wwPDB EM Validation Summary Report (i)

Sep 8, 2026 – 05:59 pm BST

PDB ID	:	7QSD / pdb_00007qsd
EMDB ID	:	EMD-14127
Title	:	Bovine complex I in the active state at 3.1 A
Authors	:	Bridges, H.R.; Blaza, J.N.; Yin, Z.; Chung, I.; Hirst, J.
Deposited on	:	2022-01-13
Resolution	:	3.10 Å(reported)

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

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

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

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

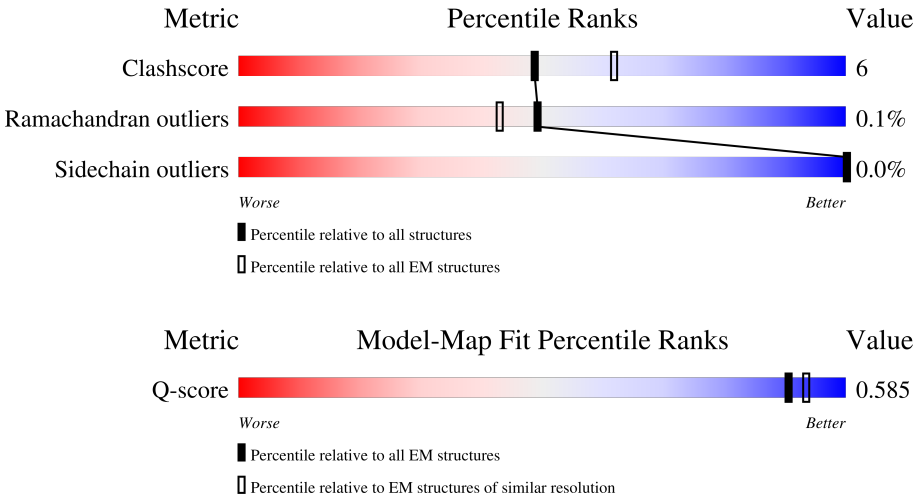
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	115	8%, 84%, 15%
2	B	216	61%, 11%, 28%
3	C	266	69%, 9%, 22%
4	D	463	78%, 15%, 7%

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Mol	Chain	Length	Quality of chain
5	E	249	6% 74% 12% 14%
6	F	464	80% 13% 7%
7	G	727	81% 14% 5%
8	H	318	78% 22%
9	I	212	71% 12% 17%
10	J	175	9% 83% 16%
11	K	98	77% 23%
12	L	606	7% 80% 20%
13	M	459	80% 20%
14	N	347	83% 17%
15	O	343	6% 76% 17% 7%
16	P	380	80% 9% 10%
17	Q	175	5% 64% 7% 29%
18	R	124	6% 74% 23%
19	S	99	8% 77% 8% 15%
20	T	156	18% 42% 7% 51%
20	U	156	6% 46% 10% 45%
21	V	116	9% 90% 8%
22	W	128	9% 77% 12% 11%
23	X	172	6% 88% 11%
24	Y	141	11% 94% 5%
25	Z	144	6% 87% 11%
26	a	70	6% 79% 21%
27	b	84	10% 92% 7%
28	c	76	7% 61% 37%

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Mol	Chain	Length	Quality of chain
29	d	120	12% 91% 9%
30	e	106	5% 86% 6% 8%
31	f	57	19% 79% 9% 12%
32	g	154	7% 53% 10% 36%
33	h	189	67% 6% 27%
34	i	127	20% 63% 20% 16%
35	j	108	7% 51% 8% 41%
36	k	98	18% 73% 8% 18%
37	l	186	8% 74% 9% 17%
38	m	129	15% 88% 10%
39	n	179	11% 81% 15%
40	o	137	20% 74% 15% 11%
41	p	176	9% 88% 10%
42	q	145	94% 5%
43	r	113	75% 8% 17%
44	s	109	32% 8% 60%

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
47	SF4	F	502	-	-	X	-

2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 67258 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	115	921	622	133	159	7	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	155	1241	792	224	211	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	207	1721	1111	296	311	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	430	3459	2209	596	629	25	0	0

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1655	1057	277	311	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	431	Total	C	N	O	S	0	0
			3319	2091	593	615	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	688	Total	C	N	O	S	0	0
			5279	3307	920	1013	39		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	174	Total	C	N	O	S	0	0
			1337	902	189	234	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			745	486	112	131	16		

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	341	Total	C	N	O	S	0	0
			2747	1777	486	479	5		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	95	Total	C	N	O	S	0	0
			730	448	137	142	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	84	Total	C	N	O	S	0	0
			677	425	126	124	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	76	Total	C	N	O	S	0	0
			612	393	90	124	5		
20	U	86	Total	C	N	O	S	0	0
			692	447	102	138	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	113	Total	C	N	O	S	0	0
			919	595	155	166	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	114	Total	C	N	O	S	0	0
			971	622	180	165	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	140	Total	C	N	O	S	0	0
			1030	657	176	191	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	141	Total	C	N	O	S	0	0
			1152	740	201	202	9		

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	48	Total	C	N	O	0	0
			405	268	69	68		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	120	Total	C	N	O	S	0	0
			993	647	169	172	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	97	Total	C	N	O	S	0	0
			819	518	156	139	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	50	Total	C	N	O	S	0	0
			437	286	77	73	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	98	Total	C	N	O	S	0	0
			824	529	137	154	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	107	Total	C	N	O	S	0	0
			920	605	158	156	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	64	Total	C	N	O	S	0	0
			556	367	90	98	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	80	Total	C	N	O	S	0	0
			644	421	108	113	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	155	Total	C	N	O	S	0	0
			1304	844	213	239	8		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
38	m	127	Total	C	N	O	0	0
			1061	681	187	193		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	172	Total	C	N	O	S	0	0
			1492	955	273	257	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	122	Total	C	N	O	S	0	0
			1048	653	201	185	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	171	Total	C	N	O	S	0	0
			1443	904	266	265	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	144	Total	C	N	O	S	0	0
			1201	773	215	209	4		

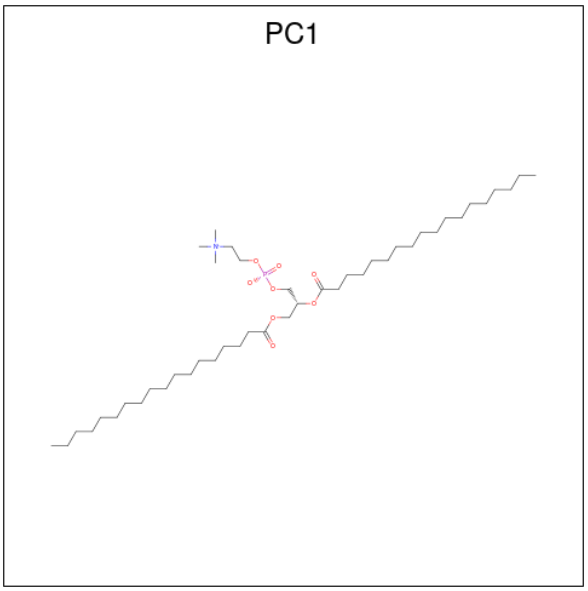
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	94	Total	C	N	O	S	0	0
			767	485	143	136	3		

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

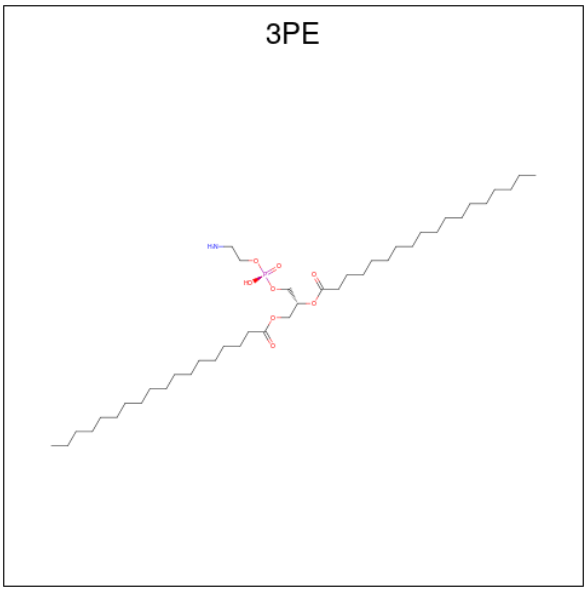
Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

- Molecule 45 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



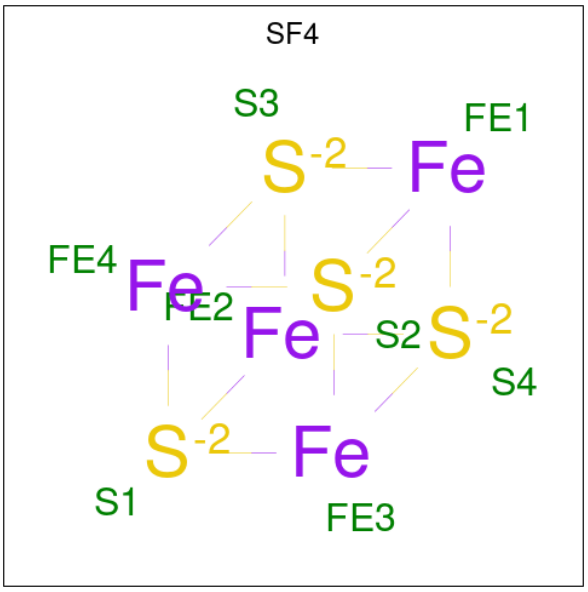
Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			21	11	1	8	1	
45	B	1	Total	C	N	O	P	0
			43	33	1	8	1	
45	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	d	1	Total	C	N	O	P	0
			26	16	1	8	1	
45	g	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



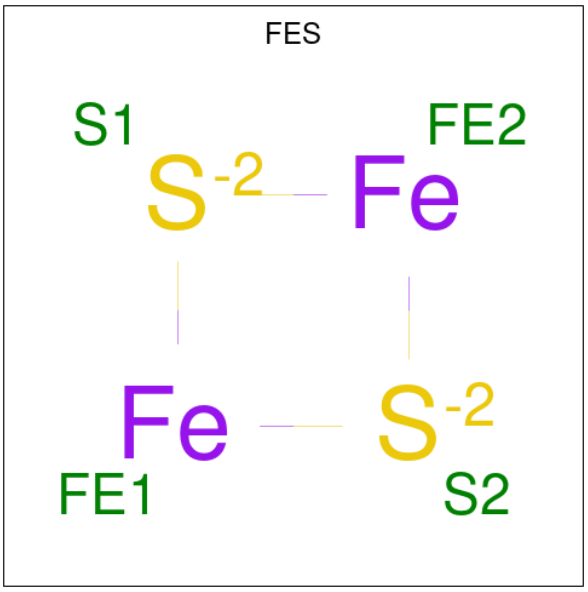
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	I	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	J	1	Total	C	N	O	P	0
			28	18	1	8	1	
46	K	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	L	1	Total	C	N	O	P	0
			38	28	1	8	1	
46	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
46	L	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	M	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	M	1	Total	C	N	O	P	0
			40	30	1	8	1	
46	N	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	N	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	X	1	Total	C	N	O	P	0
			31	21	1	8	1	
46	c	1	Total	C	N	O	P	0
			38	28	1	8	1	

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



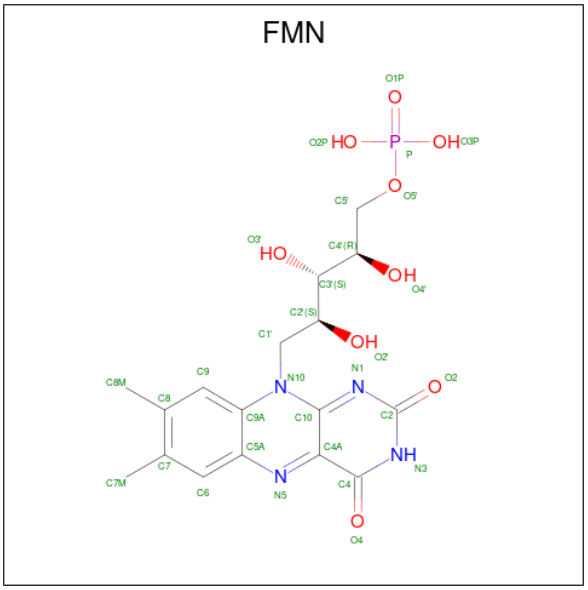
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

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



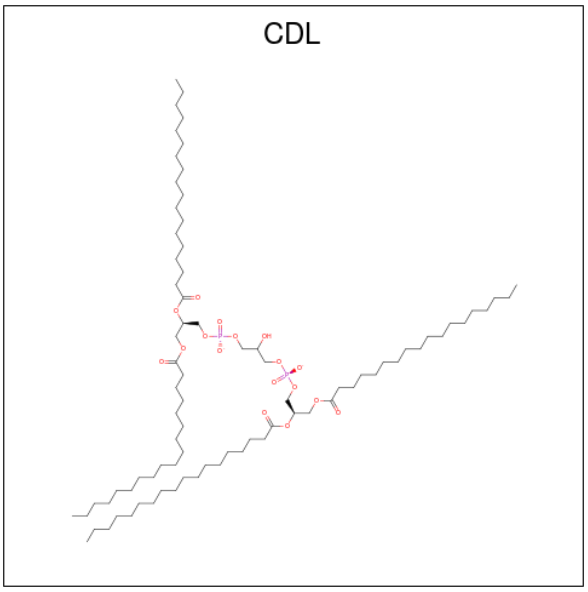
Mol	Chain	Residues	Atoms			AltConf
48	E	1	Total	Fe	S	0
			4	2	2	
48	G	1	Total	Fe	S	0
			4	2	2	

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



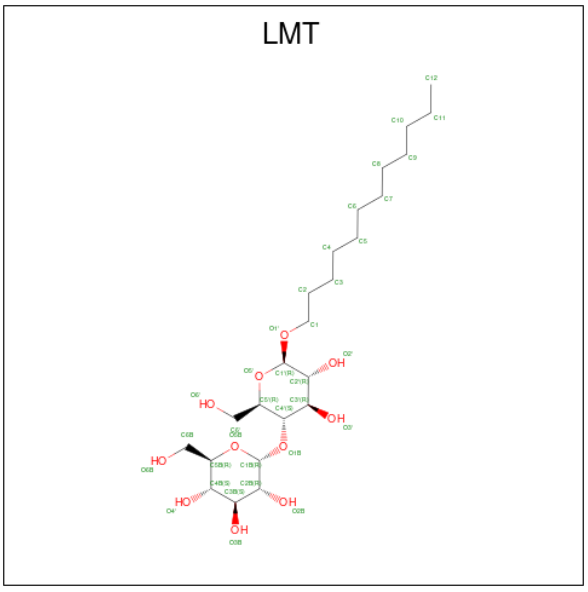
Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 50 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



