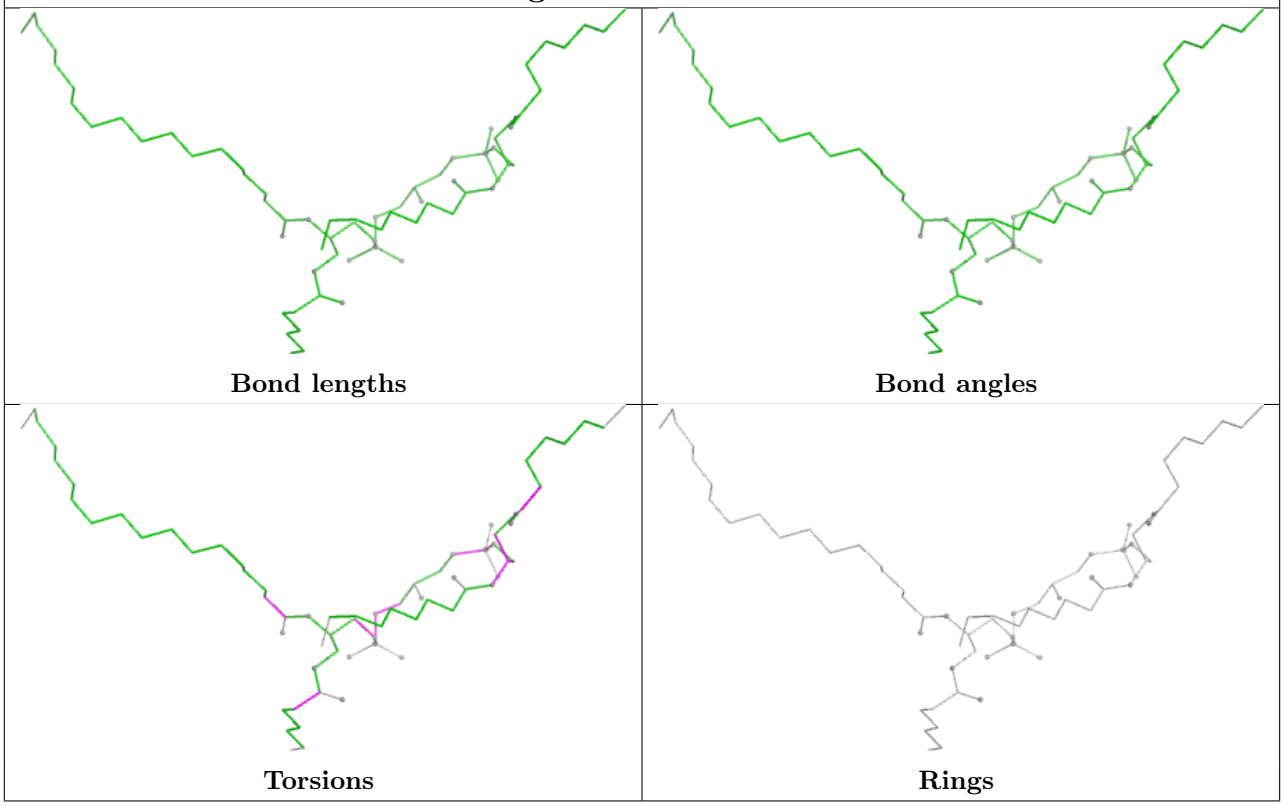
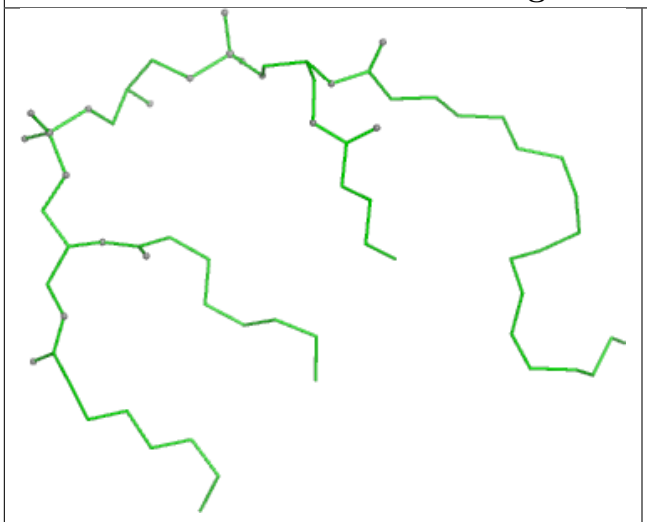


Rings

Ligand CDL h 201



Ligand CDL d 201



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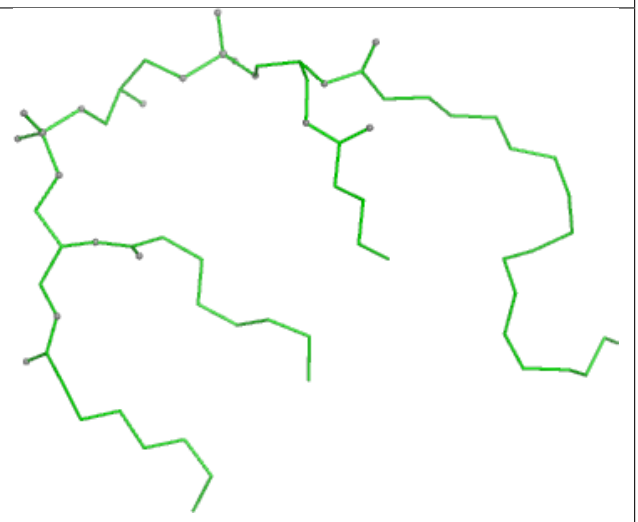
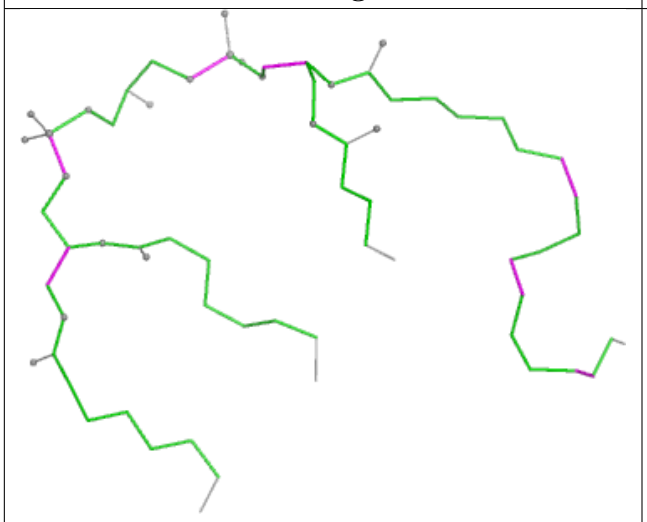