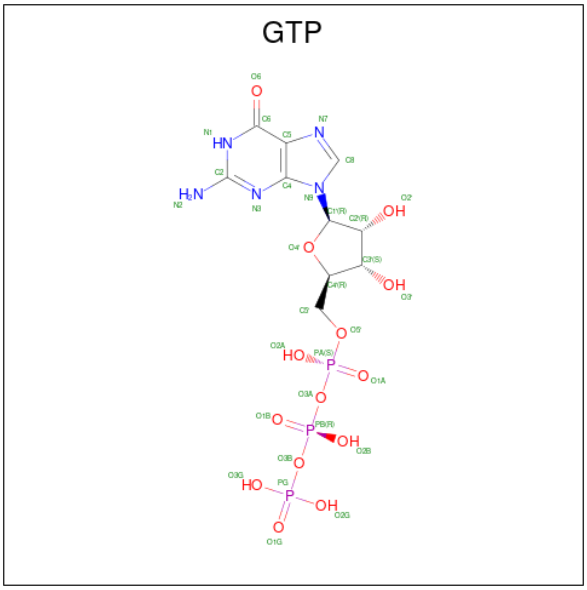
Mol	Chain	Residues	Atoms				AltConf
50	L	1	Total	C	O	P	0
			62	43	17	2	
50	Y	1	Total	C	O	P	0
			50	31	17	2	
50	h	1	Total	C	O	P	0
			64	45	17	2	
50	q	1	Total	C	O	P	0
			69	50	17	2	

- Molecule 51 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	AltConf
51	M	1	Total C O 35 24 11	0
51	N	1	Total C O 35 24 11	0
51	b	1	Total C O 35 24 11	0

- Molecule 52 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

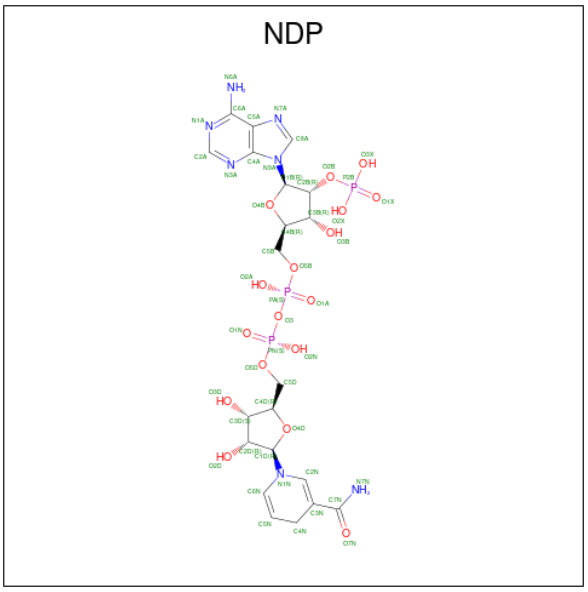


Mol	Chain	Residues	Atoms	AltConf
52	O	1	Total C N O P 32 10 5 14 3	0

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 54 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

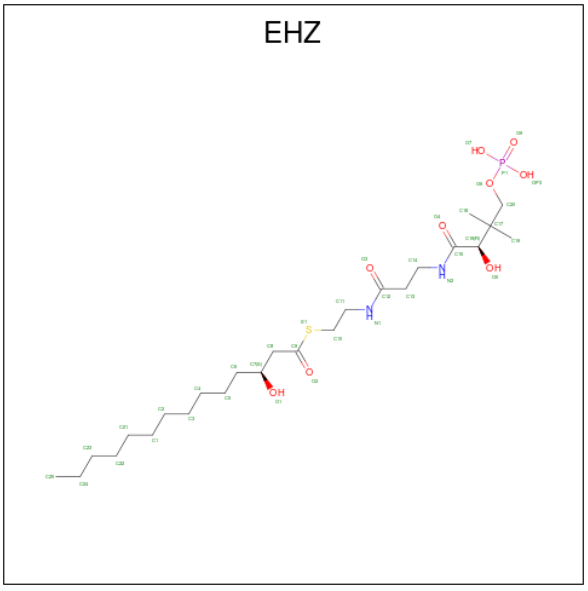


Mol	Chain	Residues	Atoms					AltConf
54	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

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

- Molecule 56 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).

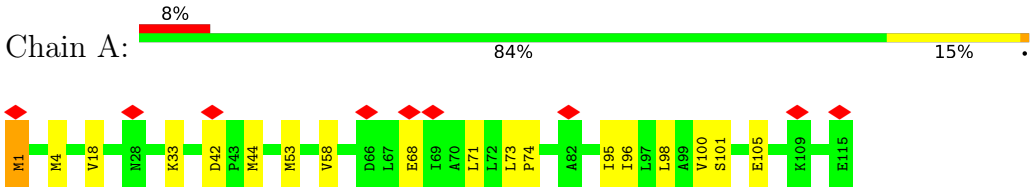


Mol	Chain	Residues	Atoms						AltConf
56	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
56	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

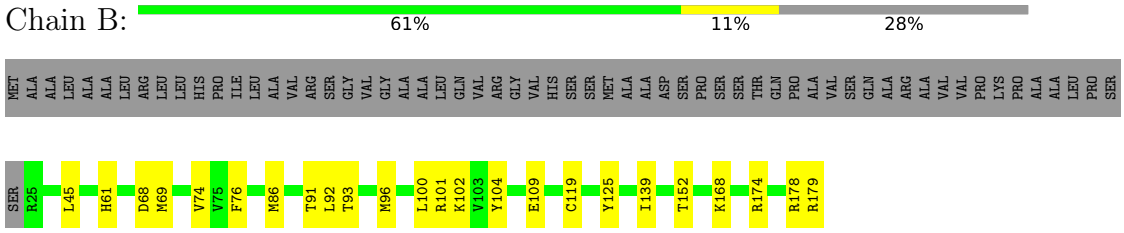
3 Residue-property plots (i)

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

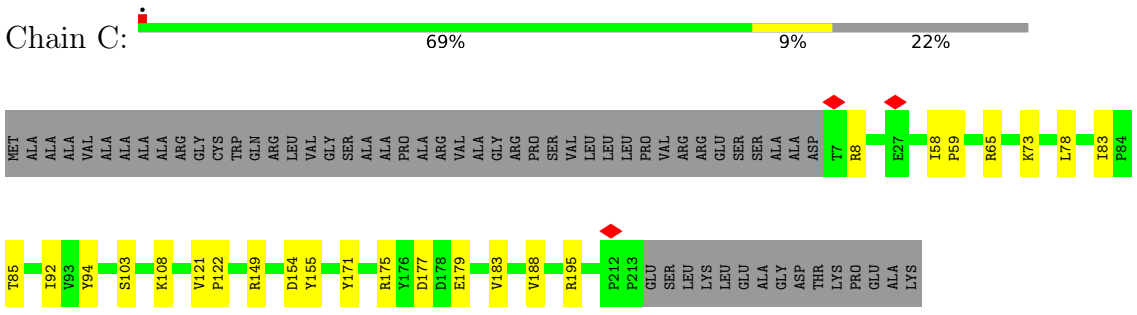
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3



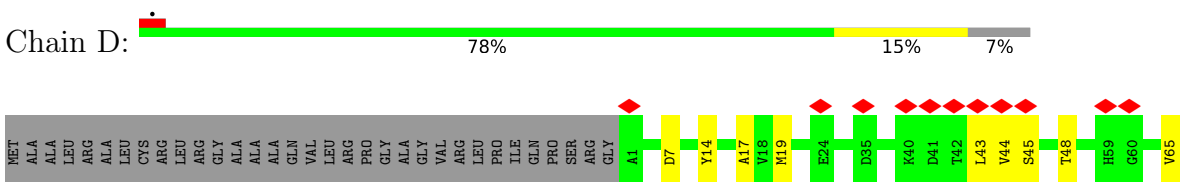
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

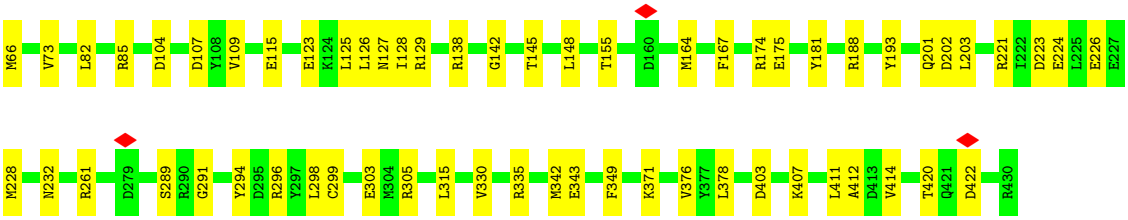


• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

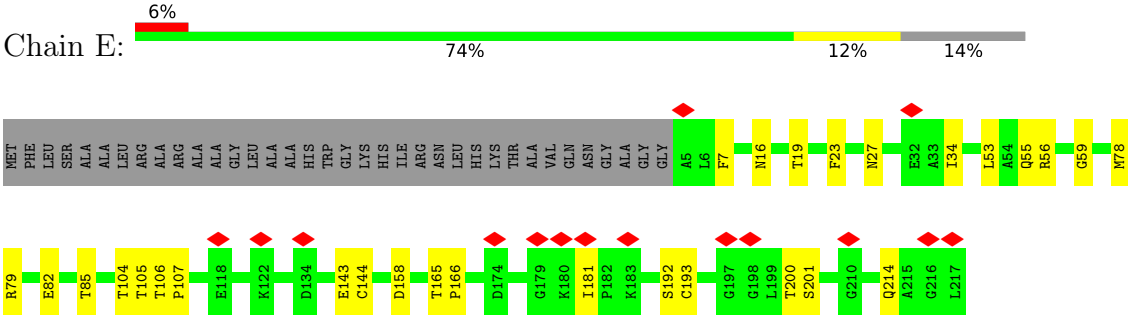


• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

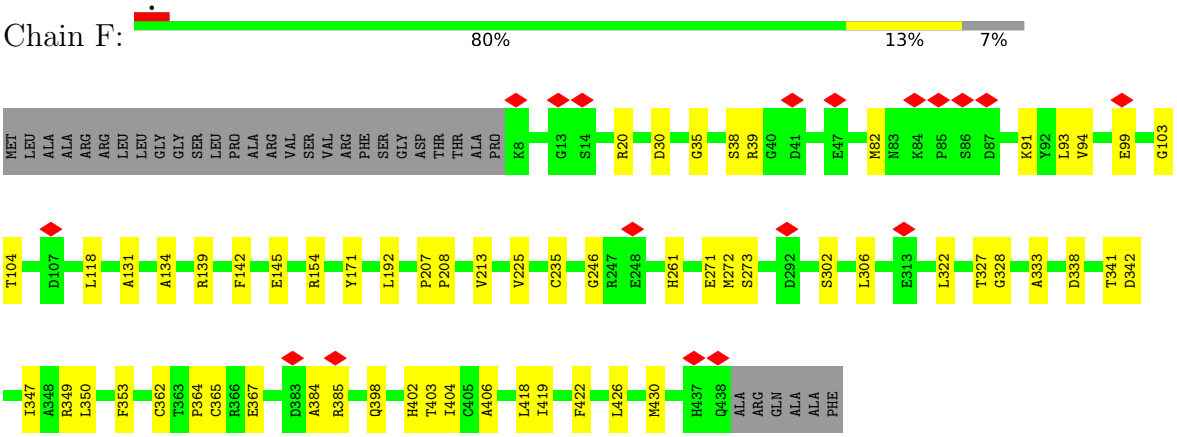




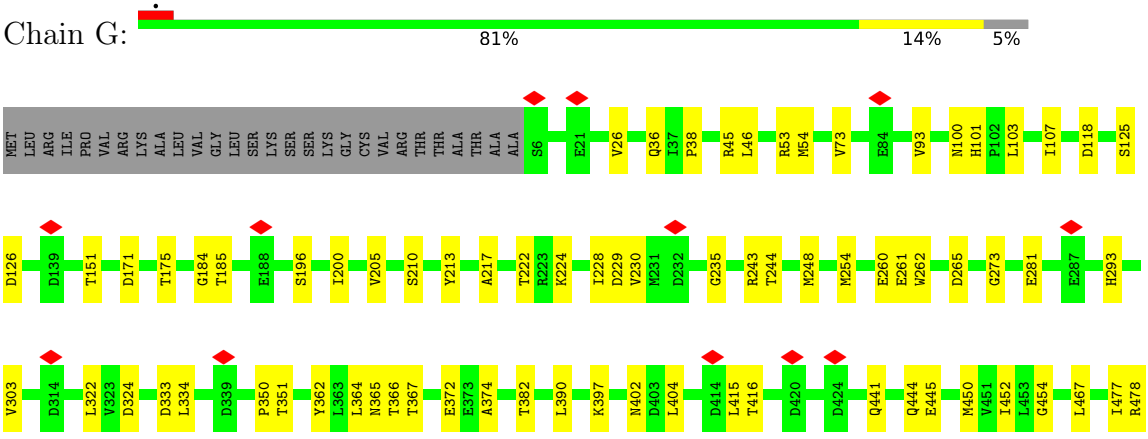
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

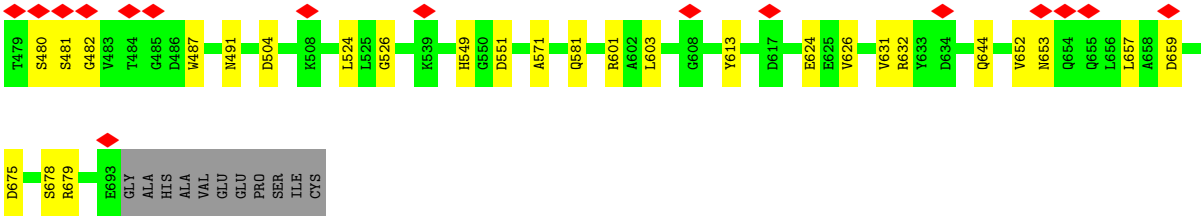


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

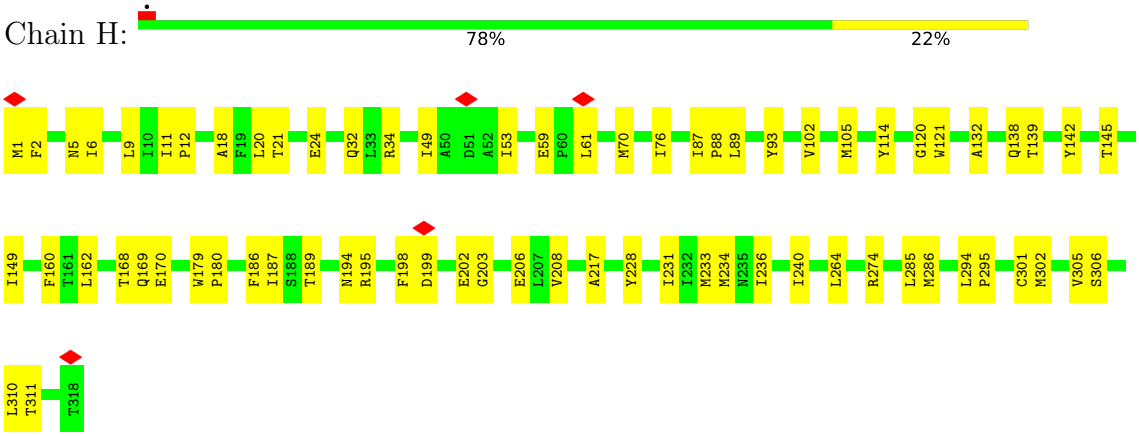


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

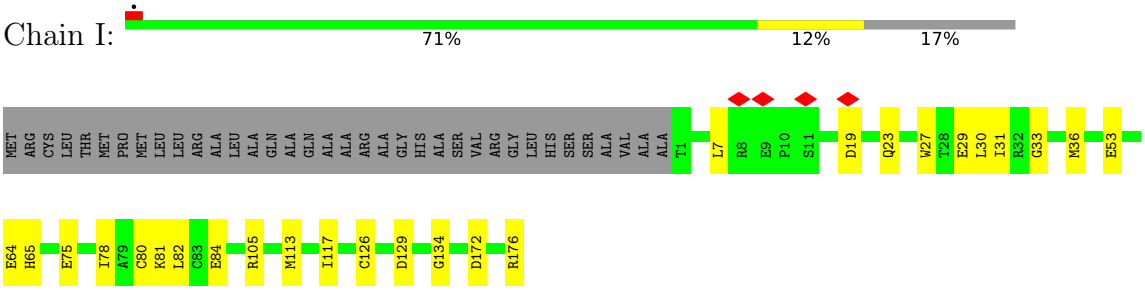




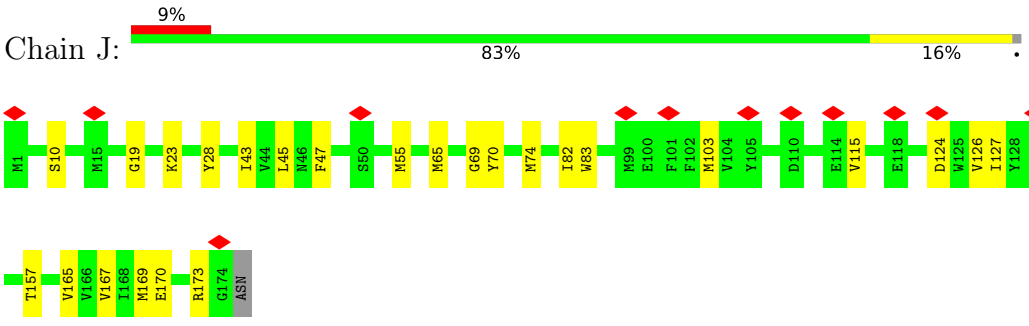
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



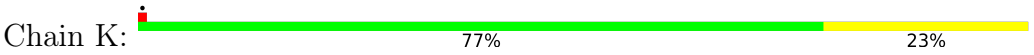
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

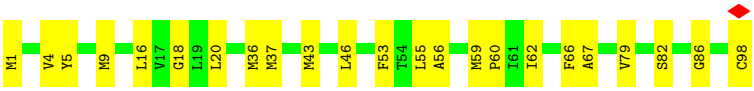


• Molecule 10: NADH-ubiquinone oxidoreductase chain 6



• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

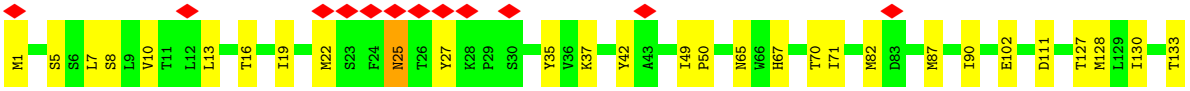


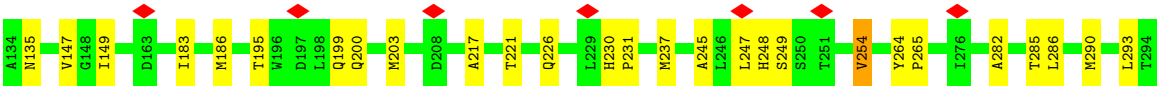


• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

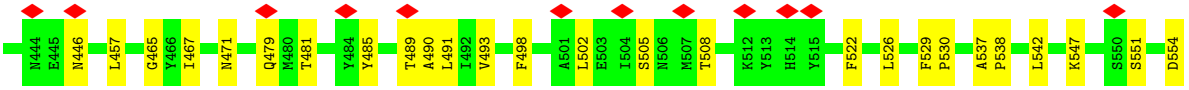
Chain L:

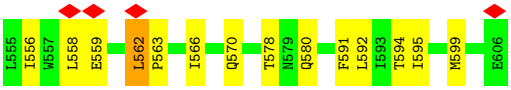










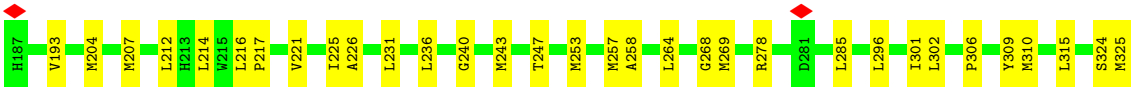


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:





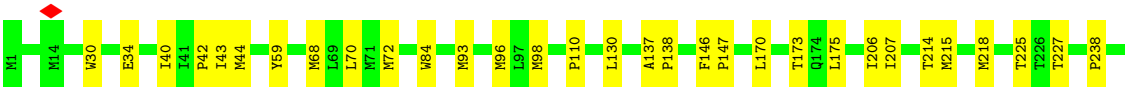


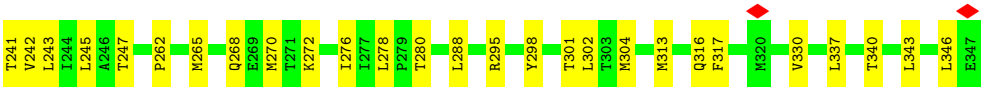


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:

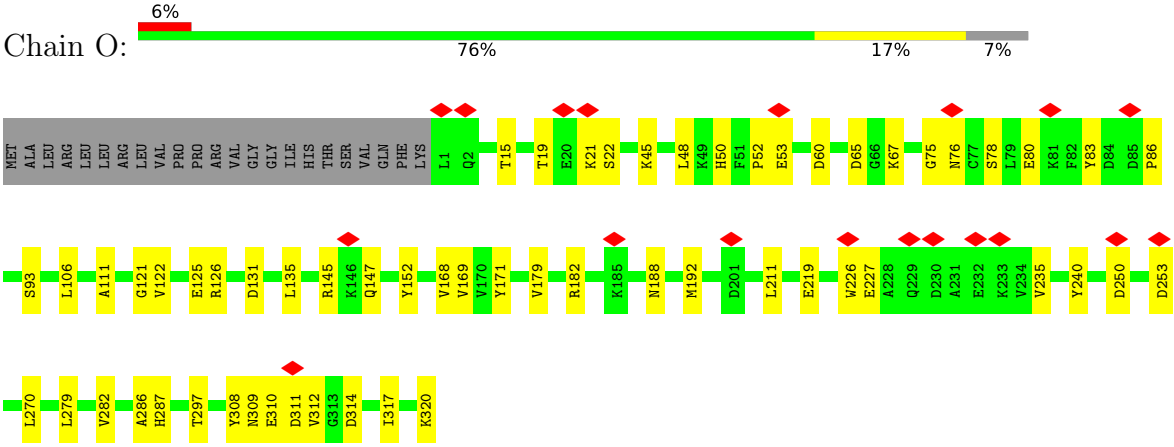






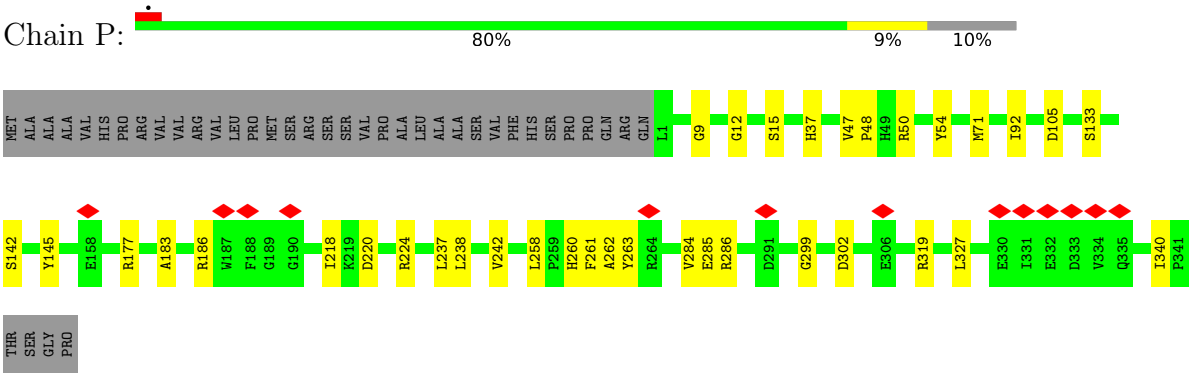
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:



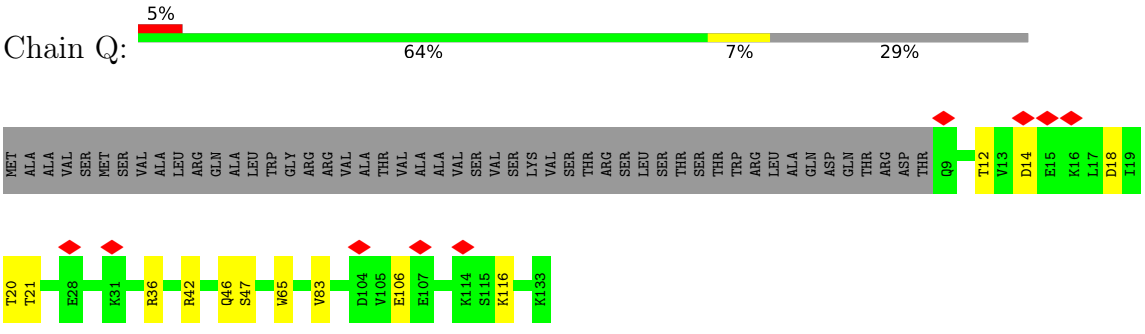
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:



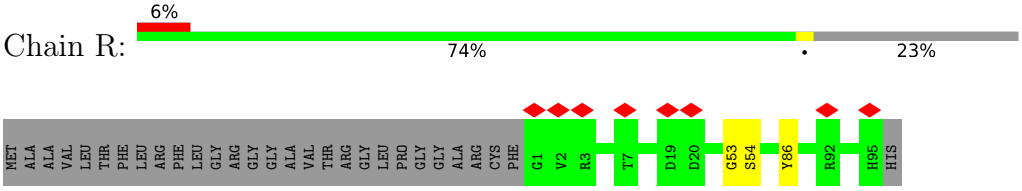
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:



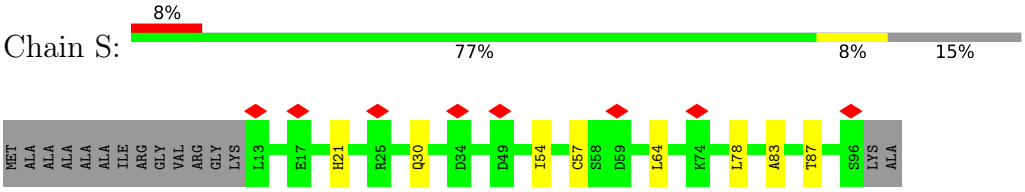
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:



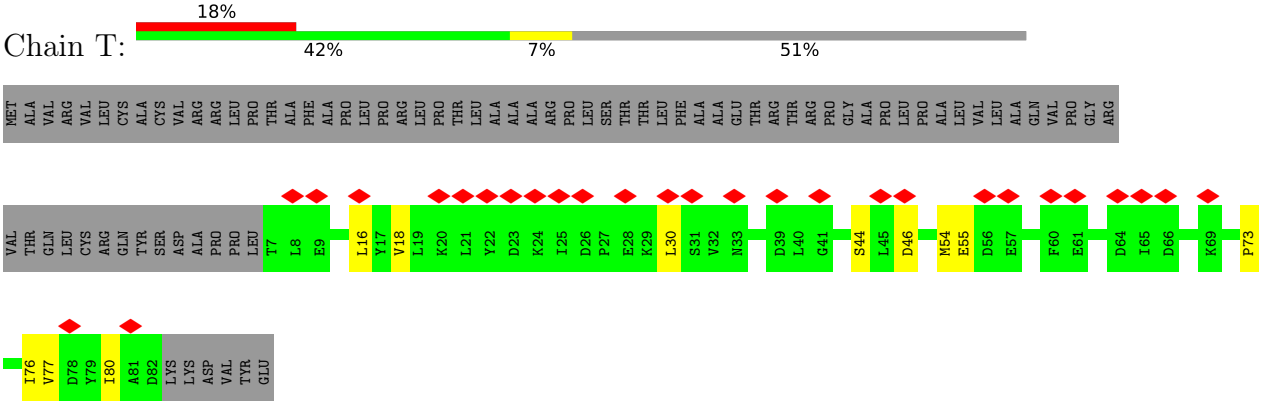
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:



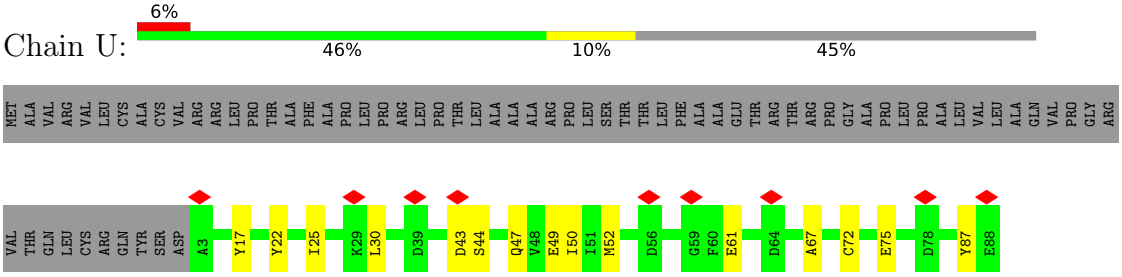
• Molecule 20: Acyl carrier protein, mitochondrial

Chain T:



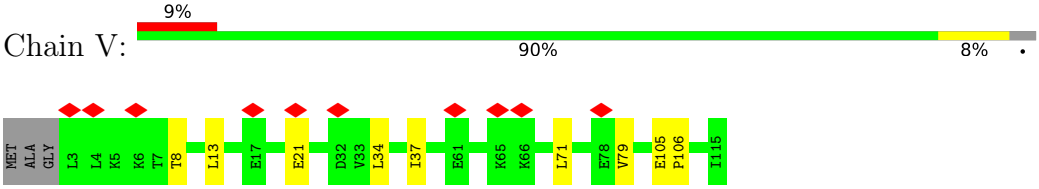
• Molecule 20: Acyl carrier protein, mitochondrial

Chain U:



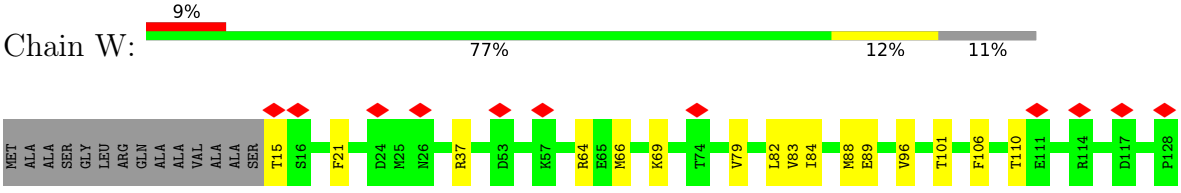
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:



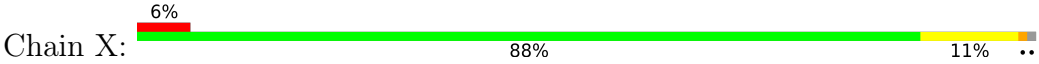
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

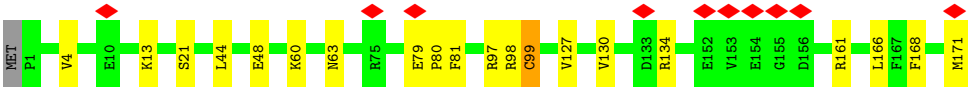
Chain W:



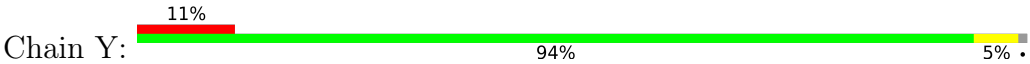
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

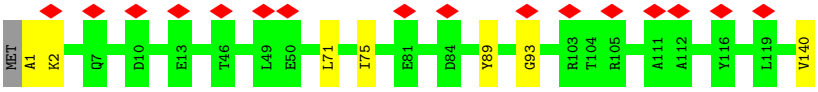
Chain X:



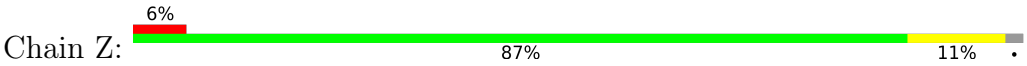


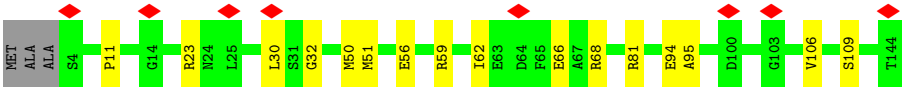
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



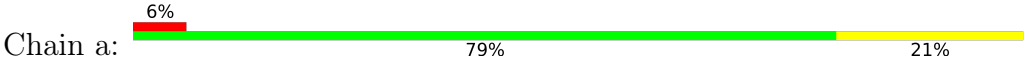


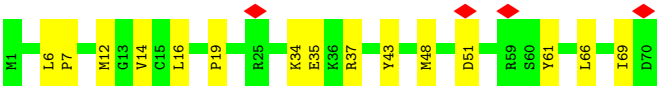
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



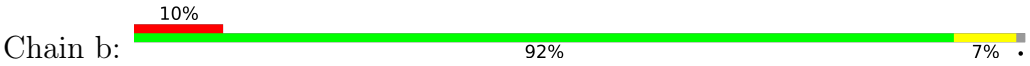


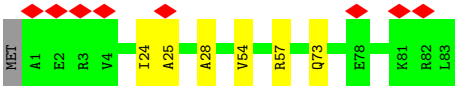
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1





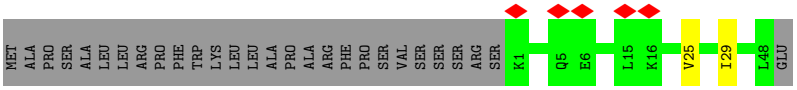
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



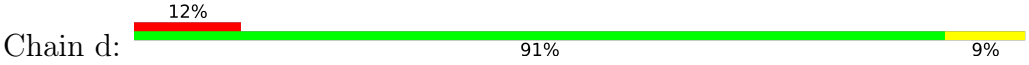


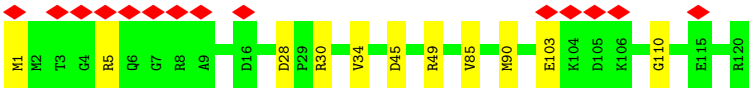
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial





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

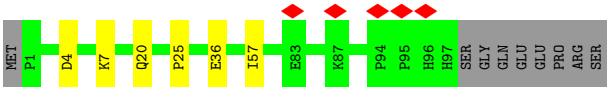




• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:

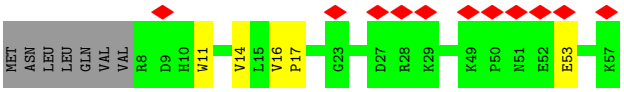




• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:

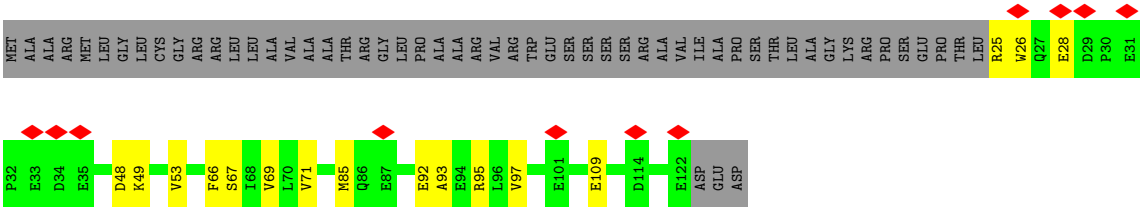




• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:

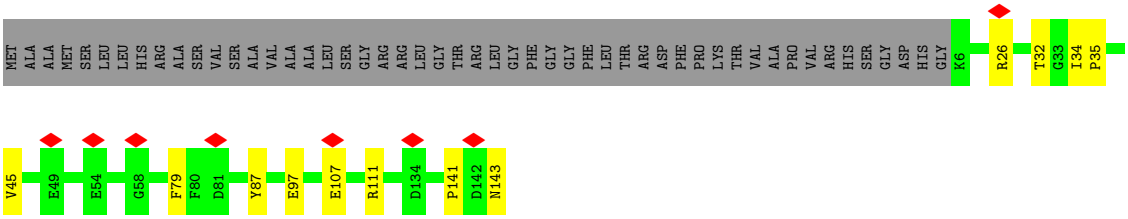




• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:

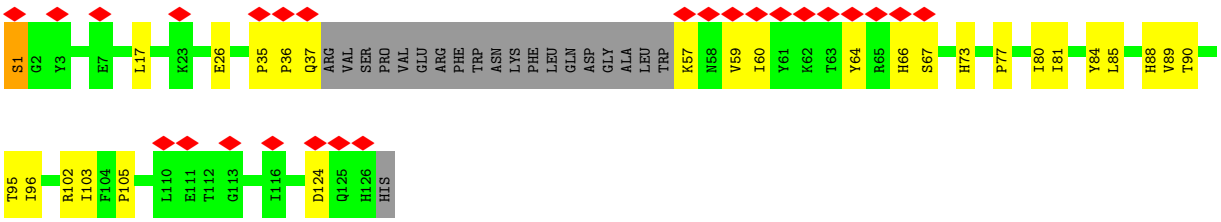




• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

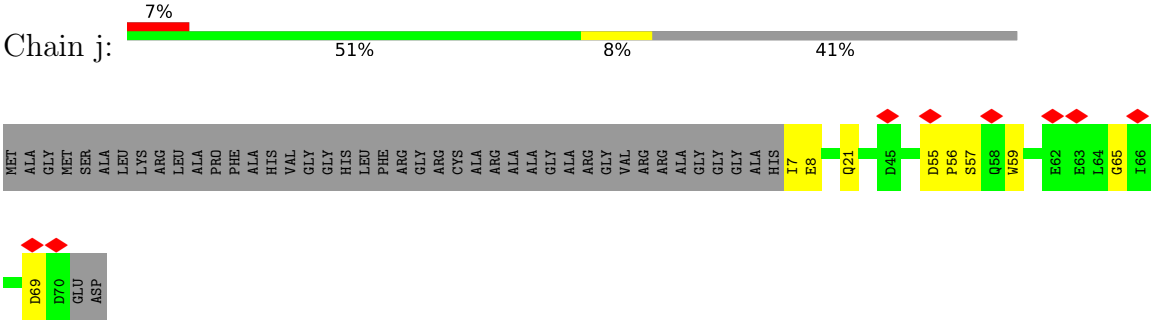
Chain i:





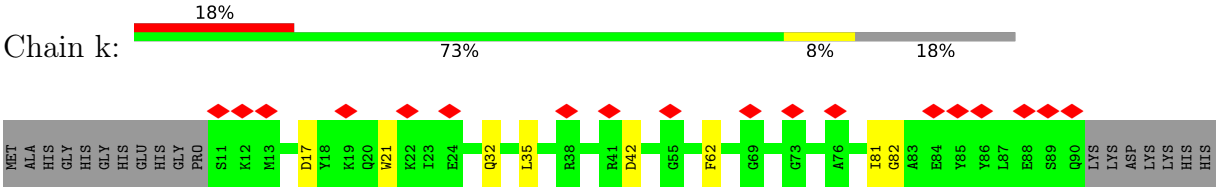
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



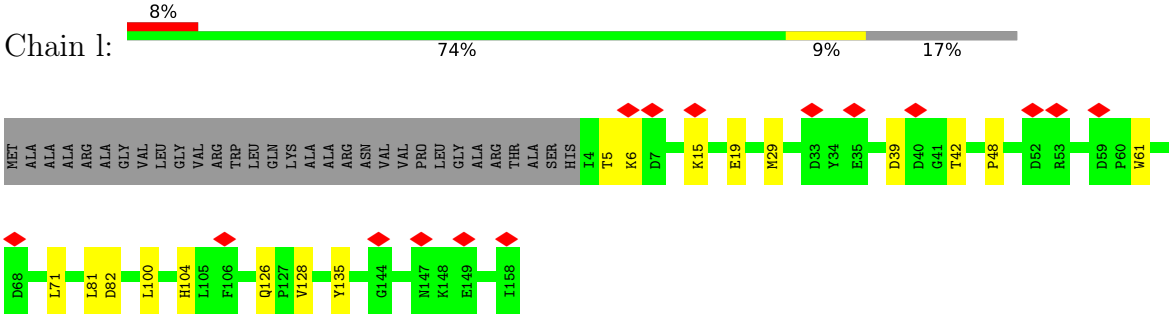
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



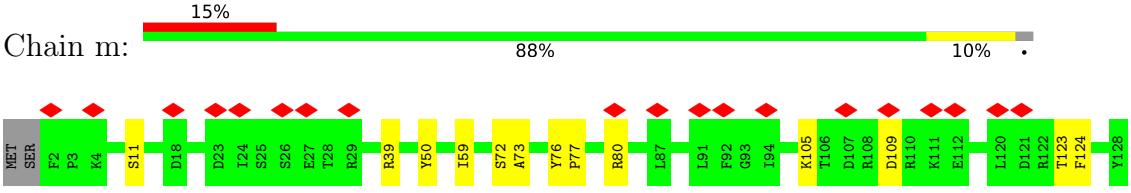
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l:



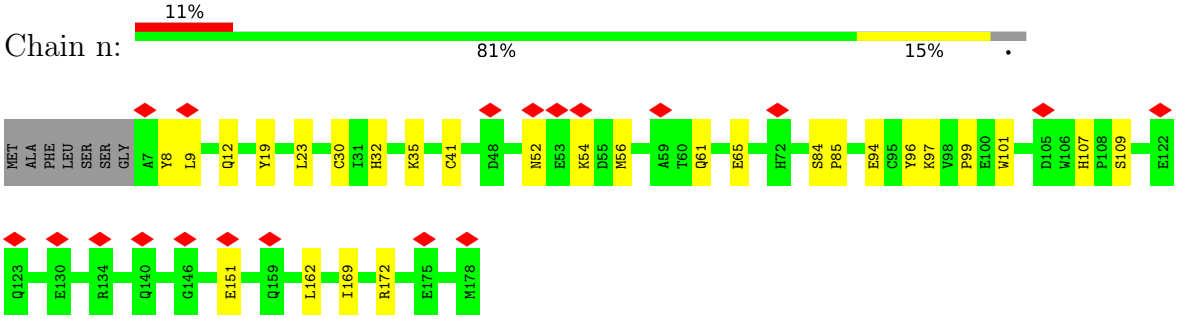
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain m:



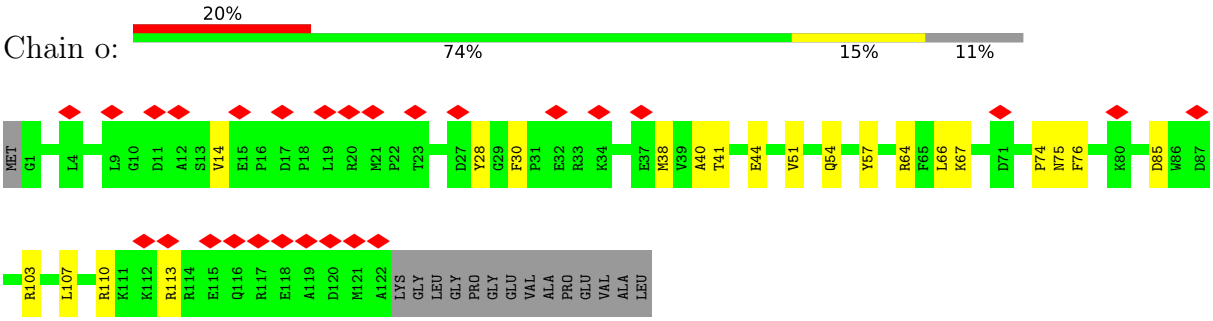
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n:



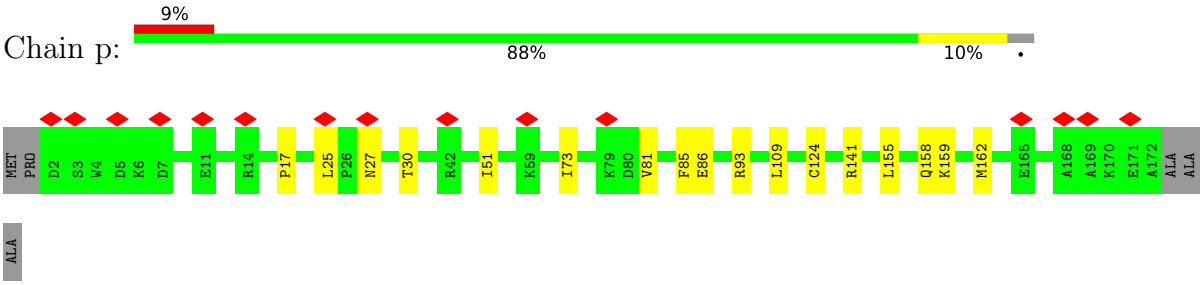
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:



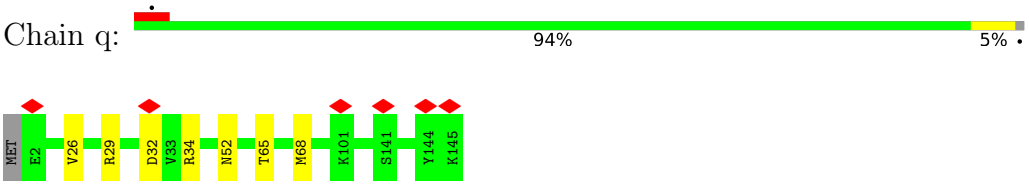
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p:



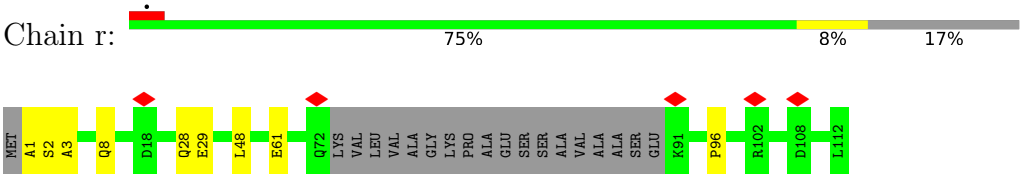
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:



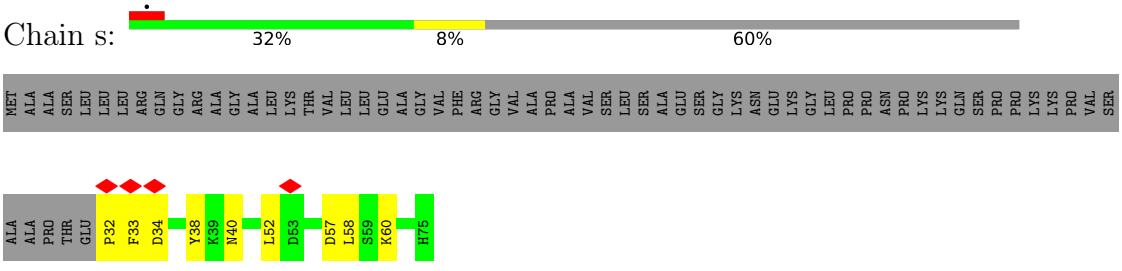
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:



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

Chain s:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18231	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	27.341	Depositor
Minimum map value	-13.287	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.973	Depositor
Recommended contour level	5.08	Depositor
Map size (Å)	475.2, 475.2, 475.2	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.056, 1.056, 1.056	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: GTP, EHZ, FME, AYA, AME, PC1, ZN, FES, SF4, FMN, 2MR, SAC, 3PE, LMT, NDP, MG, CDL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.28	0/936	0.30	0/1281
2	B	0.35	0/1272	0.41	0/1720
3	C	0.32	0/1772	0.33	0/2413
4	D	0.32	0/3537	0.33	0/4794
5	E	0.27	0/1695	0.33	0/2307
6	F	0.28	0/3393	0.38	0/4584
7	G	0.29	0/5367	0.34	0/7274
8	H	0.31	0/2571	0.37	1/3513 (0.0%)
9	I	0.35	0/1445	0.37	0/1956
10	J	0.28	0/1362	0.30	0/1848
11	K	0.31	0/745	0.32	0/1008
12	L	0.27	0/4920	0.32	0/6694
13	M	0.31	0/3738	0.33	0/5097
14	N	0.30	0/2792	0.32	0/3800
15	O	0.26	0/2651	0.30	0/3587
16	P	0.28	0/2824	0.33	0/3831
17	Q	0.29	0/1039	0.31	0/1404
18	R	0.30	0/742	0.31	0/999
19	S	0.25	0/688	0.31	0/927
20	T	0.21	0/621	0.33	0/837
20	U	0.26	0/704	0.34	0/950
21	V	0.26	0/939	0.30	0/1272
22	W	0.28	0/995	0.32	0/1337
23	X	0.28	0/1439	0.37	0/1942
24	Y	0.23	0/1042	0.28	0/1414
25	Z	0.28	0/1181	0.31	0/1592
26	a	0.29	0/584	0.33	0/786
27	b	0.25	0/672	0.32	0/923
28	c	0.24	0/418	0.26	0/567
29	d	0.29	0/1012	0.31	0/1368
30	e	0.28	0/840	0.33	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
31	f	0.23	0/450	0.36	0/606
32	g	0.27	0/850	0.31	0/1154
33	h	0.28	0/1188	0.31	0/1607
34	i	0.23	0/941	0.37	0/1279
35	j	0.25	0/582	0.29	0/799
36	k	0.21	0/663	0.31	0/895
37	l	0.26	0/1358	0.33	0/1858
38	m	0.25	0/1088	0.33	0/1472
39	n	0.25	0/1545	0.32	0/2092
40	o	0.23	0/1073	0.35	0/1437
41	p	0.27	0/1476	0.31	0/1990
42	q	0.29	0/1242	0.35	0/1688
43	r	0.28	0/780	0.30	0/1056
44	s	0.25	0/383	0.37	0/518
All	All	0.28	0/67555	0.33	1/91599 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	217	ALA	CB-CA-C	-5.01	110.82	116.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	921	0	952	21	0
2	B	1241	0	1251	20	0
3	C	1721	0	1675	16	0
4	D	3459	0	3404	55	0
5	E	1655	0	1661	25	0
6	F	3319	0	3274	44	0
7	G	5279	0	5301	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	2509	0	2621	54	0
9	I	1414	0	1370	23	0
10	J	1337	0	1346	31	0
11	K	745	0	785	26	0
12	L	4802	0	4960	100	0
13	M	3654	0	3852	68	0
14	N	2733	0	2912	51	0
15	O	2589	0	2566	39	0
16	P	2747	0	2766	25	0
17	Q	1016	0	1014	13	0
18	R	730	0	707	2	0
19	S	677	0	688	6	0
20	T	612	0	604	9	0
20	U	692	0	688	10	0
21	V	919	0	961	5	0
22	W	971	0	989	13	0
23	X	1402	0	1381	20	0
24	Y	1030	0	1039	5	0
25	Z	1152	0	1151	14	0
26	a	569	0	568	13	0
27	b	651	0	662	7	0
28	c	405	0	409	1	0
29	d	993	0	977	9	0
30	e	819	0	821	7	0
31	f	437	0	435	3	0
32	g	824	0	772	16	0
33	h	1154	0	1168	11	0
34	i	920	0	939	23	0
35	j	556	0	501	6	0
36	k	644	0	626	6	0
37	l	1304	0	1203	14	0
38	m	1061	0	1059	9	0
39	n	1492	0	1438	24	0
40	o	1048	0	1020	15	0
41	p	1443	0	1415	13	0
42	q	1201	0	1170	5	0
43	r	767	0	776	7	0
44	s	371	0	344	9	0
45	A	21	0	18	0	0
45	B	78	0	104	2	0
45	d	26	0	26	0	0
45	g	49	0	75	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	A	39	0	52	0	0
46	I	42	0	58	4	0
46	J	28	0	30	1	0
46	K	39	0	52	0	0
46	L	118	0	161	0	0
46	M	86	0	123	2	0
46	N	85	0	121	4	0
46	X	31	0	36	1	0
46	c	38	0	53	1	0
47	B	8	0	0	0	0
47	F	8	0	0	2	0
47	G	16	0	0	1	0
47	I	16	0	0	0	0
48	E	4	0	0	0	0
48	G	4	0	0	0	0
49	F	31	0	19	1	0
50	L	62	0	68	0	0
50	Y	50	0	44	1	0
50	h	64	0	75	2	0
50	q	69	0	82	1	0
51	M	35	0	46	1	0
51	N	35	0	46	0	0
51	b	35	0	46	0	0
52	O	32	0	12	3	0
53	O	1	0	0	0	0
54	P	48	0	26	4	0
55	R	1	0	0	0	0
56	T	37	0	0	0	0
56	U	37	0	0	1	0
All	All	67258	0	67594	786	0

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

The worst 5 of 786 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)
20:T:46:ASP:OD1	22:W:64:ARG:NH2	1.96	0.99
1:A:71:LEU:O	10:J:147:TYR:OH	1.83	0.96
4:D:403:ASP:OD2	4:D:407:LYS:NZ	2.01	0.93
3:C:65:ARG:O	3:C:73:LYS:NZ	2.02	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:GLU:OE1	16:P:54:TYR:OH	1.91	0.89

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
2	B	153/216 (71%)	145 (95%)	8 (5%)	0	100	100
3	C	205/266 (77%)	199 (97%)	6 (3%)	0	100	100
4	D	427/463 (92%)	397 (93%)	30 (7%)	0	100	100
5	E	211/249 (85%)	192 (91%)	19 (9%)	0	100	100
6	F	429/464 (92%)	410 (96%)	19 (4%)	0	100	100
7	G	686/727 (94%)	642 (94%)	44 (6%)	0	100	100
8	H	316/318 (99%)	293 (93%)	23 (7%)	0	100	100
9	I	174/212 (82%)	165 (95%)	9 (5%)	0	100	100
10	J	172/175 (98%)	160 (93%)	12 (7%)	0	100	100
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	604/606 (100%)	557 (92%)	44 (7%)	3 (0%)	24	57
13	M	457/459 (100%)	443 (97%)	14 (3%)	0	100	100
14	N	345/347 (99%)	333 (96%)	12 (4%)	0	100	100
15	O	318/343 (93%)	300 (94%)	18 (6%)	0	100	100
16	P	339/380 (89%)	318 (94%)	21 (6%)	0	100	100
17	Q	123/175 (70%)	117 (95%)	6 (5%)	0	100	100
18	R	93/124 (75%)	88 (95%)	5 (5%)	0	100	100
19	S	82/99 (83%)	76 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	74/156 (47%)	71 (96%)	3 (4%)	0	100	100
20	U	84/156 (54%)	82 (98%)	1 (1%)	1 (1%)	10	37
21	V	111/116 (96%)	108 (97%)	3 (3%)	0	100	100
22	W	112/128 (88%)	106 (95%)	6 (5%)	0	100	100
23	X	169/172 (98%)	154 (91%)	14 (8%)	1 (1%)	21	52
24	Y	138/141 (98%)	133 (96%)	5 (4%)	0	100	100
25	Z	139/144 (96%)	129 (93%)	10 (7%)	0	100	100
26	a	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
27	b	81/84 (96%)	73 (90%)	8 (10%)	0	100	100
28	c	46/76 (60%)	45 (98%)	1 (2%)	0	100	100
29	d	118/120 (98%)	111 (94%)	7 (6%)	0	100	100
30	e	95/106 (90%)	92 (97%)	3 (3%)	0	100	100
31	f	48/57 (84%)	44 (92%)	4 (8%)	0	100	100
32	g	96/154 (62%)	89 (93%)	7 (7%)	0	100	100
33	h	136/189 (72%)	131 (96%)	5 (4%)	0	100	100
34	i	103/127 (81%)	92 (89%)	10 (10%)	1 (1%)	12	41
35	j	62/108 (57%)	59 (95%)	2 (3%)	1 (2%)	7	30
36	k	78/98 (80%)	72 (92%)	5 (6%)	1 (1%)	9	35
37	l	153/186 (82%)	142 (93%)	11 (7%)	0	100	100
38	m	125/129 (97%)	115 (92%)	10 (8%)	0	100	100
39	n	170/179 (95%)	157 (92%)	13 (8%)	0	100	100
40	o	120/137 (88%)	107 (89%)	13 (11%)	0	100	100
41	p	169/176 (96%)	165 (98%)	4 (2%)	0	100	100
42	q	142/145 (98%)	141 (99%)	1 (1%)	0	100	100
43	r	90/113 (80%)	82 (91%)	8 (9%)	0	100	100
44	s	42/109 (38%)	38 (90%)	4 (10%)	0	100	100
All	All	8112/9212 (88%)	7640 (94%)	464 (6%)	8 (0%)	49	78

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	X	99	CYS
12	L	562	LEU

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Mol	Chain	Res	Type
20	U	43	ASP
35	j	8	GLU
12	L	25	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	100/100 (100%)	100 (100%)	0	100	100
2	B	131/175 (75%)	131 (100%)	0	100	100
3	C	188/228 (82%)	188 (100%)	0	100	100
4	D	370/392 (94%)	370 (100%)	0	100	100
5	E	183/205 (89%)	183 (100%)	0	100	100
6	F	345/368 (94%)	345 (100%)	0	100	100
7	G	578/608 (95%)	578 (100%)	0	100	100
8	H	274/274 (100%)	274 (100%)	0	100	100
9	I	151/175 (86%)	151 (100%)	0	100	100
10	J	140/141 (99%)	140 (100%)	0	100	100
11	K	85/85 (100%)	85 (100%)	0	100	100
12	L	533/533 (100%)	533 (100%)	0	100	100
13	M	412/412 (100%)	412 (100%)	0	100	100
14	N	315/315 (100%)	315 (100%)	0	100	100
15	O	283/303 (93%)	283 (100%)	0	100	100
16	P	295/327 (90%)	295 (100%)	0	100	100
17	Q	112/153 (73%)	112 (100%)	0	100	100
18	R	78/97 (80%)	78 (100%)	0	100	100
19	S	75/82 (92%)	75 (100%)	0	100	100
20	T	70/135 (52%)	69 (99%)	1 (1%)	59	76
20	U	79/135 (58%)	78 (99%)	1 (1%)	61	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	V	101/102 (99%)	101 (100%)	0	100	100
22	W	107/114 (94%)	107 (100%)	0	100	100
23	X	154/155 (99%)	154 (100%)	0	100	100
24	Y	101/102 (99%)	101 (100%)	0	100	100
25	Z	120/121 (99%)	120 (100%)	0	100	100
26	a	59/59 (100%)	59 (100%)	0	100	100
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	44/68 (65%)	44 (100%)	0	100	100
29	d	104/105 (99%)	104 (100%)	0	100	100
30	e	88/96 (92%)	88 (100%)	0	100	100
31	f	47/54 (87%)	47 (100%)	0	100	100
32	g	89/131 (68%)	89 (100%)	0	100	100
33	h	121/158 (77%)	121 (100%)	0	100	100
34	i	102/120 (85%)	102 (100%)	0	100	100
35	j	59/84 (70%)	59 (100%)	0	100	100
36	k	62/76 (82%)	62 (100%)	0	100	100
37	l	139/159 (87%)	139 (100%)	0	100	100
38	m	113/115 (98%)	113 (100%)	0	100	100
39	n	156/161 (97%)	156 (100%)	0	100	100
40	o	110/120 (92%)	110 (100%)	0	100	100
41	p	155/157 (99%)	155 (100%)	0	100	100
42	q	130/131 (99%)	130 (100%)	0	100	100
43	r	84/97 (87%)	84 (100%)	0	100	100
44	s	43/92 (47%)	43 (100%)	0	100	100
All	All	7156/7892 (91%)	7154 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	T	44	SER
20	U	44	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	235	ASN
44	s	43	HIS
17	Q	50	ASN
43	r	107	GLN
37	l	132	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

12 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	$\#\|Z\| > 2$
34	SAC	i	1	34	7,8,9	0.91	0	8,9,11	1.02	1 (12%)
14	FME	N	1	14	8,9,10	0.96	0	7,9,11	0.94	0
10	FME	J	1	10	8,9,10	0.91	0	7,9,11	0.89	0
24	AYA	Y	1	24	6,7,8	1.29	1 (16%)	5,8,10	1.54	1 (20%)
29	AME	d	1	29	9,10,11	1.48	1 (11%)	9,11,13	1.54	2 (22%)
13	FME	M	1	13	8,9,10	0.94	0	7,9,11	0.96	0
8	FME	H	1	8	8,9,10	0.90	0	7,9,11	1.08	1 (14%)
43	AYA	r	1	43	6,7,8	1.41	1 (16%)	5,8,10	0.98	0
4	2MR	D	85	4	10,12,13	2.40	2 (20%)	5,13,15	1.30	0
1	FME	A	1	1	8,9,10	1.03	1 (12%)	7,9,11	0.61	0
11	FME	K	1	11	8,9,10	0.97	0	7,9,11	0.72	0
12	FME	L	1	12	8,9,10	1.00	1 (12%)	7,9,11	0.75	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
34	SAC	i	1	34	-	2/7/8/10	-
14	FME	N	1	14	-	3/7/9/11	-
10	FME	J	1	10	-	3/7/9/11	-
24	AYA	Y	1	24	-	0/4/6/8	-
29	AME	d	1	29	-	6/9/10/12	-
13	FME	M	1	13	-	0/7/9/11	-
8	FME	H	1	8	-	3/7/9/11	-
43	AYA	r	1	43	-	0/4/6/8	-
4	2MR	D	85	4	-	1/10/13/15	-
1	FME	A	1	1	-	0/7/9/11	-
11	FME	K	1	11	-	2/7/9/11	-
12	FME	L	1	12	-	2/7/9/11	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.30	1.45	1.33
4	D	85	2MR	CZ-NE	4.89	1.44	1.34
29	d	1	AME	CT1-N	3.38	1.46	1.34
43	r	1	AYA	CA-N	-2.99	1.43	1.46
24	Y	1	AYA	CA-N	-2.67	1.43	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	1	AYA	CB-CA-N	3.29	113.27	109.61
29	d	1	AME	CE-SD-CG	2.60	109.32	100.40
29	d	1	AME	CT2-CT1-N	2.36	120.10	116.10
34	i	1	SAC	OG-CB-CA	-2.23	105.27	110.97
8	H	1	FME	C-CA-N	2.08	113.48	109.73