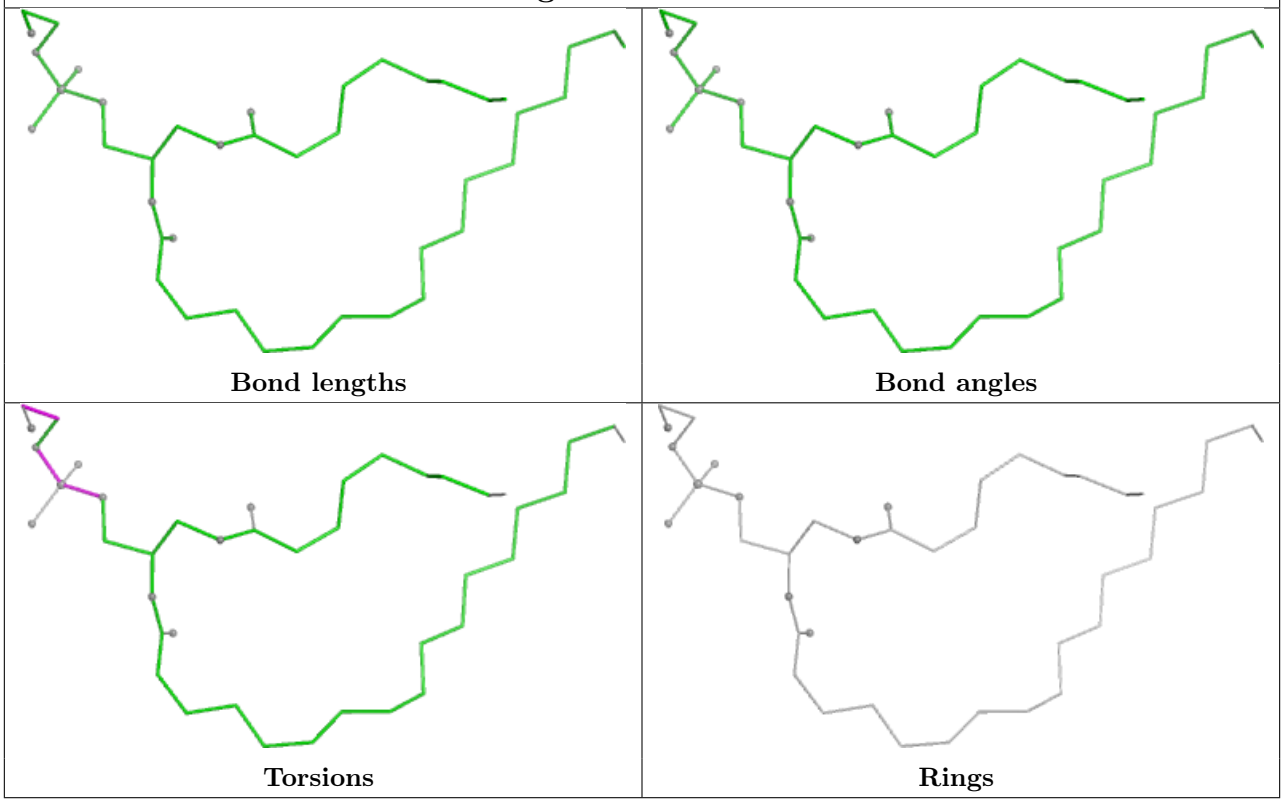
Bond angles



Torsions

Rings

Ligand 3PE i 201



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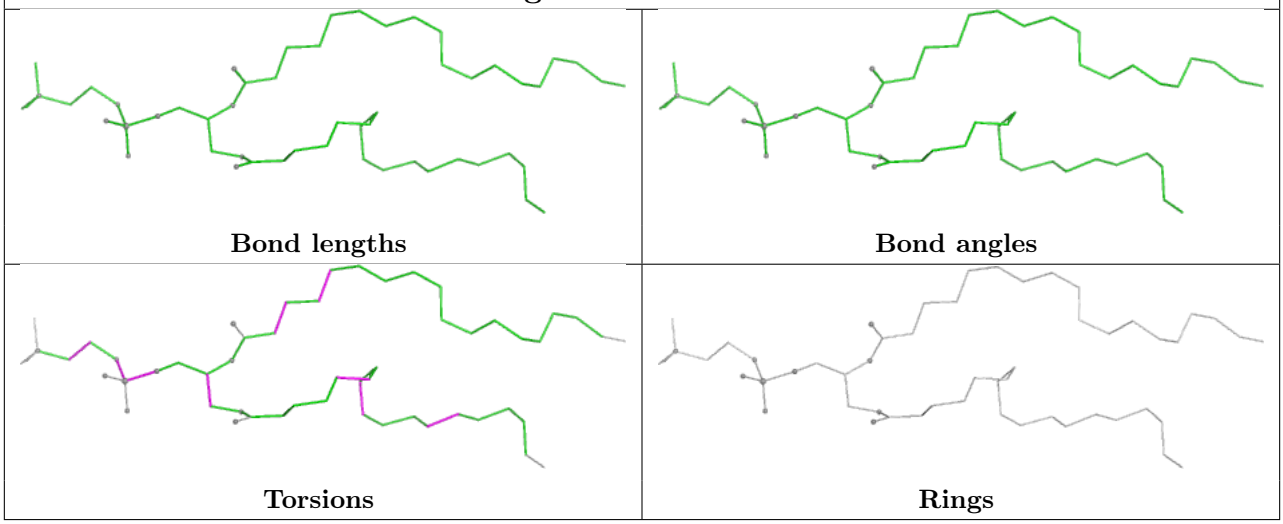
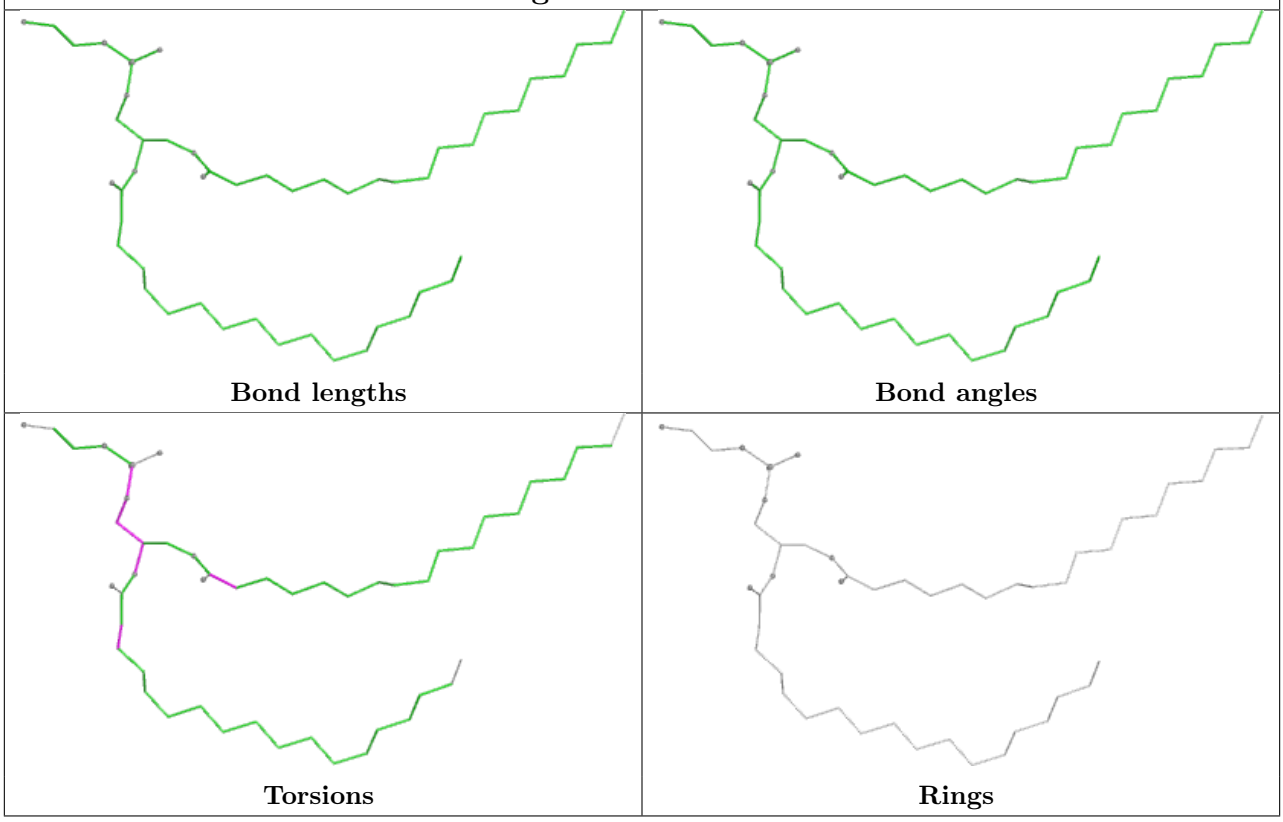
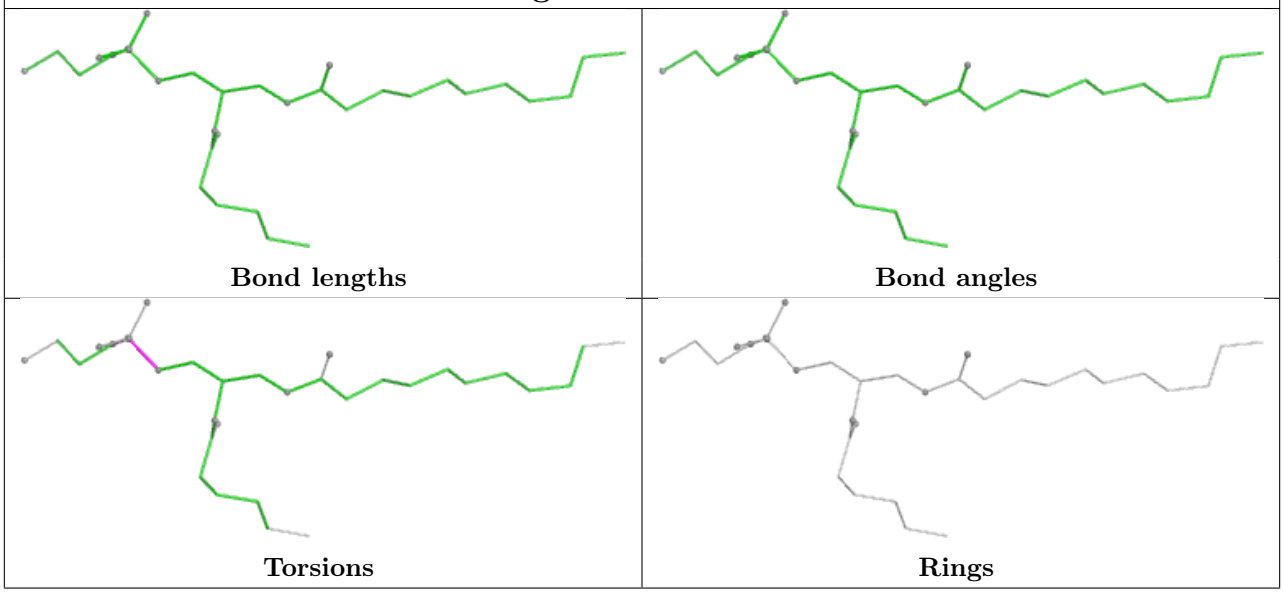


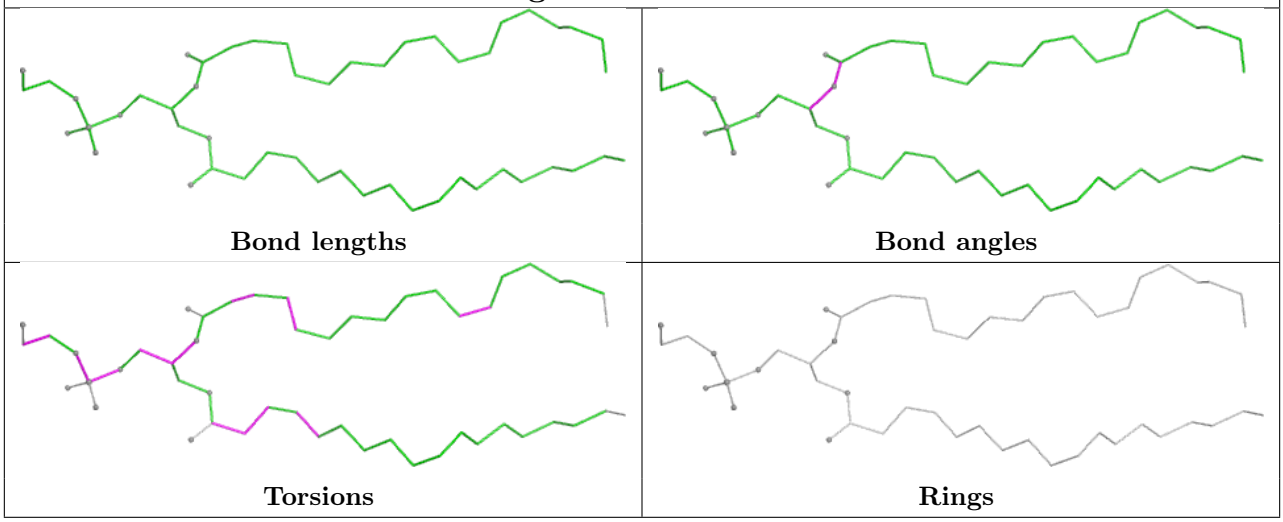
Ligand 3PE L 701



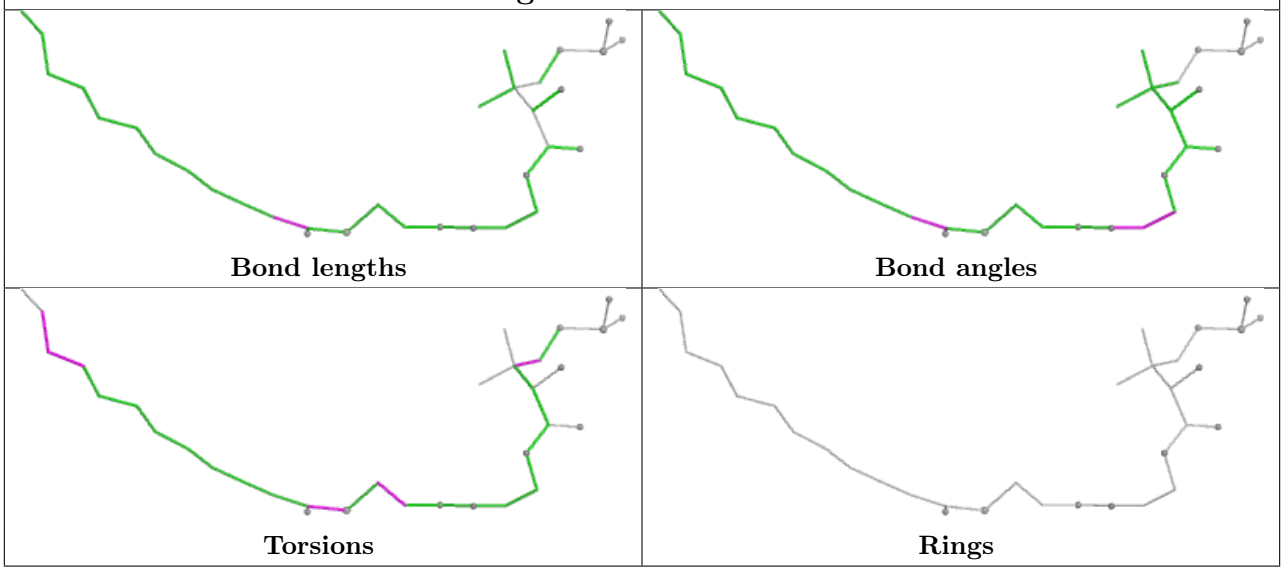
Ligand 3PE d 203



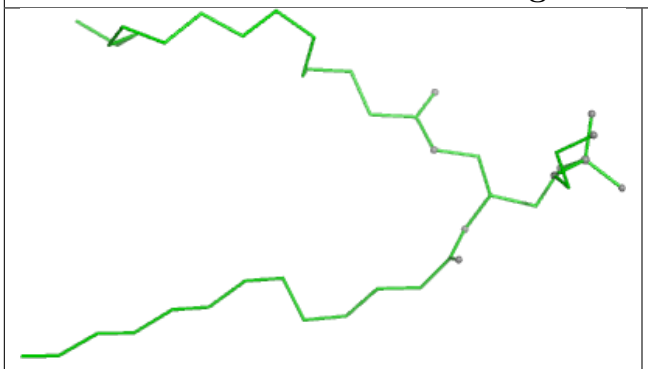
Ligand 3PE H 401



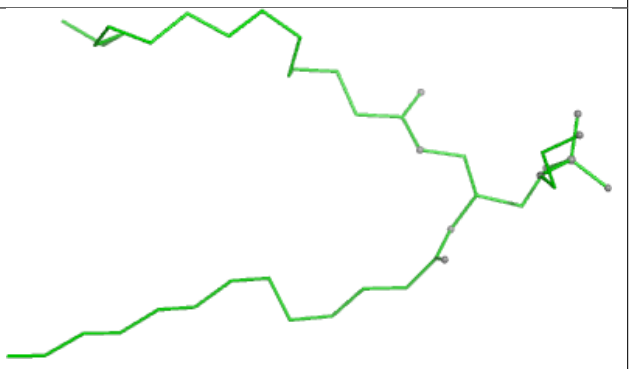
Ligand ZMP W 201



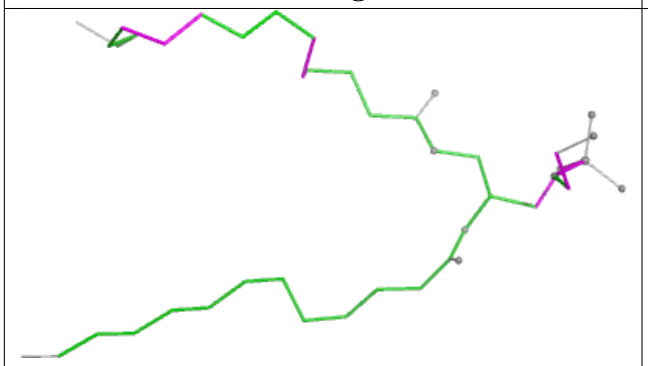
Ligand 3PE A 201



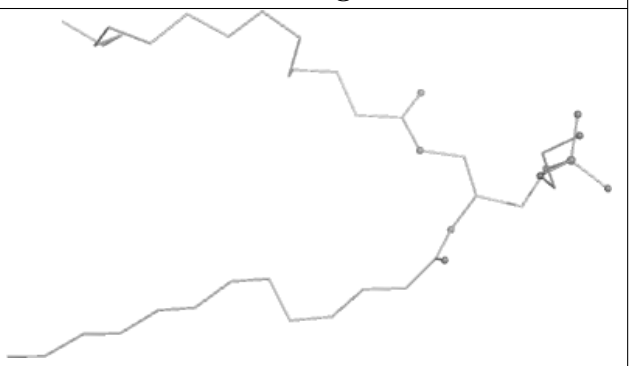
Bond lengths



Bond angles

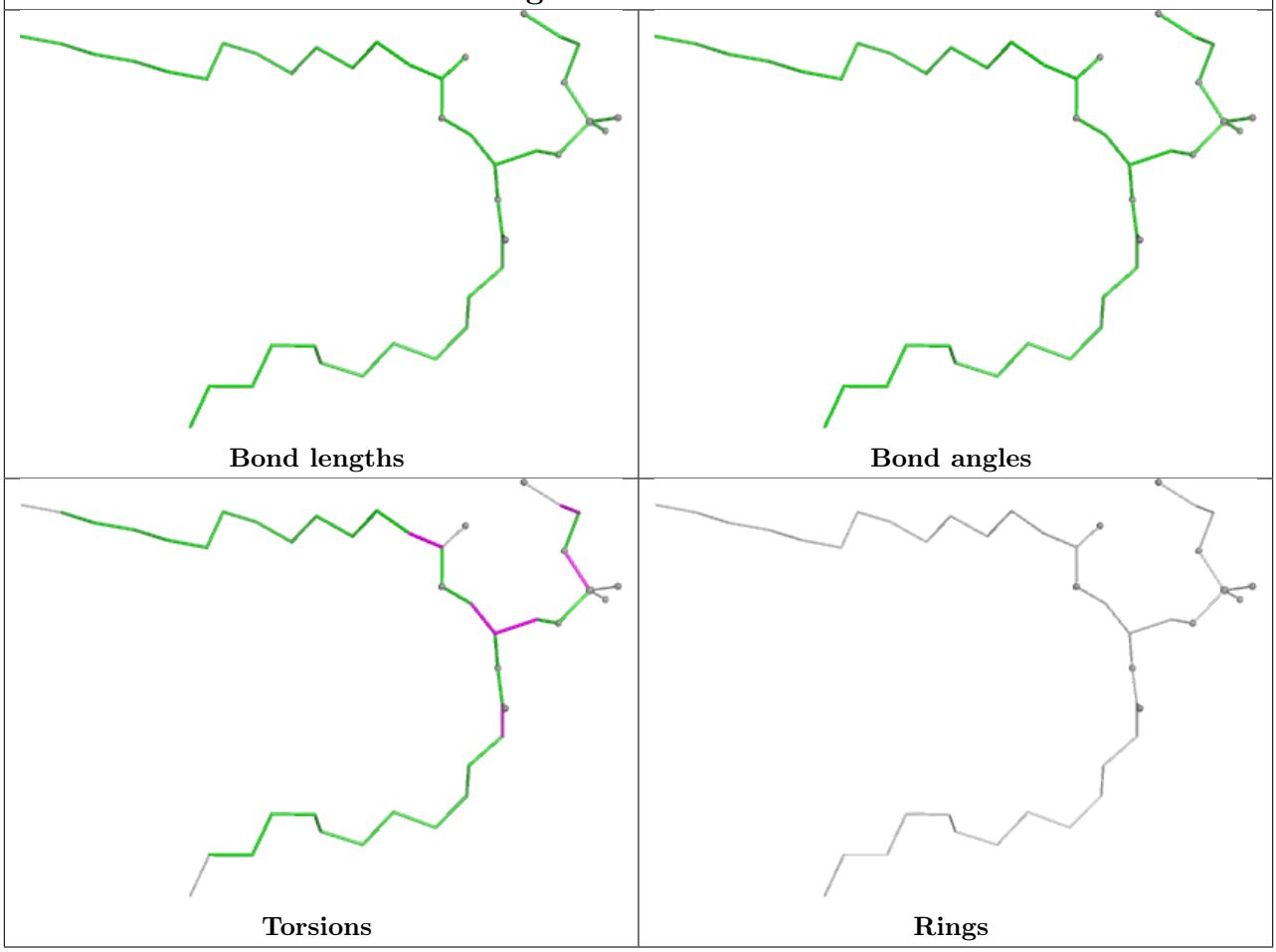


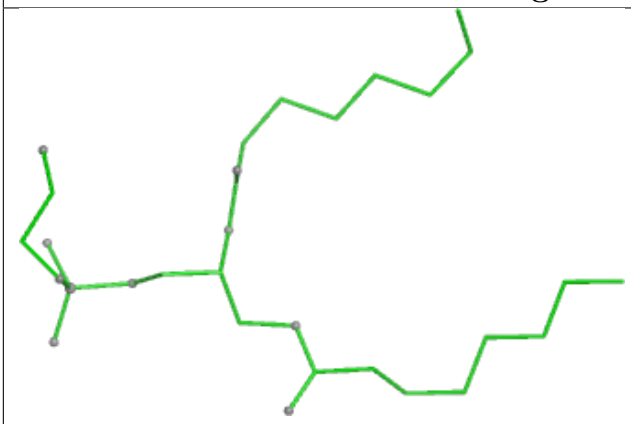
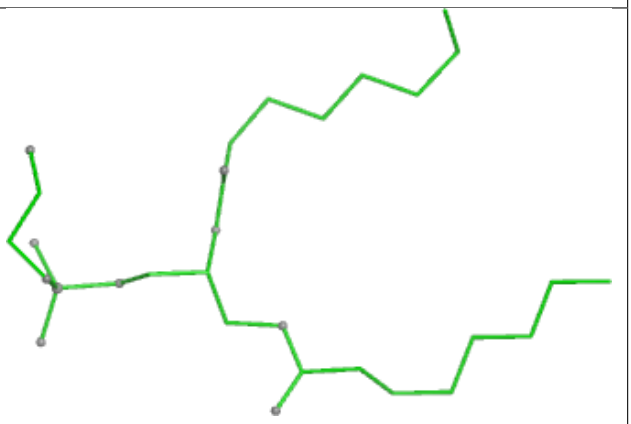
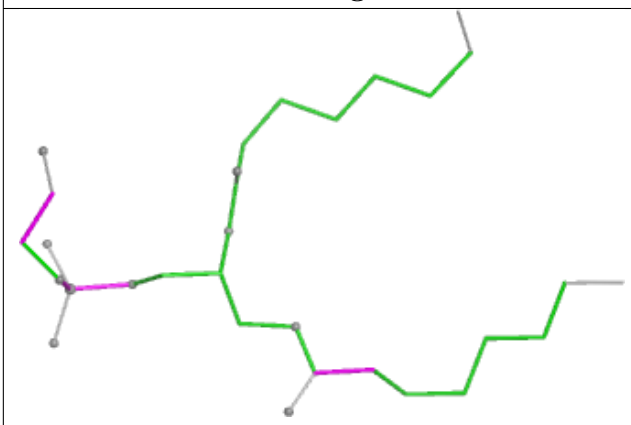
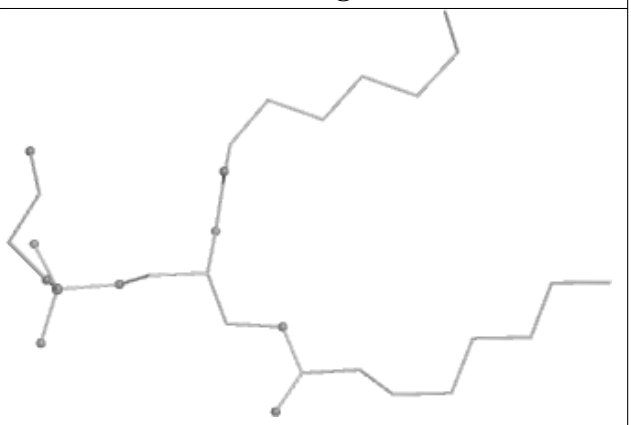
Torsions



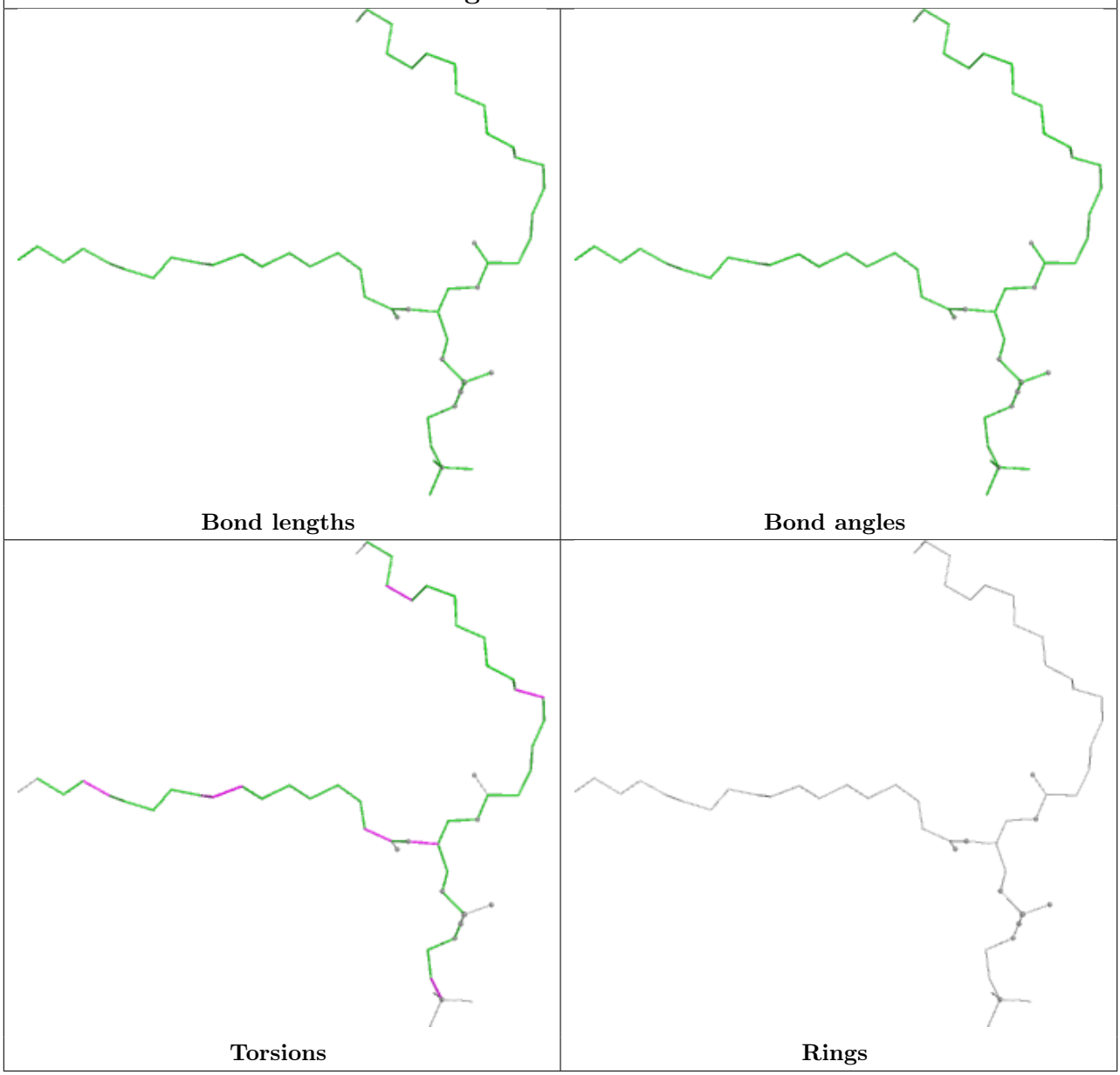
Rings

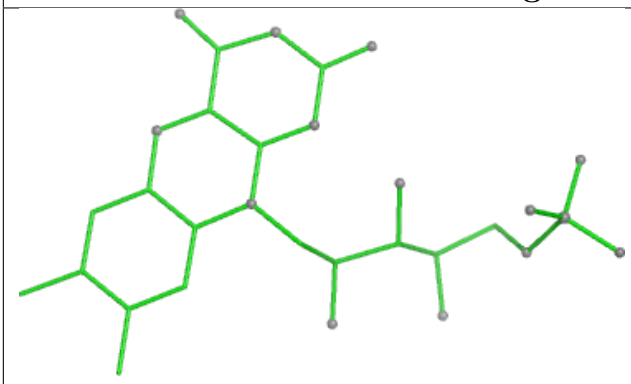
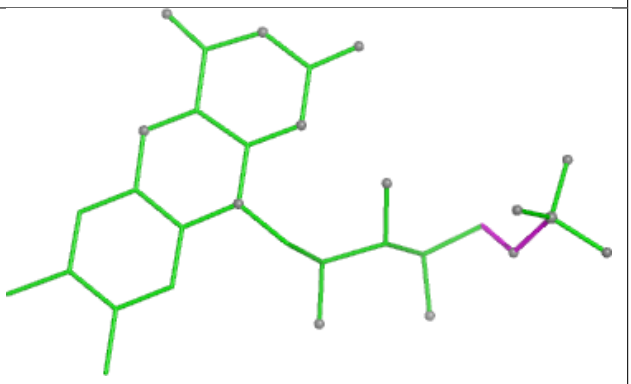
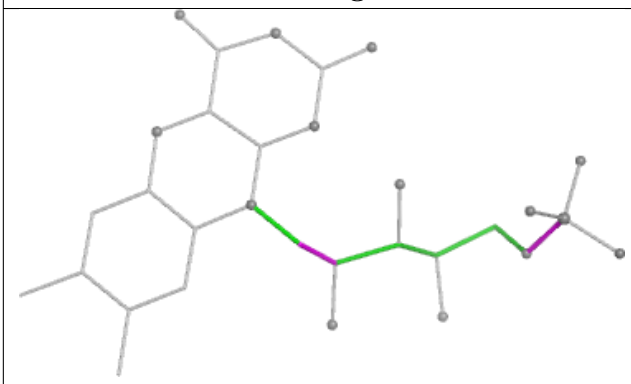
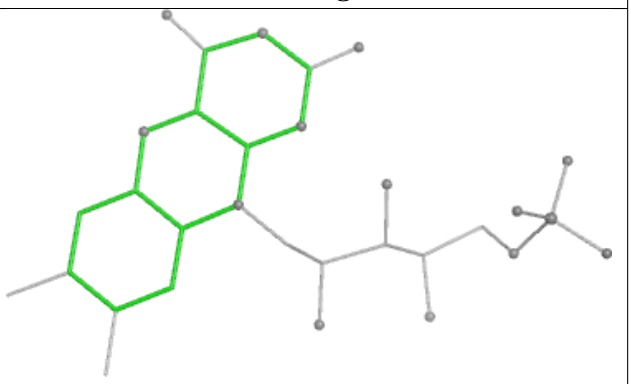
Ligand 3PE Y 202