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	85	2MR	O-C-CA-CB
8	H	1	FME	O-C-CA-CB
10	J	1	FME	O1-CN-N-CA
12	L	1	FME	O1-CN-N-CA
12	L	1	FME	CA-CB-CG-SD

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	i	1	SAC	1	0
13	M	1	FME	1	0
1	A	1	FME	1	0
11	K	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 40 ligands modelled in this entry, 2 are monoatomic - leaving 38 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	PC1	g	1501	-	48,48,53	1.00	3 (6%)	54,56,61	1.08	2 (3%)
50	CDL	Y	701	-	49,49,99	1.21	8 (16%)	55,61,111	1.31	4 (7%)
46	3PE	A	702	-	38,38,50	0.98	4 (10%)	41,43,55	1.11	2 (4%)
51	LMT	b	301	-	36,36,36	1.19	3 (8%)	47,47,47	1.34	5 (10%)
47	SF4	F	502	6	0,12,12	-	-	-		
46	3PE	J	401	-	27,27,50	1.08	3 (11%)	30,32,55	1.10	1 (3%)
47	SF4	B	201	2	0,12,12	-	-	-		
56	EHZ	U	101	20	29,36,37	1.64	5 (17%)	35,44,47	1.35	3 (8%)
51	LMT	M	602	-	36,36,36	1.15	2 (5%)	47,47,47	1.02	1 (2%)
46	3PE	L	701	-	37,37,50	1.01	4 (10%)	40,42,55	1.13	2 (5%)
46	3PE	I	201	-	41,41,50	0.93	3 (7%)	44,46,55	1.18	2 (4%)
49	FMN	F	501	-	33,33,33	1.10	2 (6%)	48,50,50	1.32	7 (14%)
46	3PE	N	902	-	43,43,50	0.92	3 (6%)	46,48,55	1.04	2 (4%)
48	FES	G	803	7	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
46	3PE	X	401	-	30,30,50	1.09	3 (10%)	33,35,55	1.24	2 (6%)
45	PC1	B	202	-	42,42,53	1.05	4 (9%)	48,50,61	1.04	2 (4%)
46	3PE	M	601	-	45,45,50	0.91	4 (8%)	48,50,55	1.22	2 (4%)
50	CDL	L	702	-	61,61,99	1.12	8 (13%)	67,73,111	1.14	4 (5%)
52	GTP	O	401	53	30,34,34	3.05	11 (36%)	46,54,54	1.98	16 (34%)
45	PC1	d	501	-	25,25,53	1.37	4 (16%)	31,33,61	1.03	2 (6%)
45	PC1	A	701	-	20,20,53	1.89	3 (15%)	24,27,61	1.13	1 (4%)
54	NDP	P	501	-	49,52,52	2.03	8 (16%)	66,80,80	1.66	13 (19%)
47	SF4	G	802	7	0,12,12	-	-	-		
47	SF4	I	202	9	0,12,12	-	-	-		
46	3PE	c	301	-	37,37,50	0.99	3 (8%)	40,42,55	0.99	2 (5%)
47	SF4	G	801	7	0,12,12	-	-	-		
46	3PE	K	101	-	38,38,50	1.00	4 (10%)	41,43,55	1.11	2 (4%)
48	FES	E	301	5	0,4,4	-	-	-		
50	CDL	h	1001	-	63,63,99	1.10	8 (12%)	69,75,111	1.22	5 (7%)
47	SF4	I	203	9	0,12,12	-	-	-		
46	3PE	N	903	-	40,40,50	0.95	4 (10%)	43,45,55	1.20	2 (4%)
56	EHZ	T	101	20	29,36,37	1.69	5 (17%)	35,44,47	1.73	7 (20%)
46	3PE	L	704	-	34,34,50	1.03	4 (11%)	37,39,55	1.16	2 (5%)
46	3PE	L	703	-	44,44,50	0.90	4 (9%)	47,49,55	1.14	3 (6%)
51	LMT	N	901	-	36,36,36	1.13	2 (5%)	47,47,47	1.17	3 (6%)
46	3PE	M	603	-	39,39,50	0.96	4 (10%)	42,44,55	1.07	2 (4%)
50	CDL	q	201	-	68,68,99	1.03	8 (11%)	74,80,111	1.11	4 (5%)
45	PC1	B	203	-	34,34,53	1.19	4 (11%)	40,42,61	1.09	2 (5%)

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	PC1	g	1501	-	-	23/52/52/57	-
50	CDL	Y	701	-	-	23/59/59/110	-
46	3PE	A	702	-	-	16/42/42/54	-
51	LMT	b	301	-	-	8/21/61/61	0/2/2/2
47	SF4	F	502	6	-	-	0/6/5/5
46	3PE	J	401	-	-	12/30/30/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	SF4	B	201	2	-	-	0/6/5/5
56	EHZ	U	101	20	-	7/42/44/45	-
51	LMT	M	602	-	-	6/21/61/61	0/2/2/2
46	3PE	L	701	-	-	19/41/41/54	-
49	FMN	F	501	-	-	3/18/18/18	0/3/3/3
46	3PE	I	201	-	-	18/45/45/54	-
46	3PE	N	902	-	-	24/47/47/54	-
48	FES	G	803	7	-	-	0/1/1/1
46	3PE	X	401	-	-	16/34/34/54	-
45	PC1	B	202	-	-	22/46/46/57	-
46	3PE	M	601	-	-	20/49/49/54	-
50	CDL	L	702	-	-	34/72/72/110	-
52	GTP	O	401	53	-	0/22/38/38	0/3/3/3
45	PC1	d	501	-	-	11/29/29/57	-
45	PC1	A	701	-	-	13/22/22/57	-
54	NDP	P	501	-	-	9/34/77/77	0/5/5/5
47	SF4	G	802	7	-	-	0/6/5/5
47	SF4	I	202	9	-	-	0/6/5/5
46	3PE	c	301	-	-	22/41/41/54	-
47	SF4	G	801	7	-	-	0/6/5/5
46	3PE	K	101	-	-	19/42/42/54	-
48	FES	E	301	5	-	-	0/1/1/1
50	CDL	h	1001	-	-	28/74/74/110	-
47	SF4	I	203	9	-	-	0/6/5/5
46	3PE	N	903	-	-	19/44/44/54	-
56	EHZ	T	101	20	-	11/42/44/45	-
46	3PE	L	704	-	-	20/38/38/54	-
46	3PE	L	703	-	-	23/48/48/54	-
51	LMT	N	901	-	-	5/21/61/61	0/2/2/2
46	3PE	M	603	-	-	20/43/43/54	-
50	CDL	q	201	-	-	35/79/79/110	-
45	PC1	B	203	-	-	12/38/38/57	-

The worst 5 of 135 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	P	501	NDP	P2B-O2B	10.95	1.80	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	O	401	GTP	O6-C6	8.67	1.40	1.23
52	O	401	GTP	C5-N7	6.83	1.52	1.39
45	A	701	PC1	O21-C2	-5.79	1.40	1.46
56	T	101	EHZ	C12-N1	5.29	1.45	1.33

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	O	401	GTP	C8-N9-C4	7.41	120.16	106.05
54	P	501	NDP	PN-O3-PA	-7.29	107.80	132.83
56	T	101	EHZ	C8-C9-S1	6.21	121.31	113.63
50	Y	701	CDL	OB6-CB5-C51	5.54	121.29	111.09
56	U	101	EHZ	C8-C9-S1	5.06	119.89	113.63

There are no chirality outliers.

5 of 498 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	701	PC1	C1-O11-P-O14
45	A	701	PC1	O13-C11-C12-N
45	A	701	PC1	C1-C2-O21-C21
45	A	701	PC1	O22-C21-O21-C2
45	B	202	PC1	C11-O13-P-O14

There are no ring outliers.

17 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	Y	701	CDL	1	0
47	F	502	SF4	2	0
46	J	401	3PE	1	0
56	U	101	EHZ	1	0
51	M	602	LMT	1	0
46	I	201	3PE	4	0
49	F	501	FMN	1	0
46	N	902	3PE	4	0
46	X	401	3PE	1	0
52	O	401	GTP	3	0
54	P	501	NDP	4	0
46	c	301	3PE	1	0
47	G	801	SF4	1	0

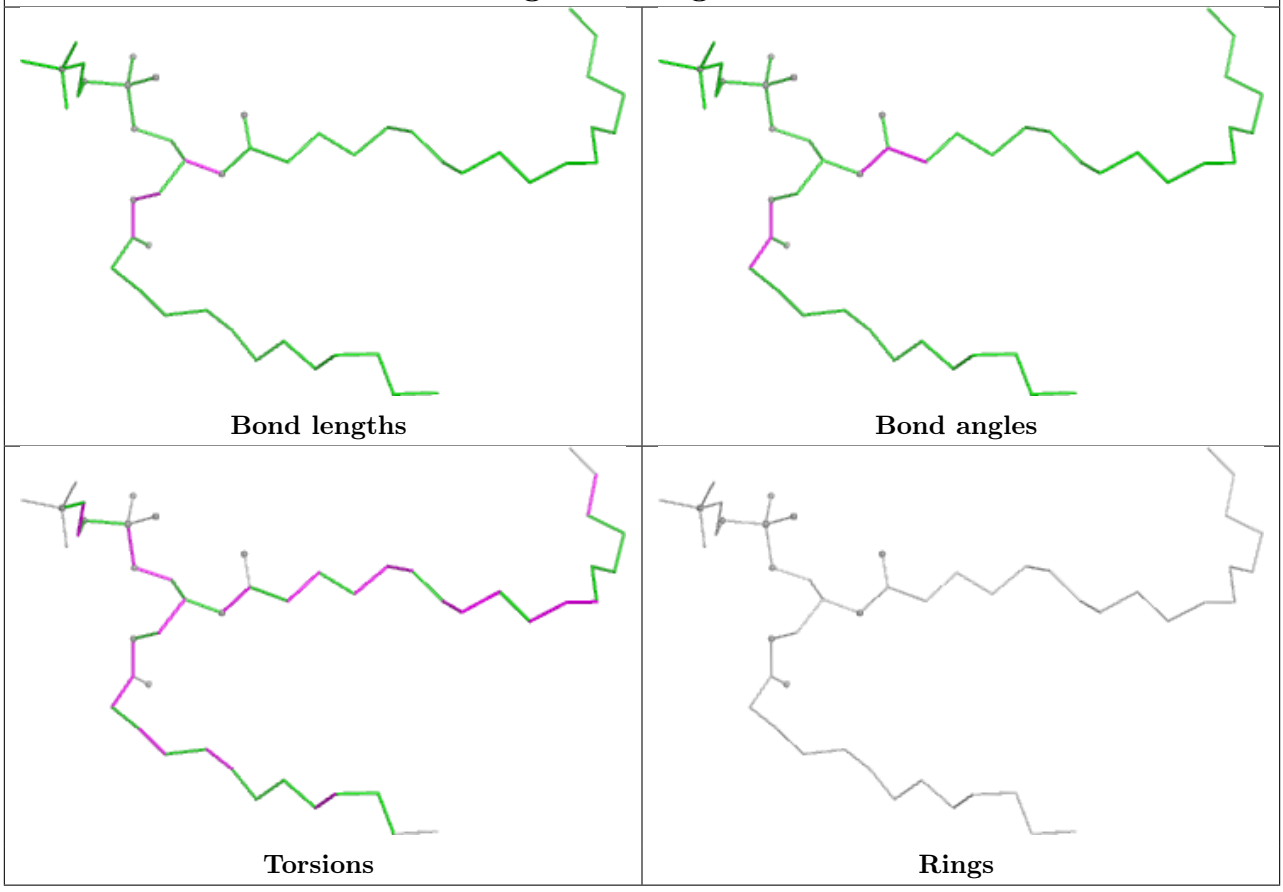
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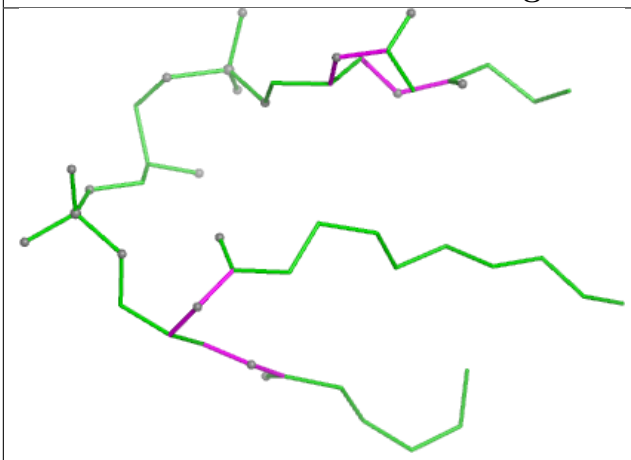
Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	h	1001	CDL	2	0
46	M	603	3PE	2	0
50	q	201	CDL	1	0
45	B	203	PC1	2	0