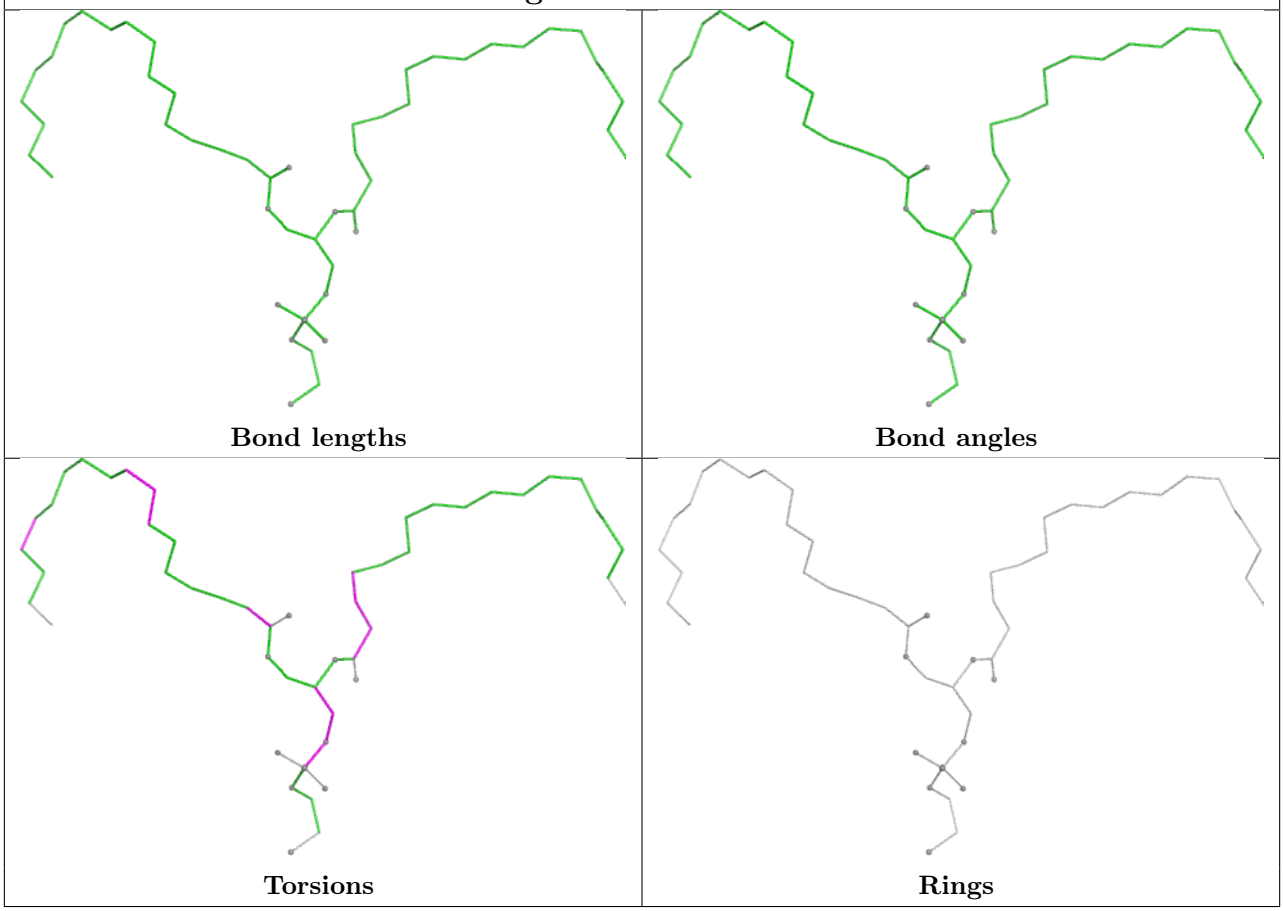
Ligand 3PE d 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 9 203

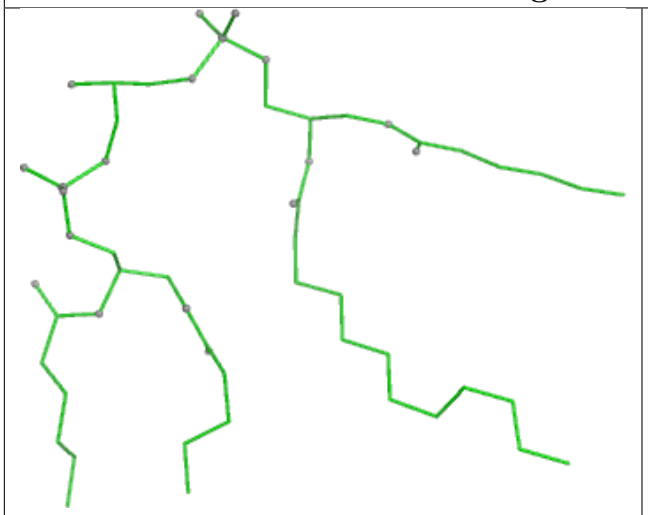


Ligand FMN 1 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

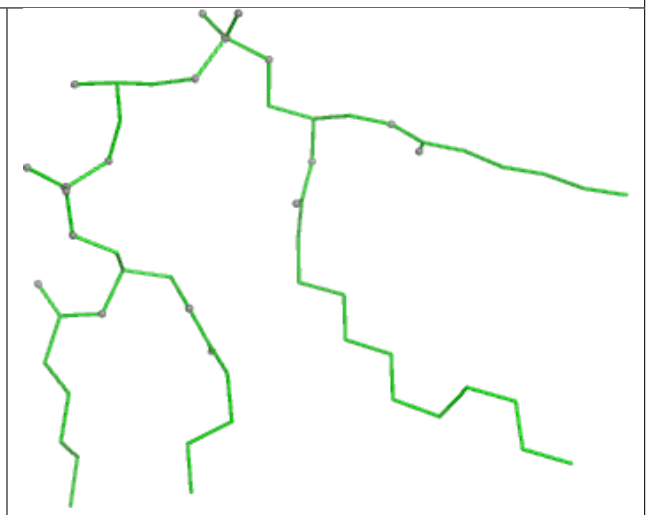
Ligand 3PE M 502



Ligand CDL r 202



Bond lengths

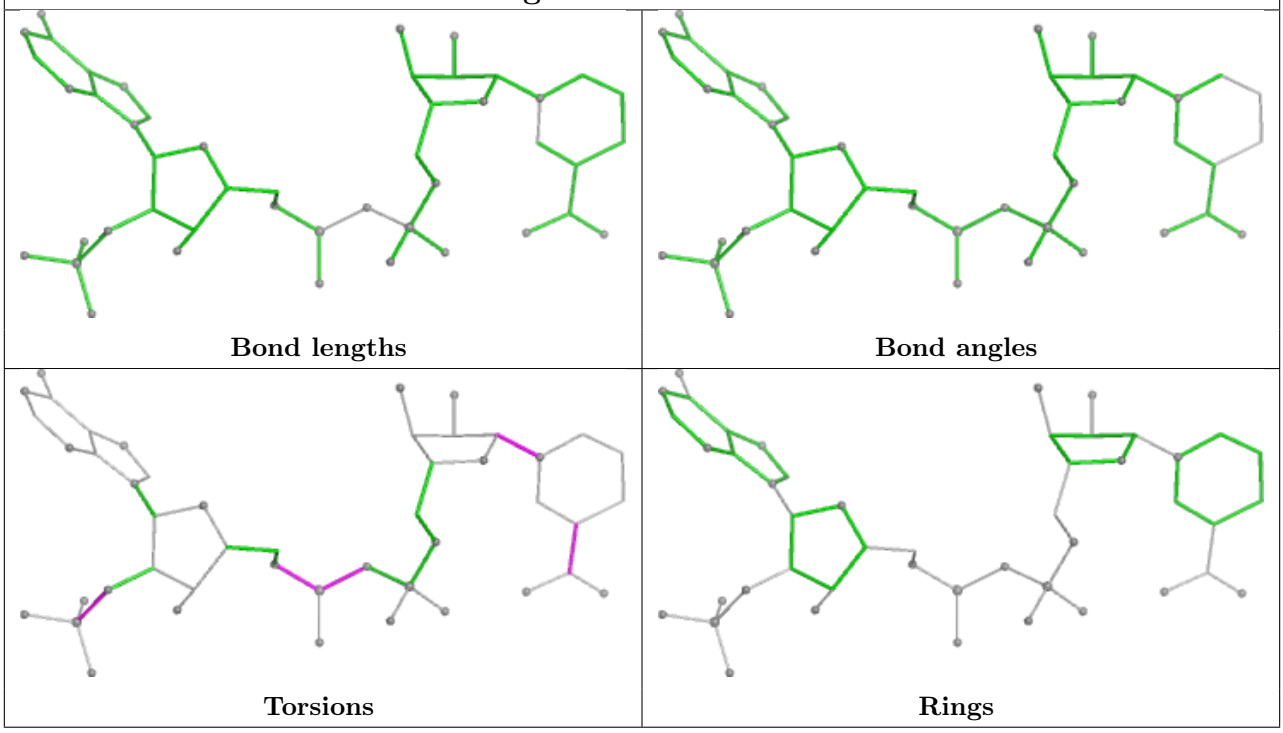


Bond angles

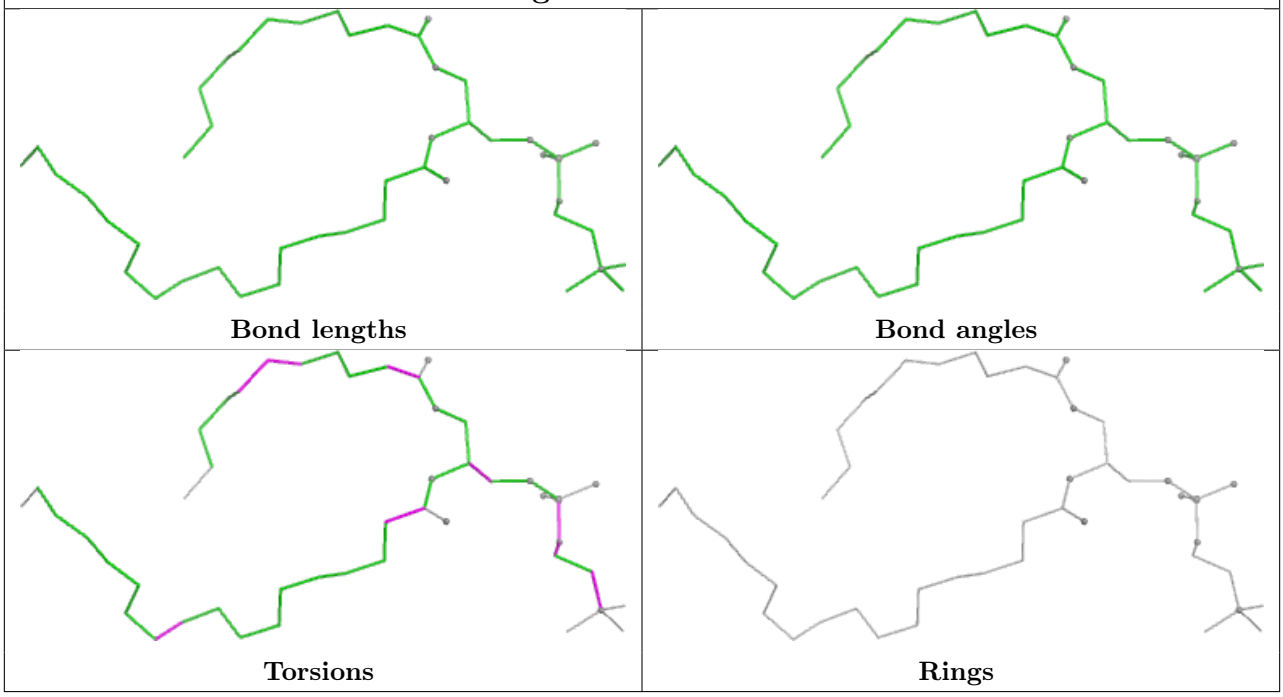
Torsions

Rings

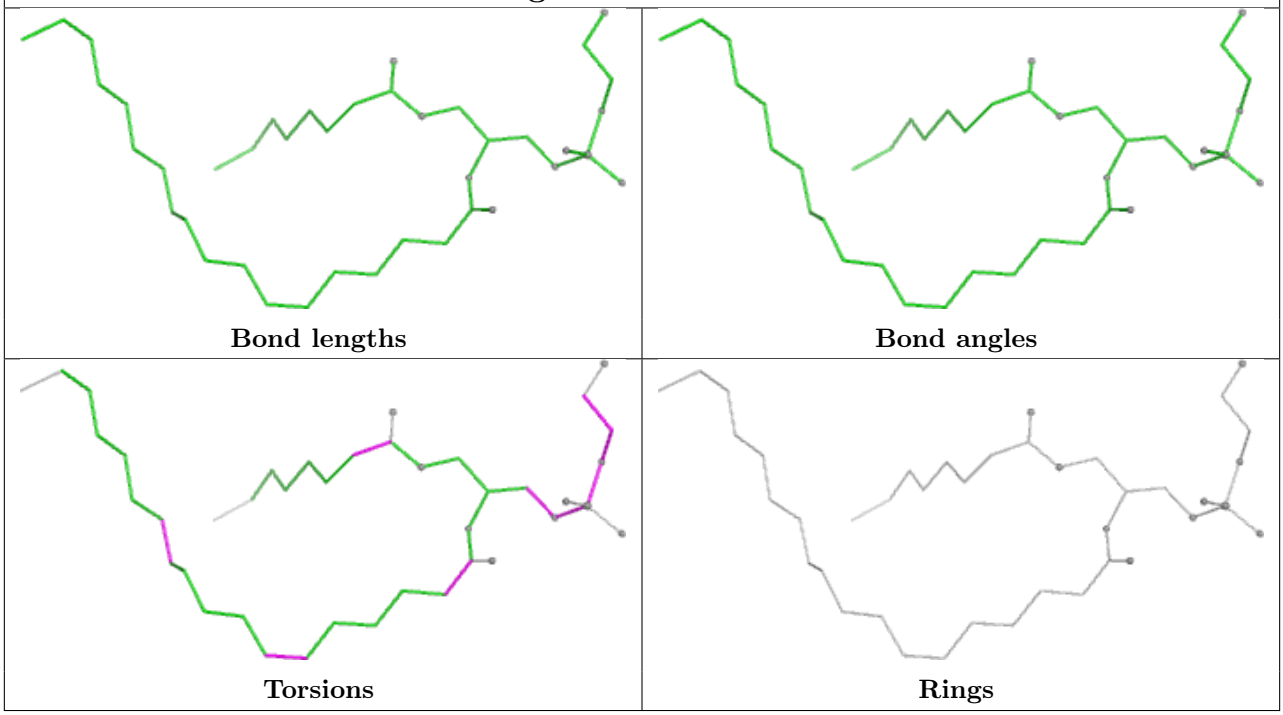
Ligand NDP P 501



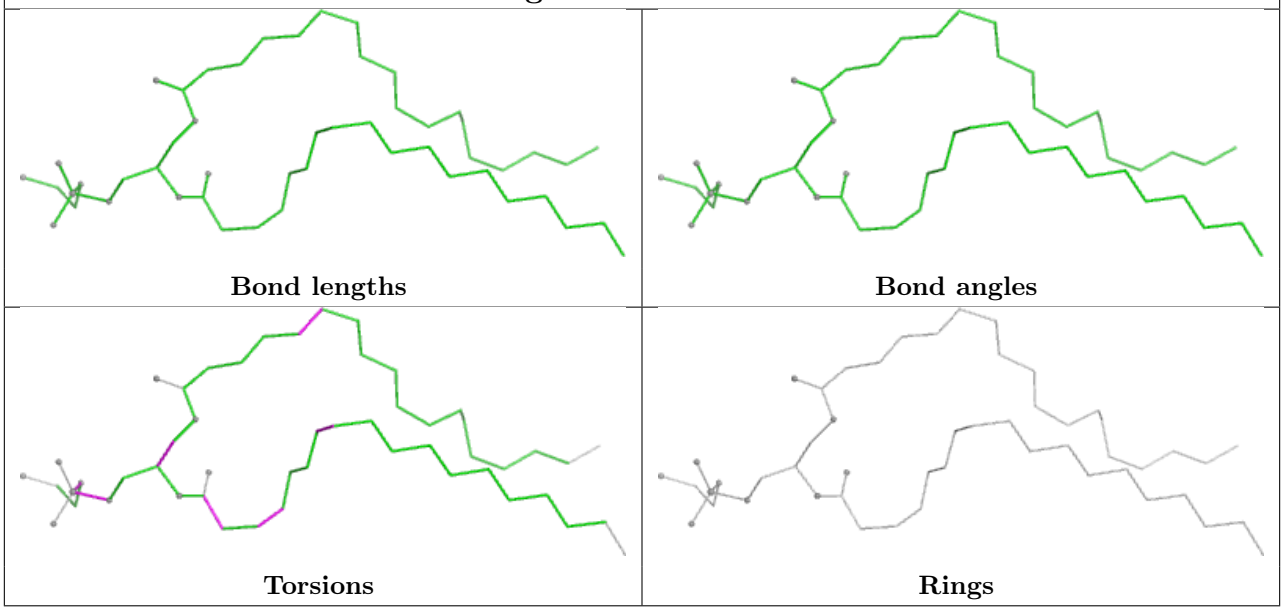
Ligand PC1 9 204



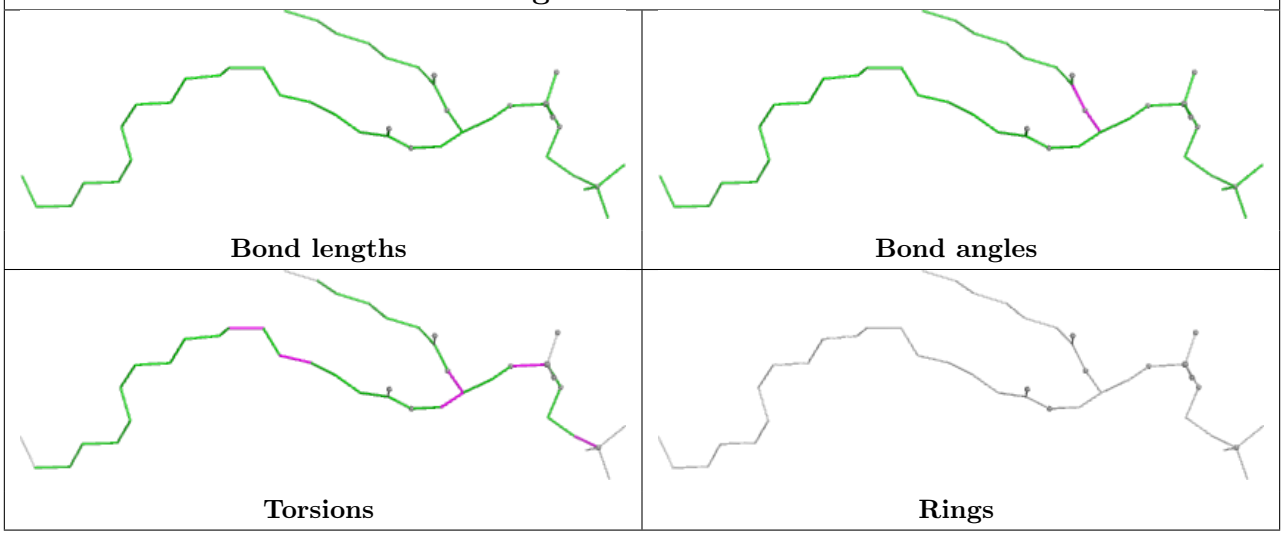
Ligand 3PE K 201



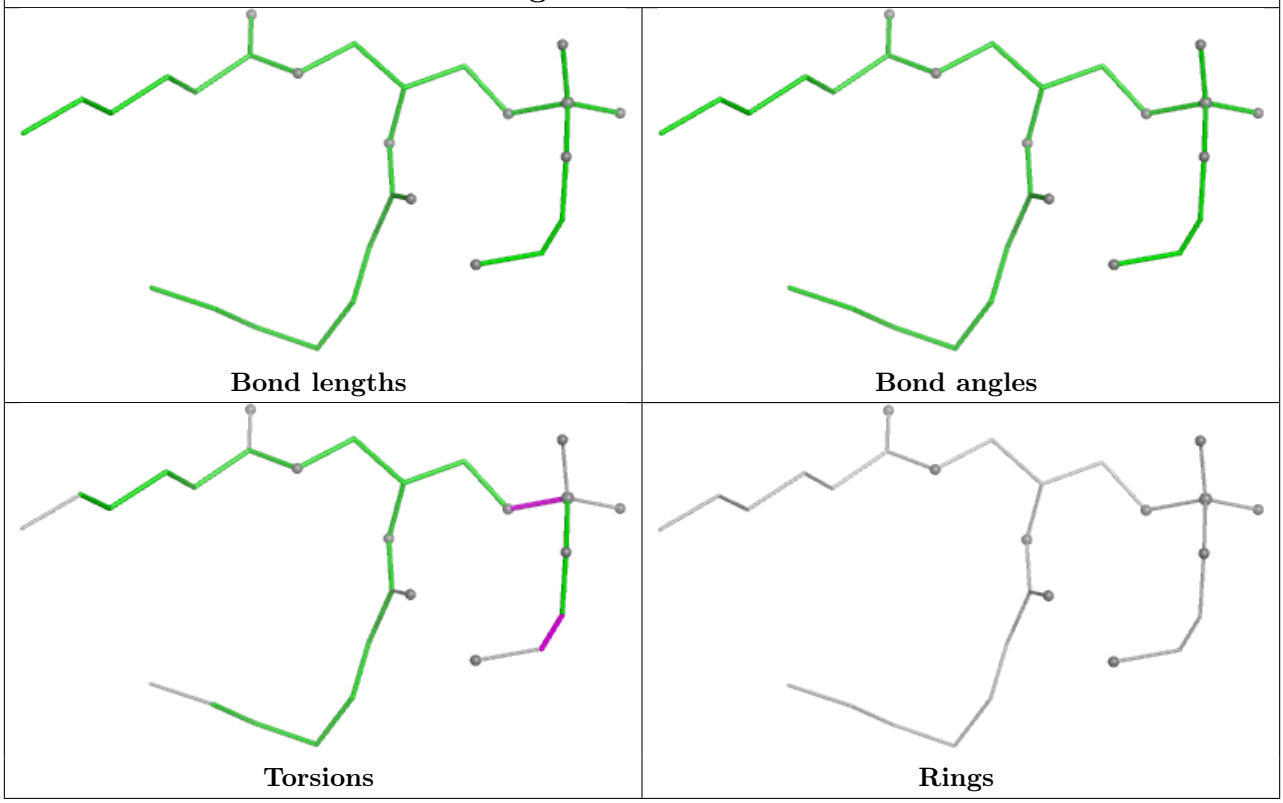
Ligand 3PE M 503



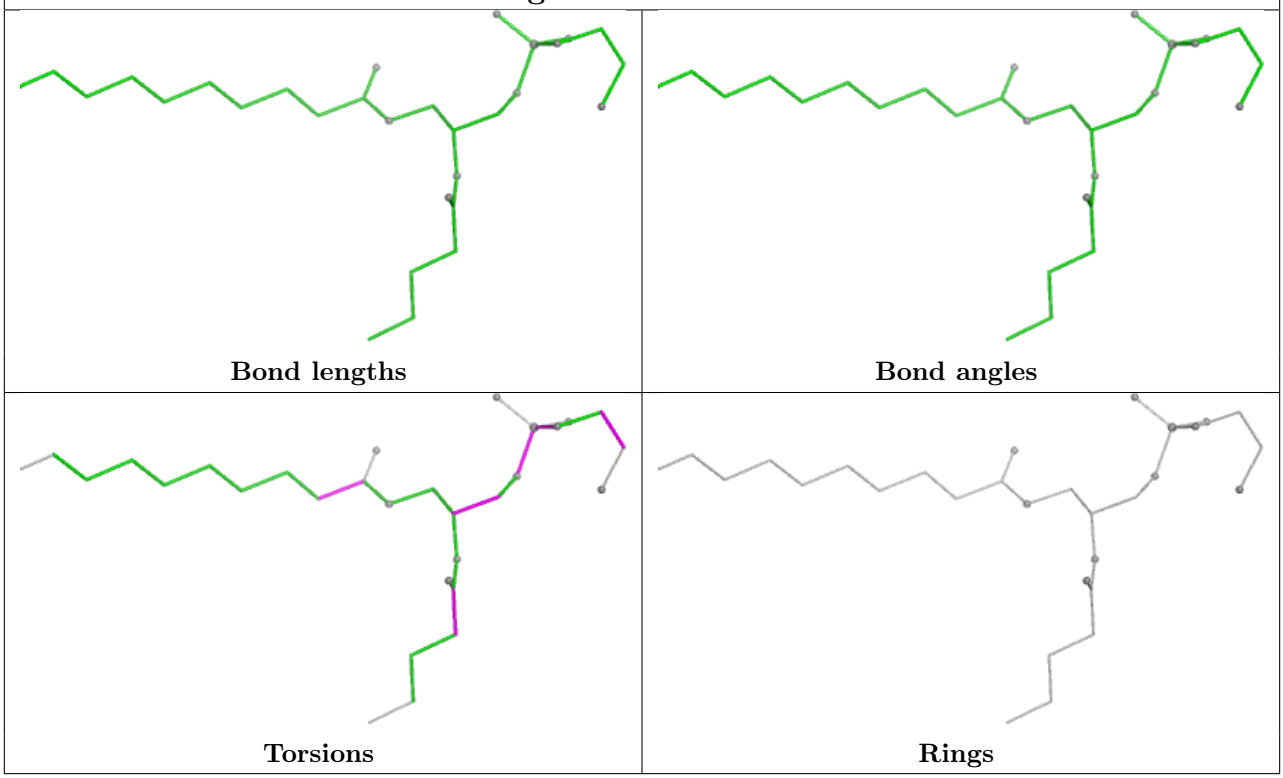
Ligand PC1 6 203