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

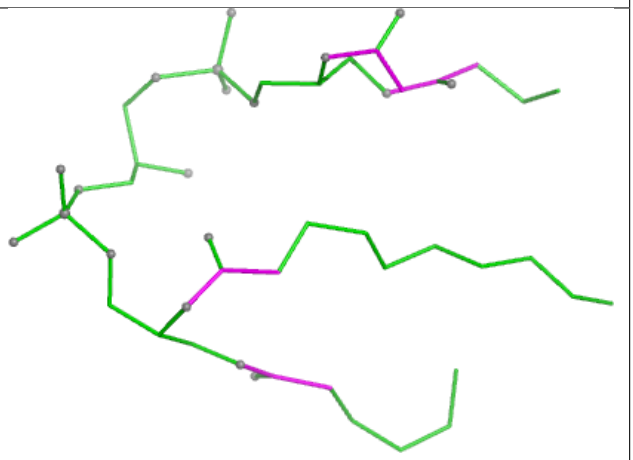
Ligand PC1 g 1501



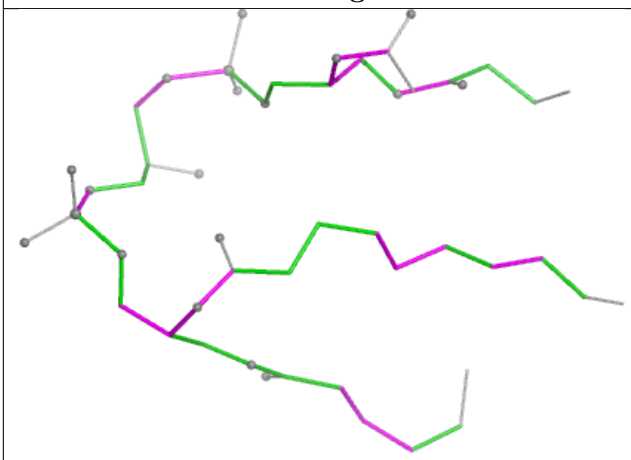
Ligand CDL Y 701



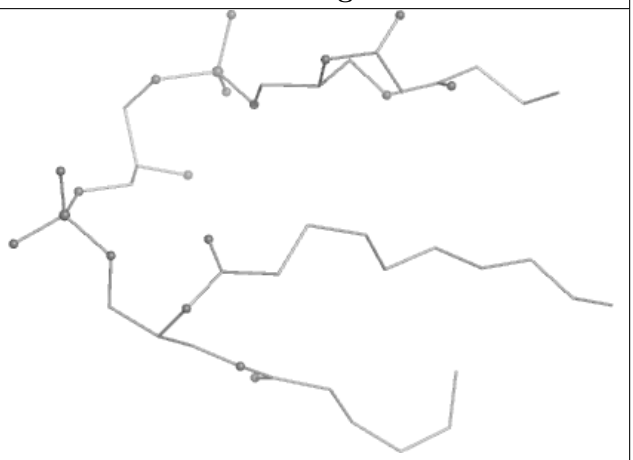
Bond lengths



Bond angles

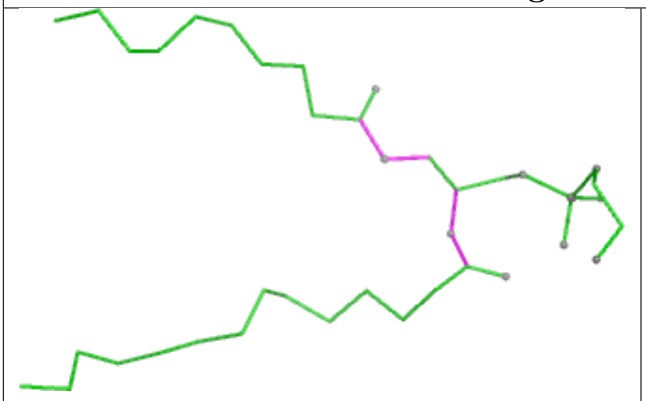


Torsions

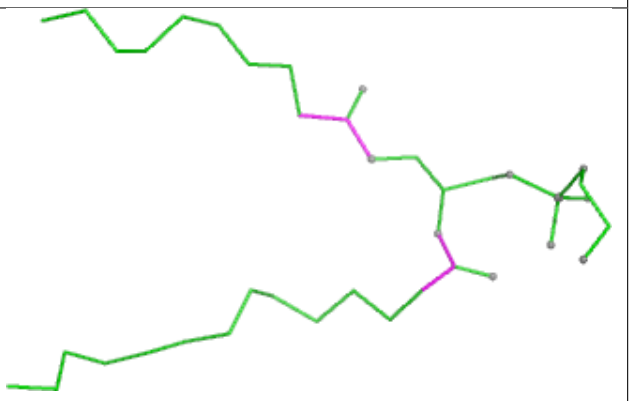


Rings

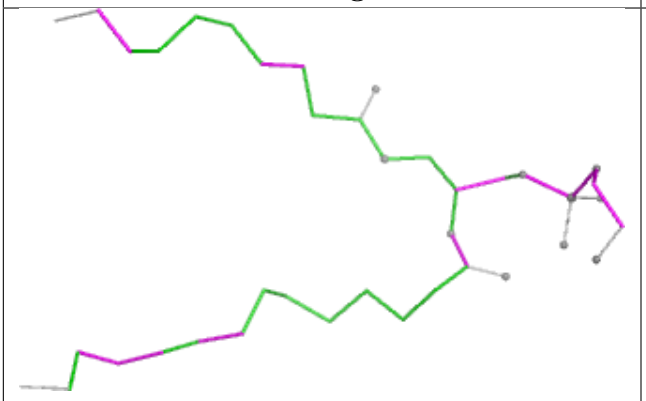
Ligand 3PE A 702



Bond lengths



Bond angles

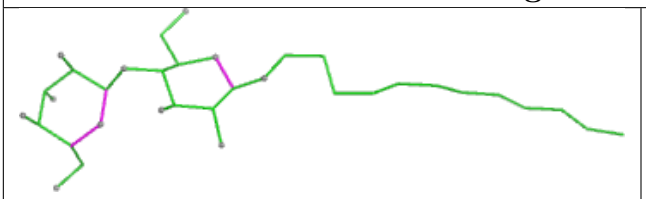


Torsions

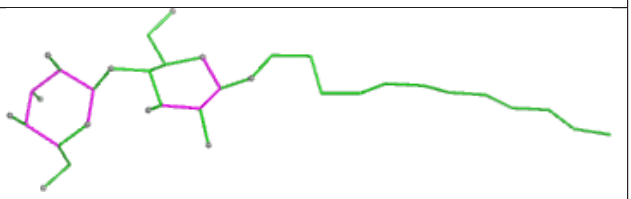


Rings

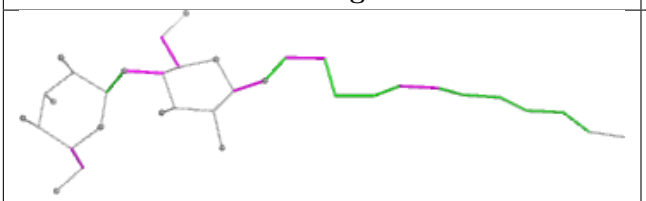
Ligand LMT b 301



Bond lengths



Bond angles

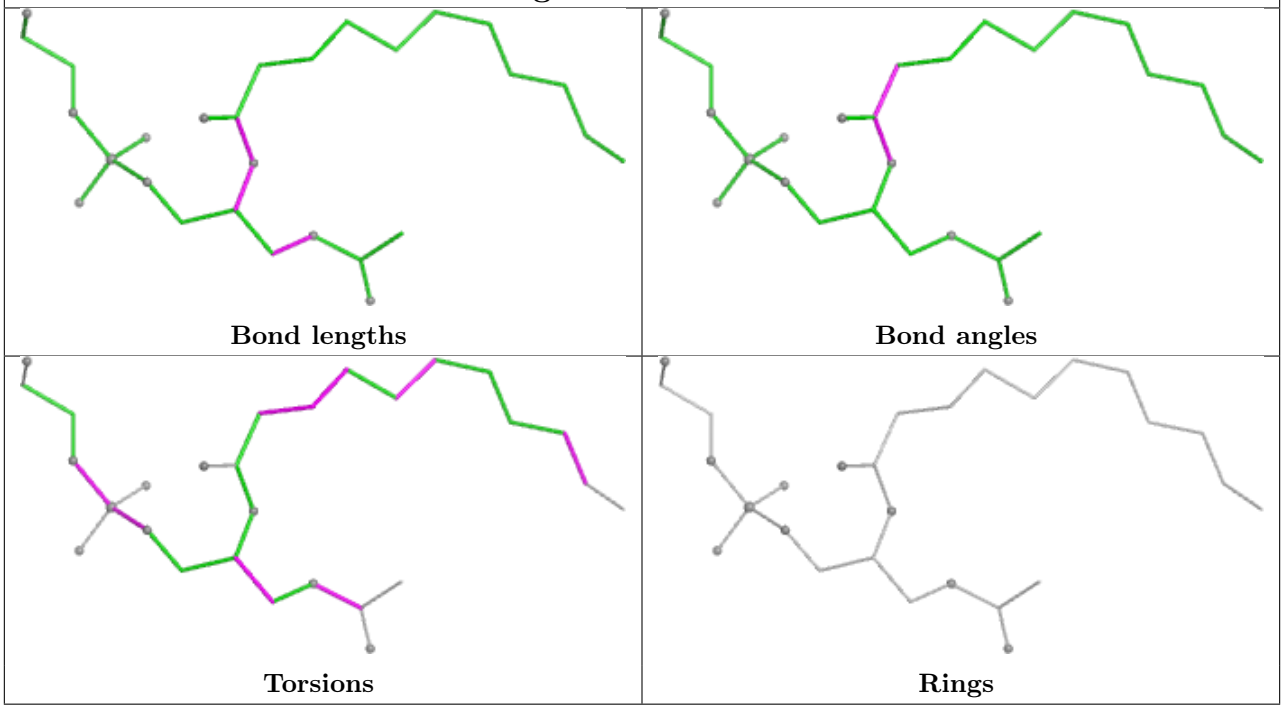


Torsions

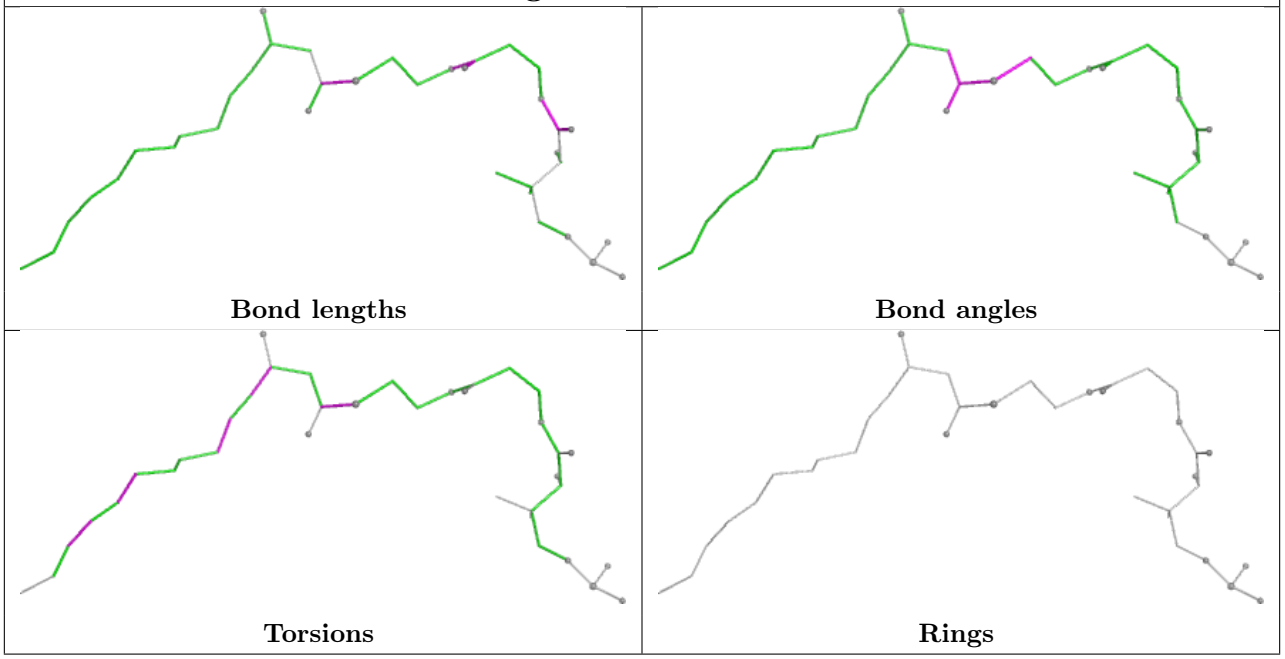


Rings

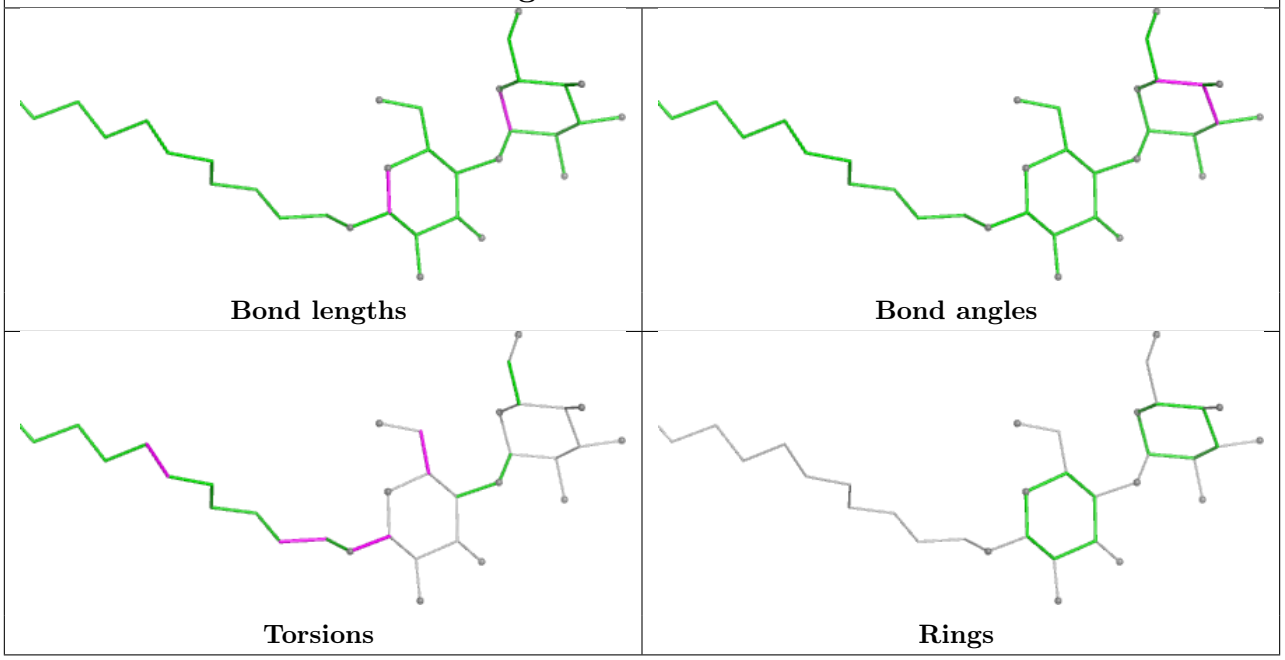
Ligand 3PE J 401