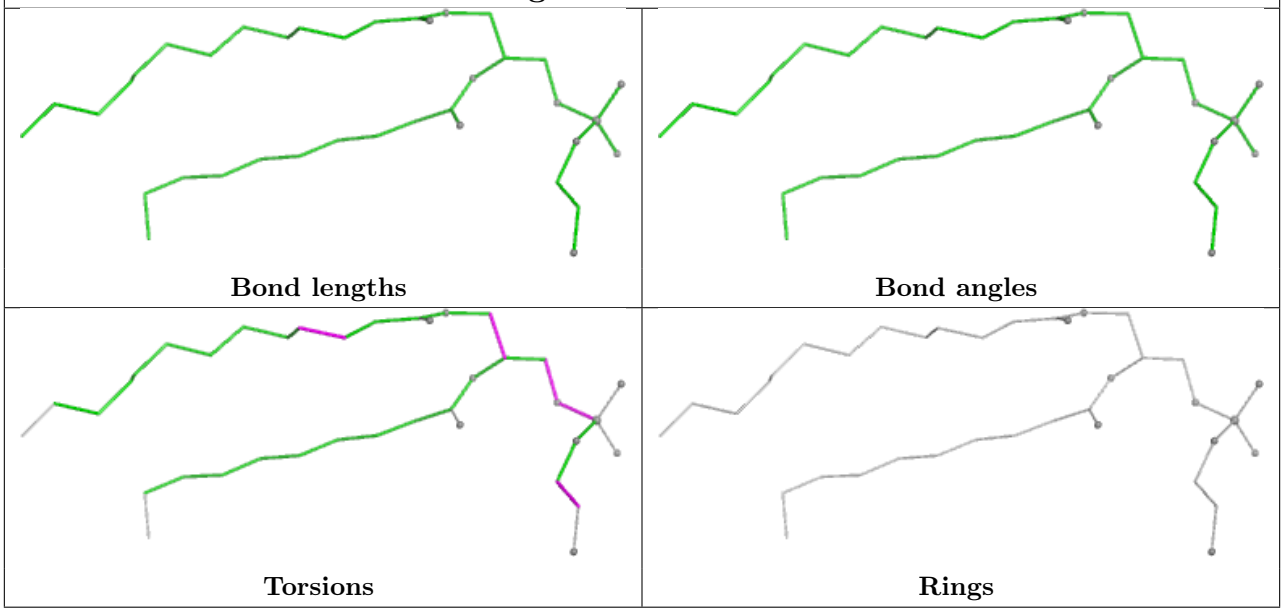
Ligand 3PE Y 201



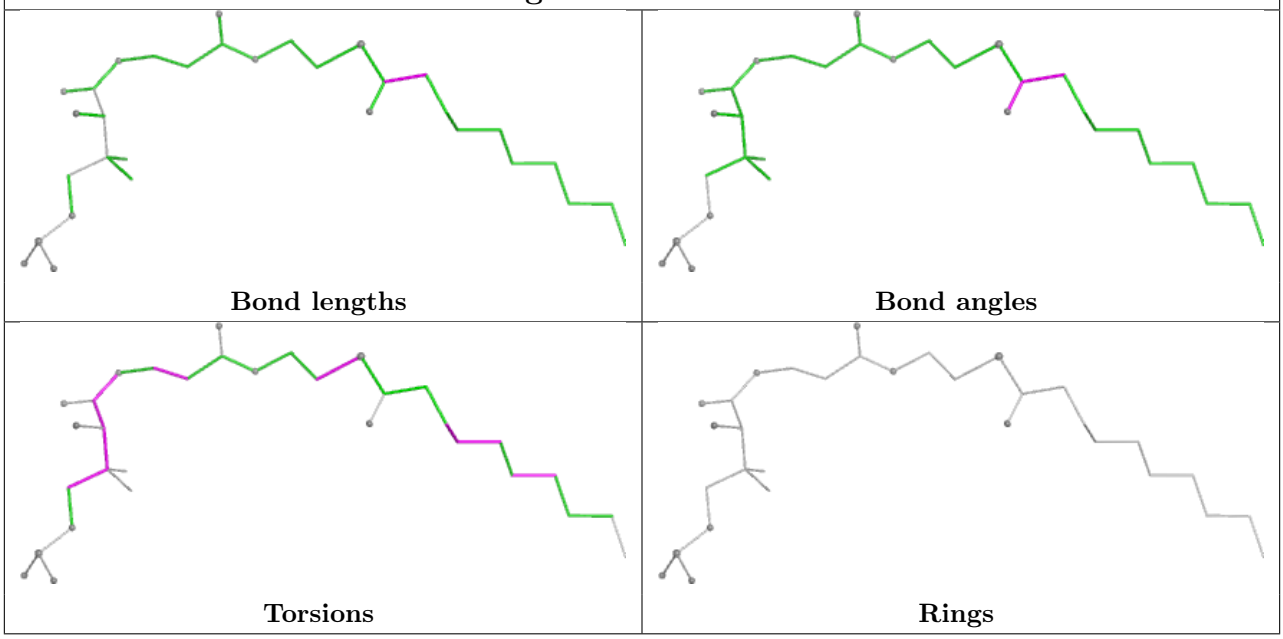
Ligand 3PE m 202



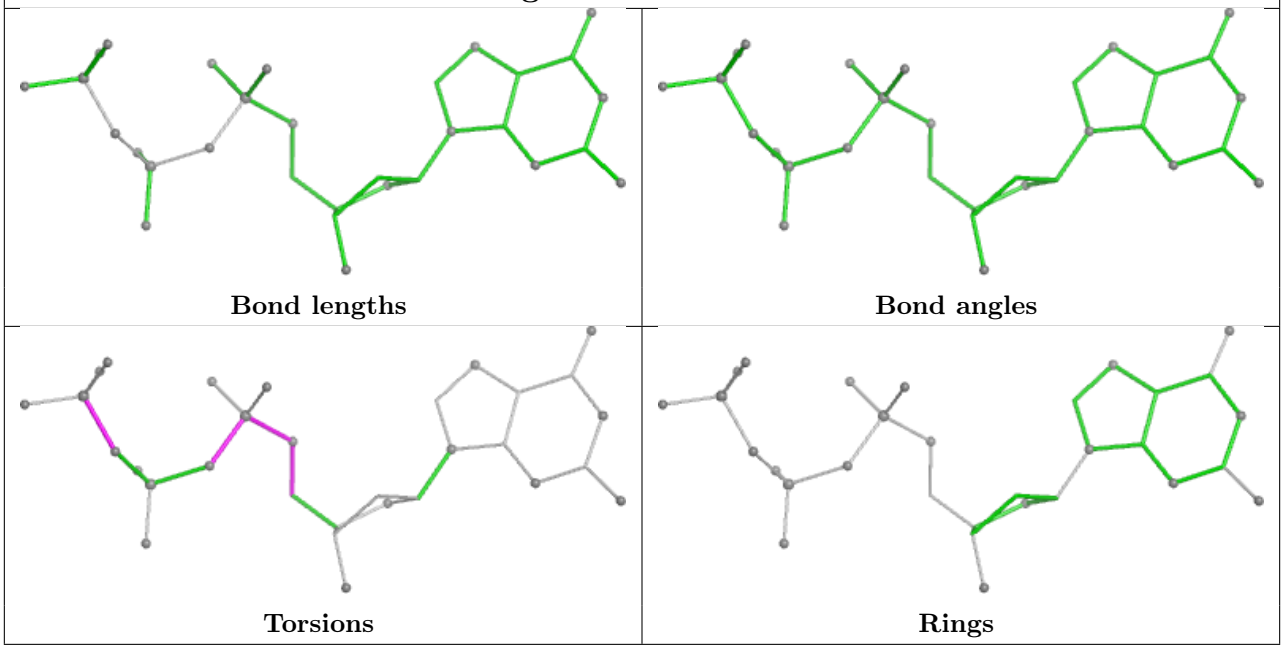
Ligand 3PE N 402

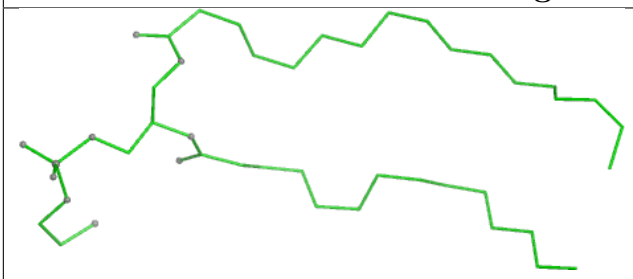
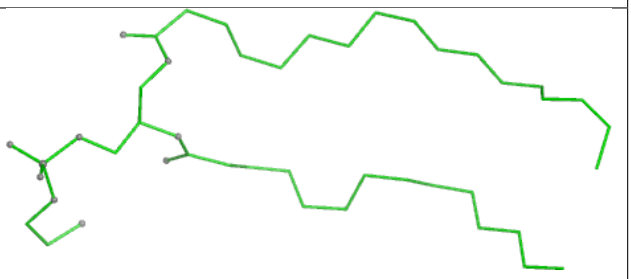
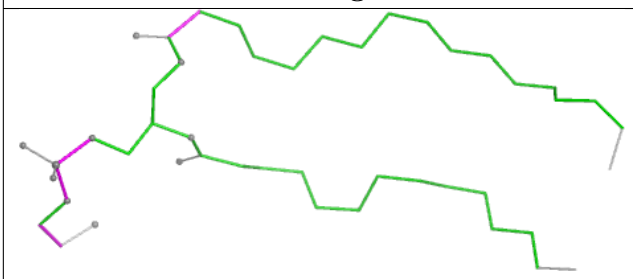
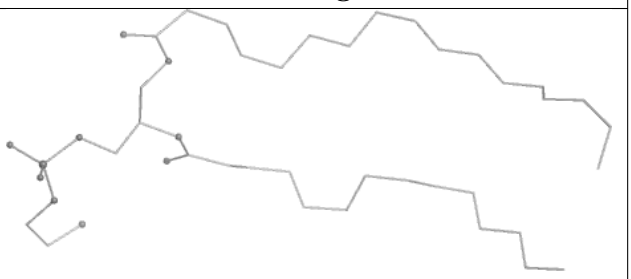


Ligand ZMP n 201



Ligand DGT O 401



Ligand 3PE r 201	
 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.

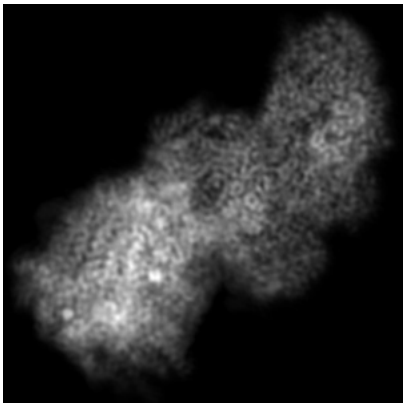
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-19146. These allow visual inspection of the internal detail of the map and identification of artifacts.

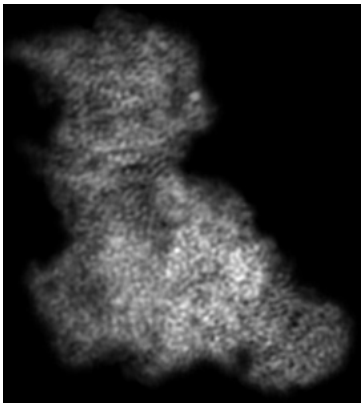
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

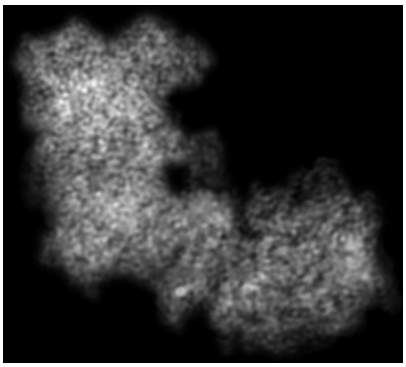
6.1.1 Primary map



X



Y

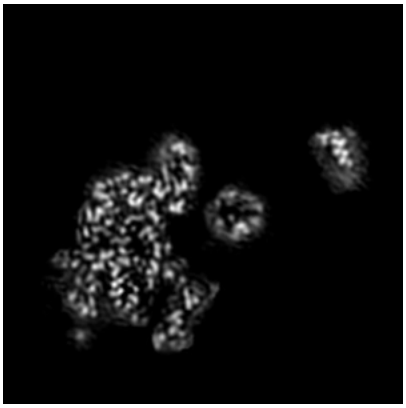


Z

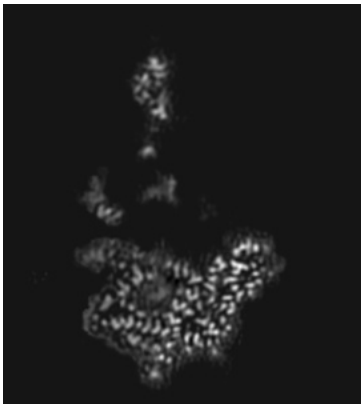
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

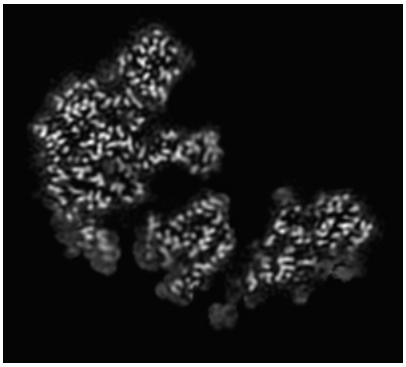
6.2.1 Primary map



X Index: 109



Y Index: 98

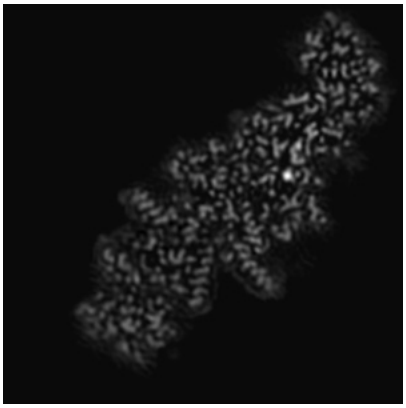


Z Index: 98

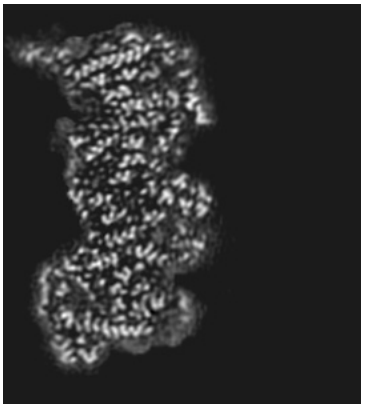
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

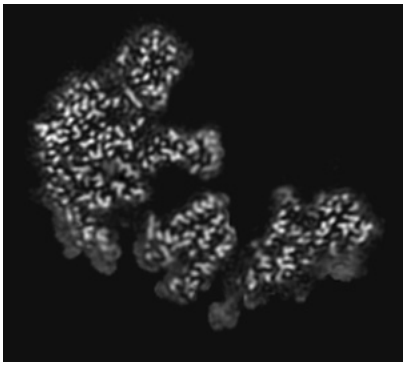
6.3.1 Primary map



X Index: 45



Y Index: 63

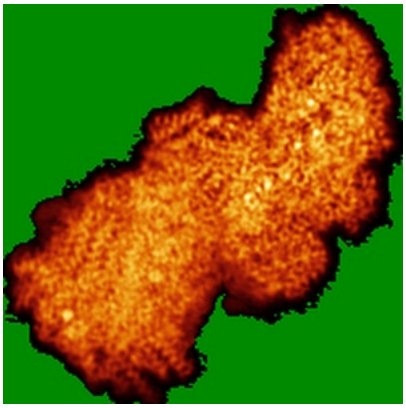


Z Index: 97

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

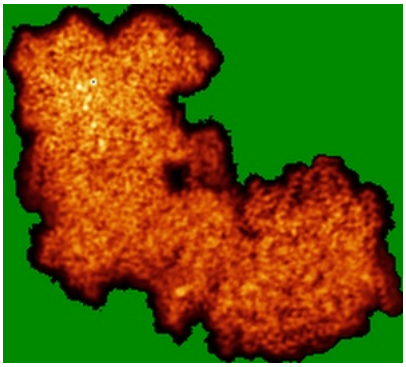
6.4 Orthogonal standard-deviation projections (False-color) (i)

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

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

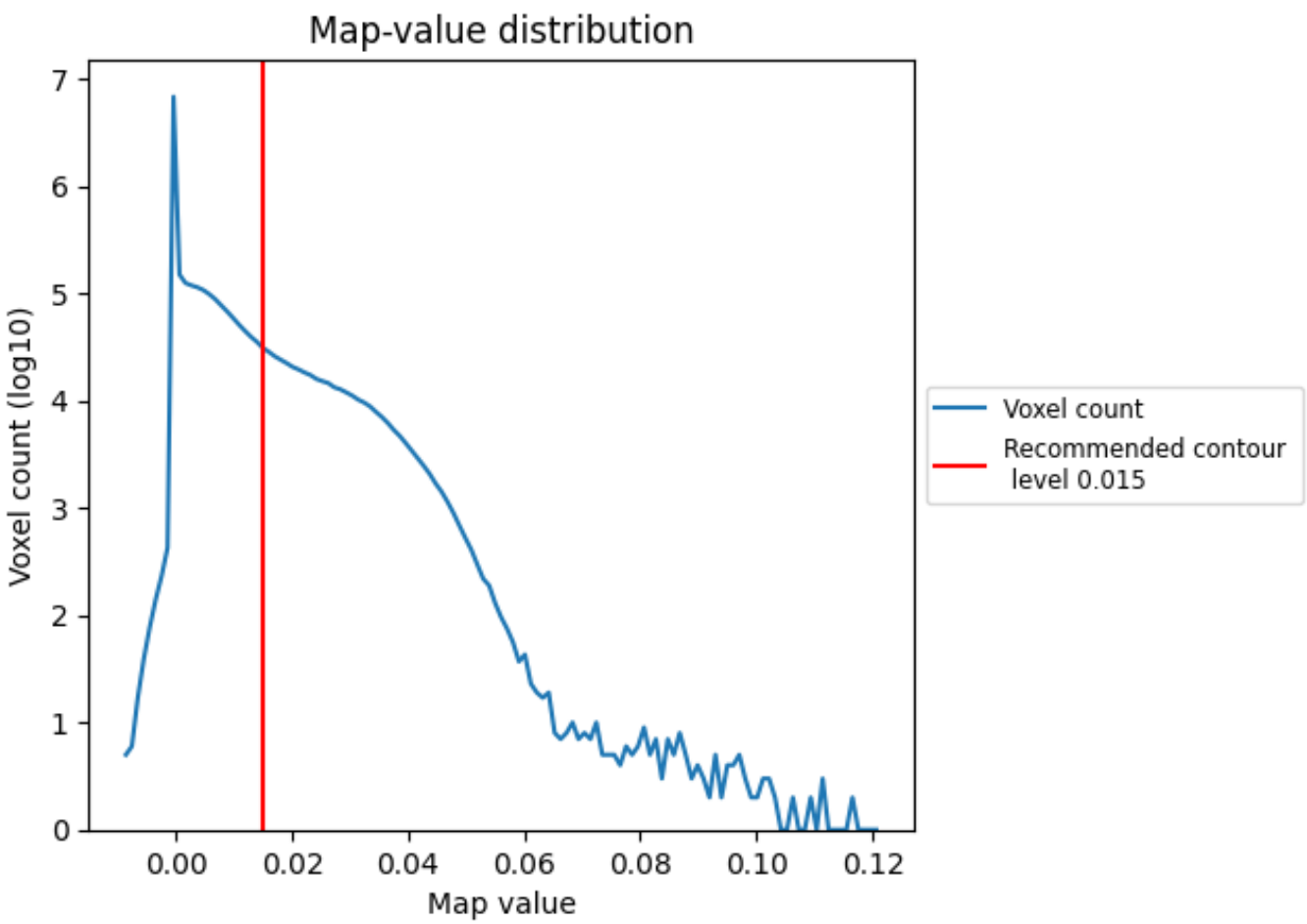
6.6 Mask visualisation (i)

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

7 Map analysis (i)

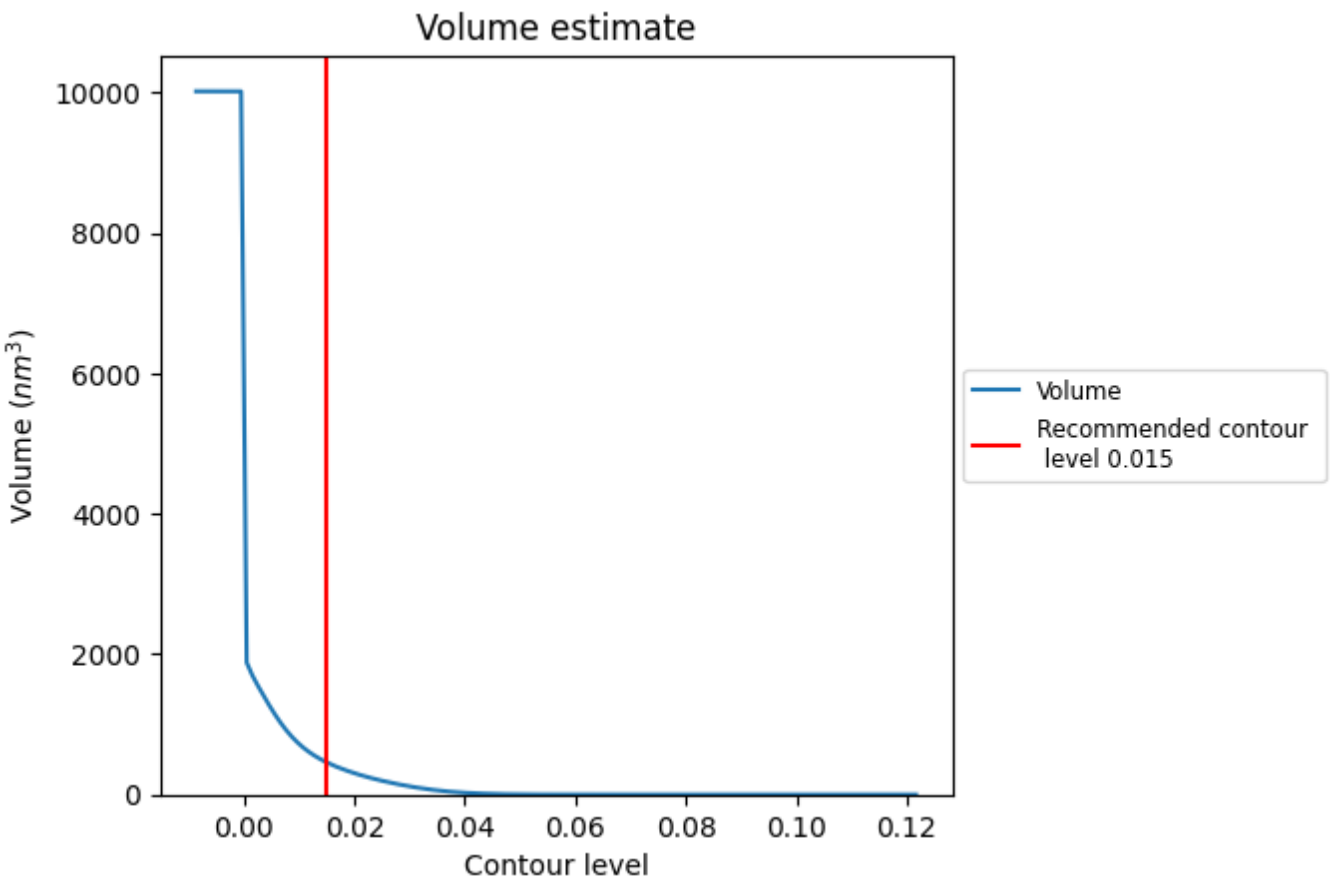
This section contains the results of statistical analysis of the map.

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 460 nm^3; this corresponds to an approximate mass of 416 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.

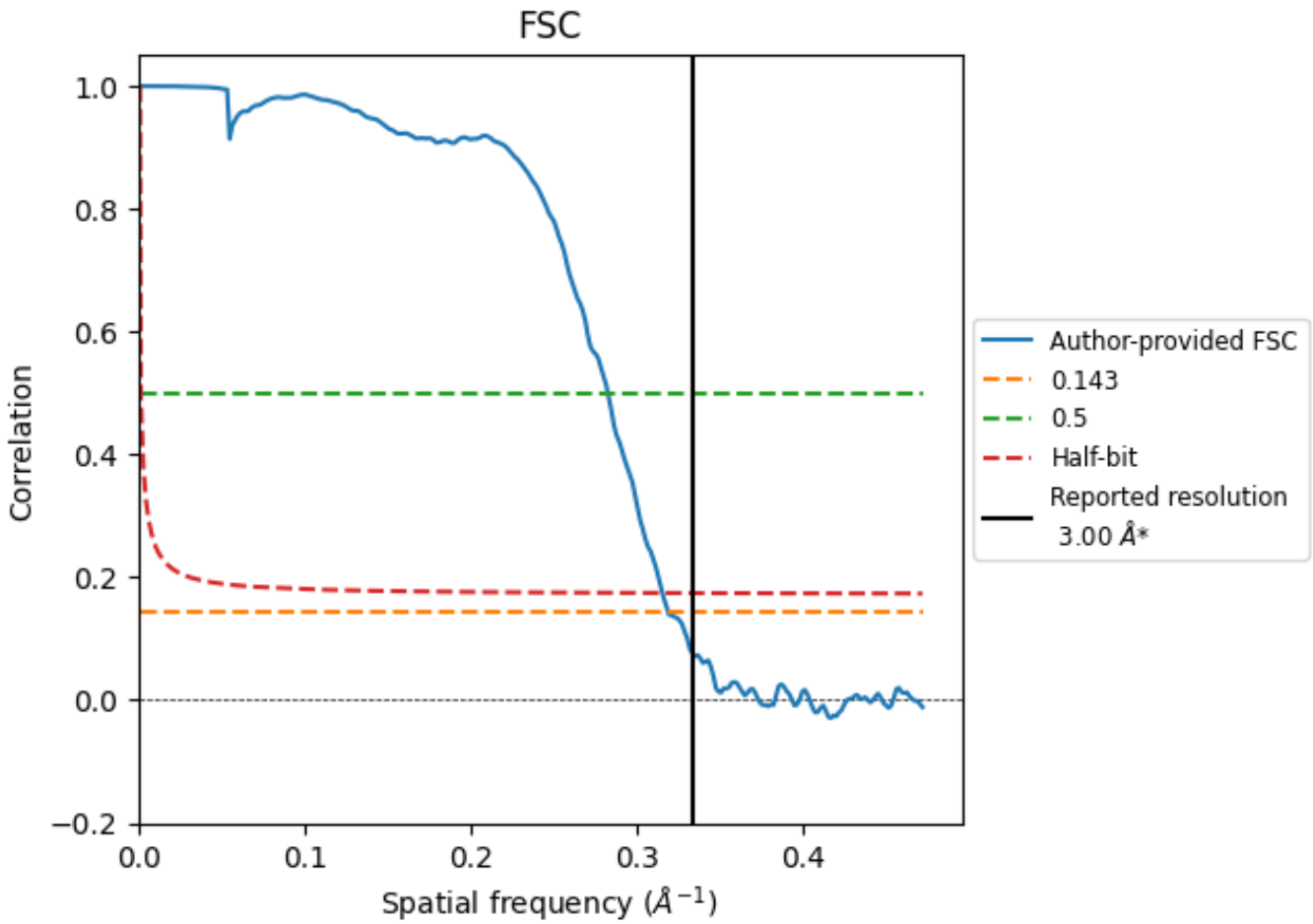
7.3 Rotationally averaged power spectrum (i)

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

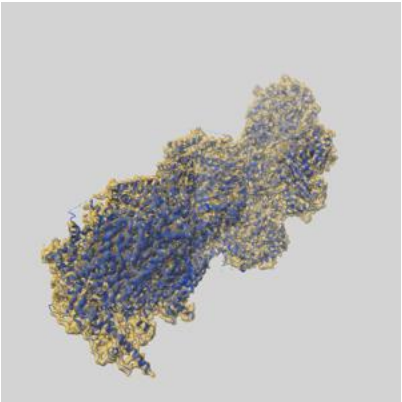
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.14	3.54	3.17
Unmasked-calculated*	-	-	-

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

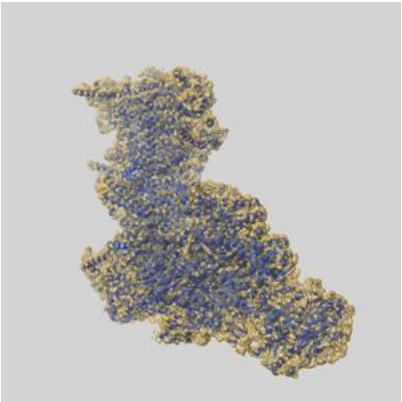
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-19146 and PDB model 8RGQ. Per-residue inclusion information can be found in section 3 on page 19.

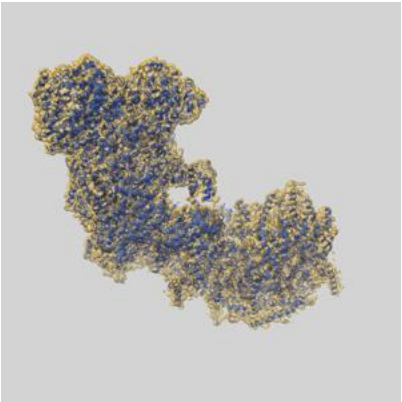
9.1 Map-model overlay (i)



X



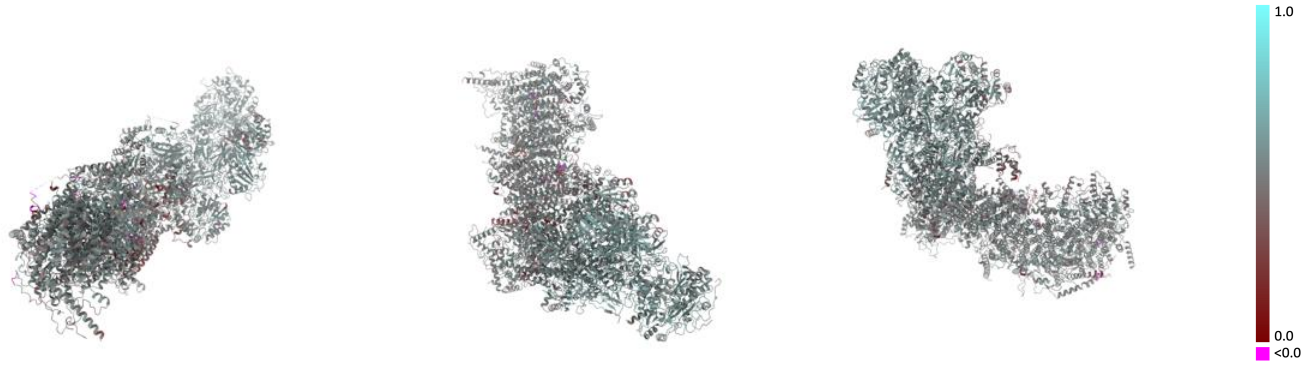
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

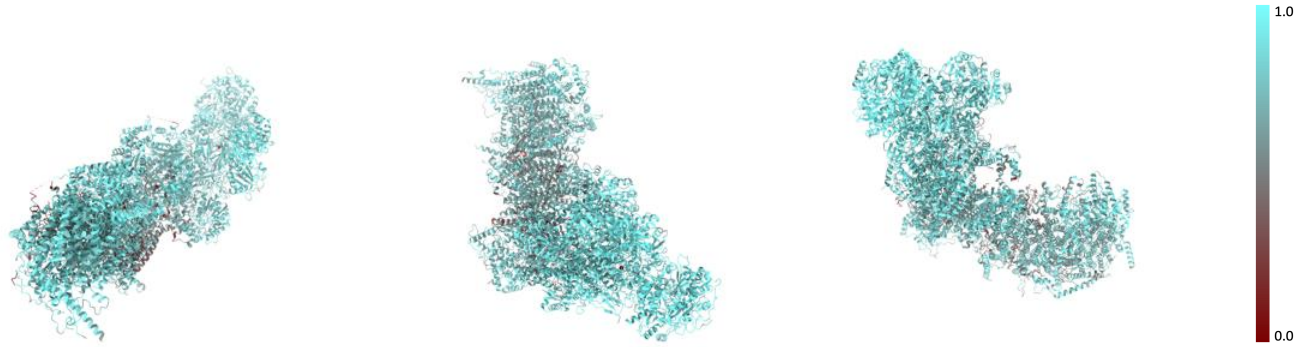
9.2 Q-score mapped to coordinate model (i)



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.

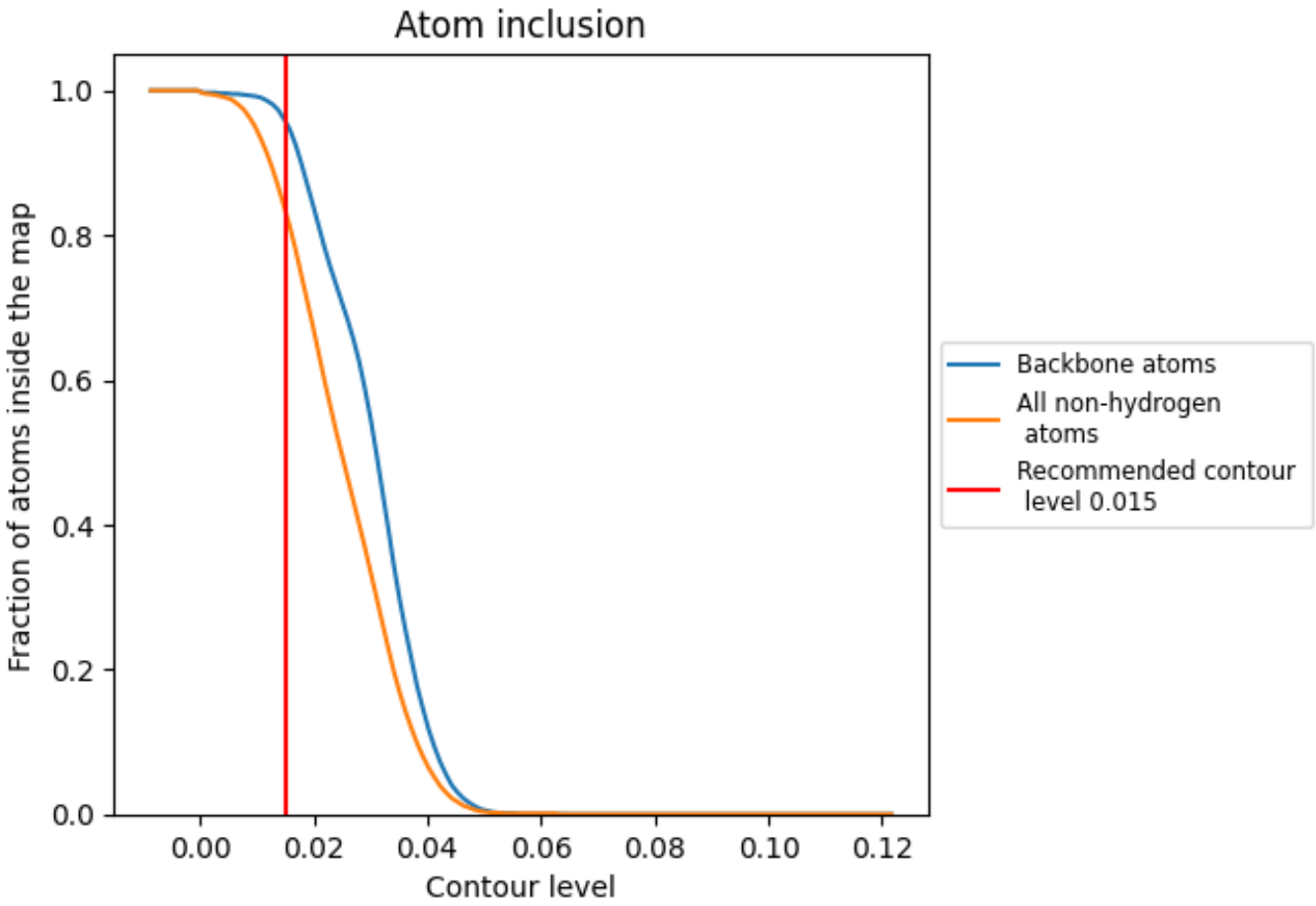
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 84% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8350	0.5150
1	0.9300	0.5540
2	0.9220	0.5480
3	0.9120	0.5550
6	0.8500	0.5210
7	0.9190	0.5580
9	0.8890	0.5510
A	0.7160	0.4950
C	0.9140	0.5670
D	0.8470	0.5240
H	0.7960	0.4970
J	0.6600	0.4530
K	0.7030	0.4900
L	0.7970	0.5080
M	0.7900	0.5170
N	0.7750	0.5120
O	0.8510	0.5030
P	0.8070	0.5000
Q	0.8800	0.5670
S	0.8790	0.4970
T	0.7180	0.3940
U	0.8400	0.5000
V	0.8740	0.5270
W	0.8870	0.5350
X	0.8630	0.5020
Y	0.7090	0.4690
Z	0.8650	0.5080
a	0.8450	0.5090
b	0.8310	0.4760
c	0.7930	0.4890
d	0.7680	0.5080
e	0.8120	0.5070
f	0.7700	0.4850
g	0.7820	0.4840
h	0.8430	0.5010

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Chain	Atom inclusion	Q-score
i	0.7480	0.4570
j	0.8360	0.4780
k	0.8410	0.4970
l	0.8500	0.5170
m	0.7190	0.4480
n	0.8550	0.5090
o	0.8330	0.4820
p	0.8710	0.5110
q	0.9170	0.5540
r	0.8510	0.5470
s	0.8920	0.5290