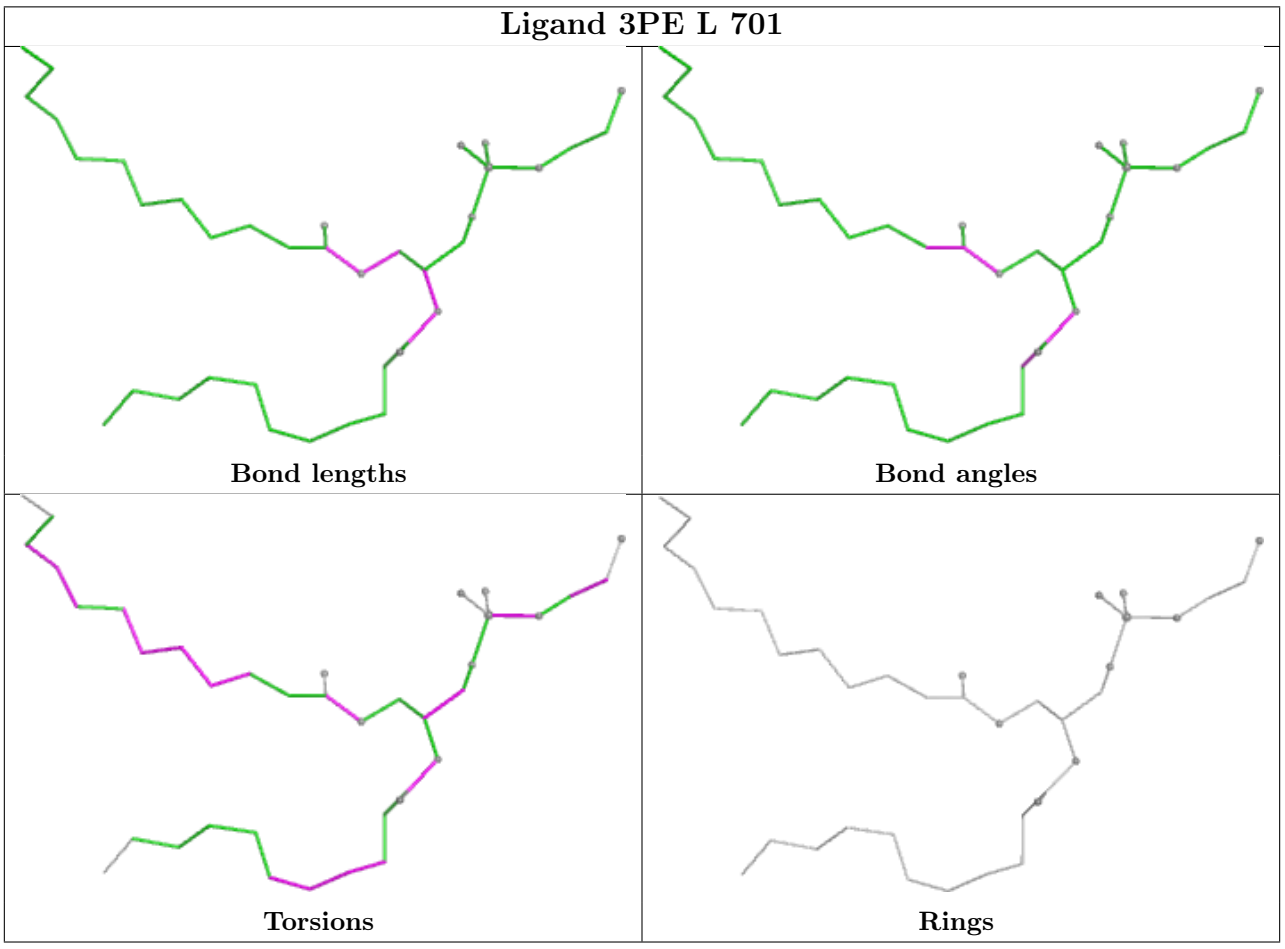
Ligand EHZ U 101



Ligand LMT M 602



Ligand 3PE L 701



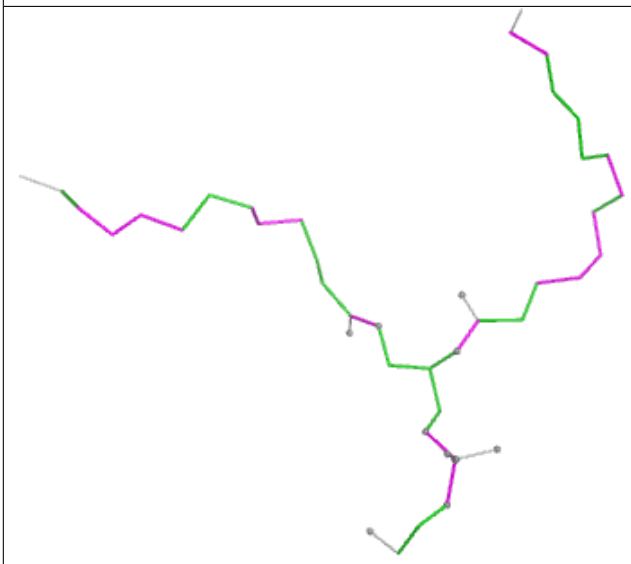
Ligand 3PE I 201



Bond lengths



Bond angles

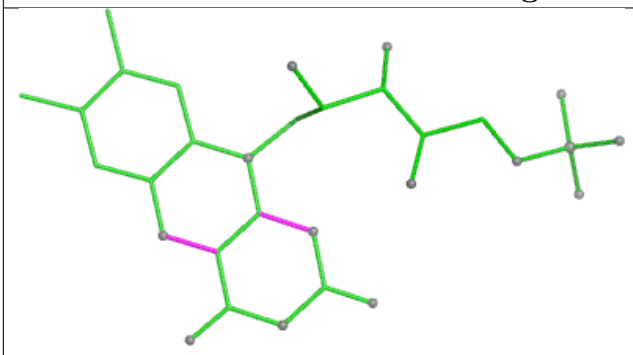


Torsions

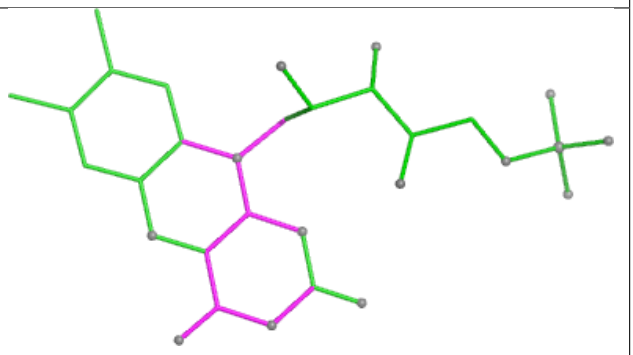


Rings

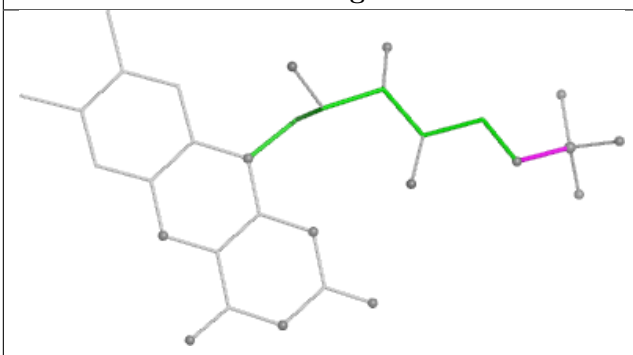
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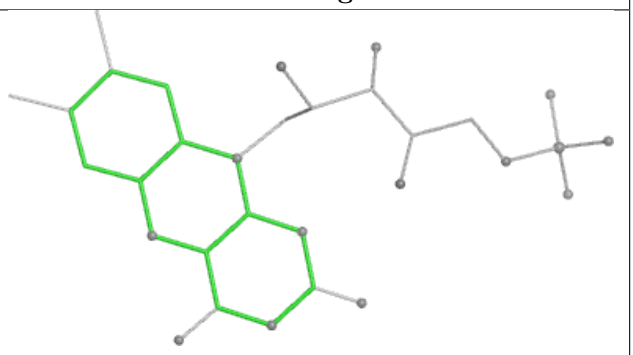
Bond lengths



Bond angles

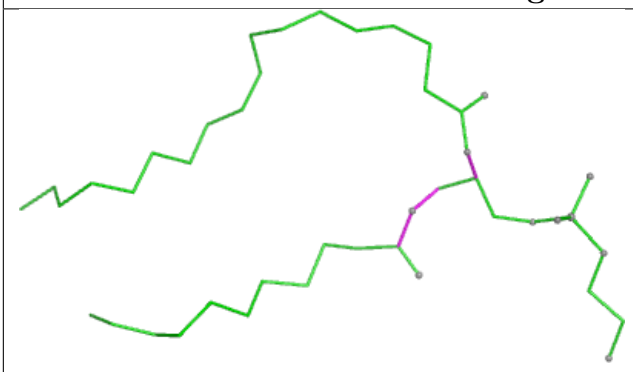


Torsions

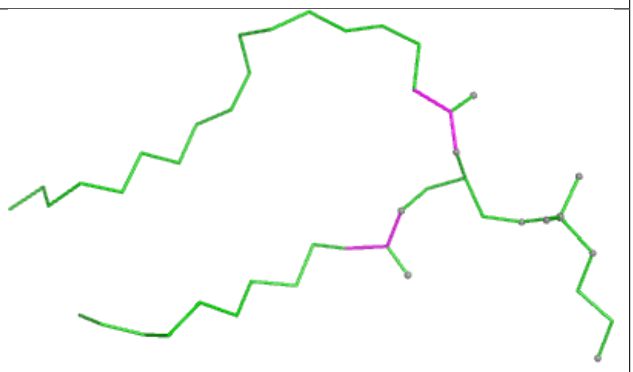


Rings

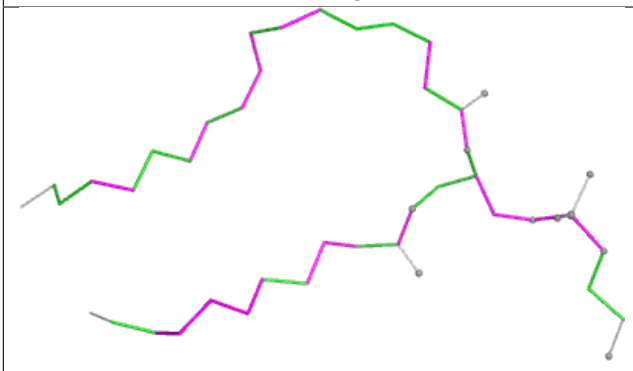
Ligand 3PE N 902



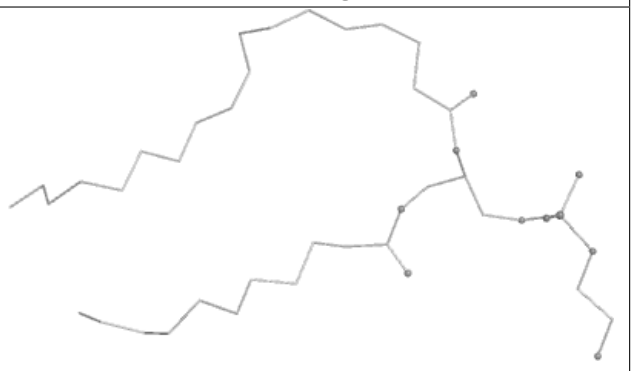
Bond lengths



Bond angles

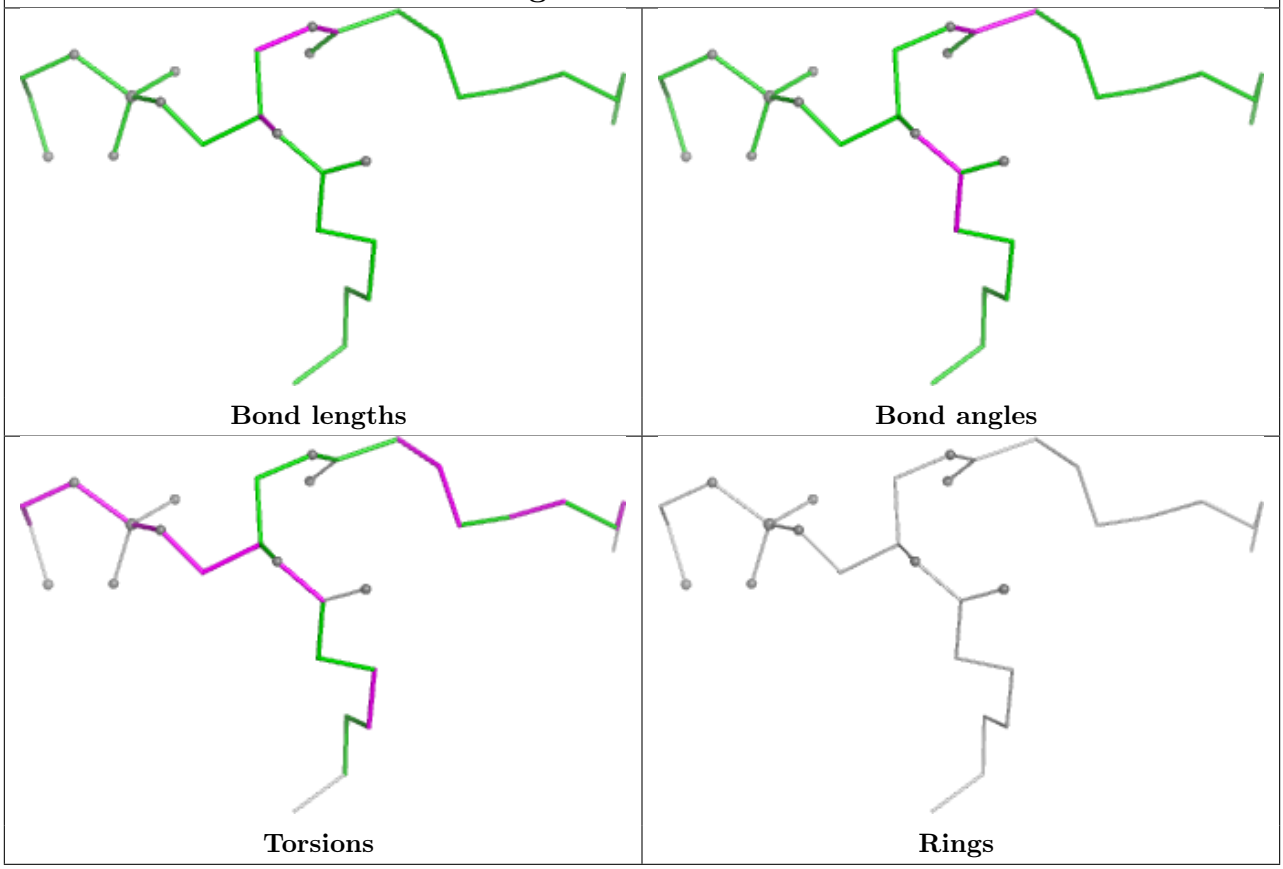


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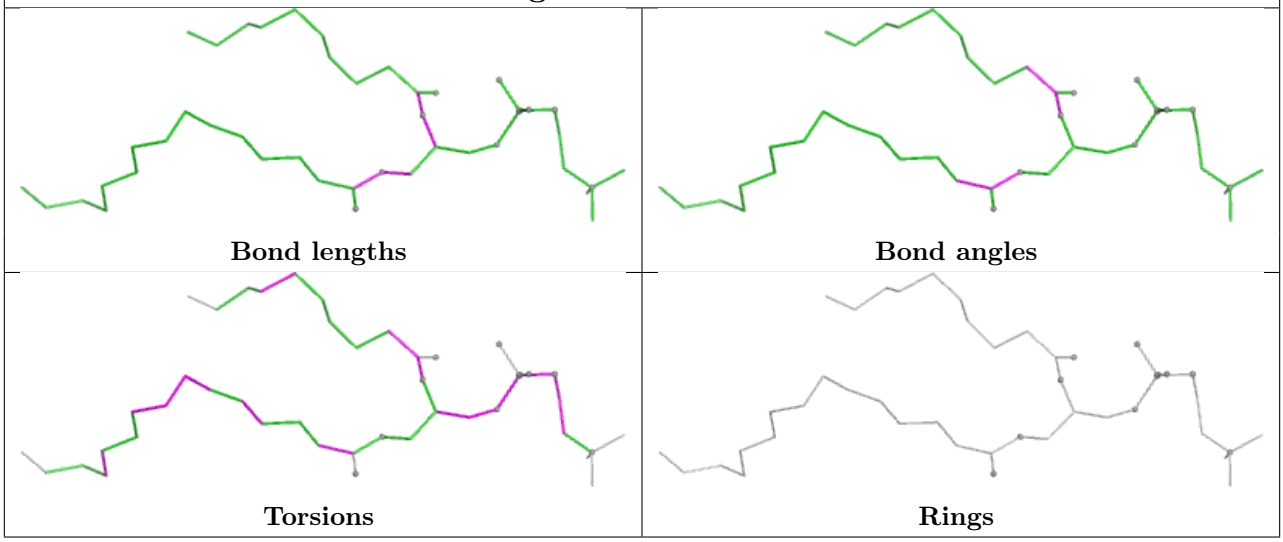


Rings

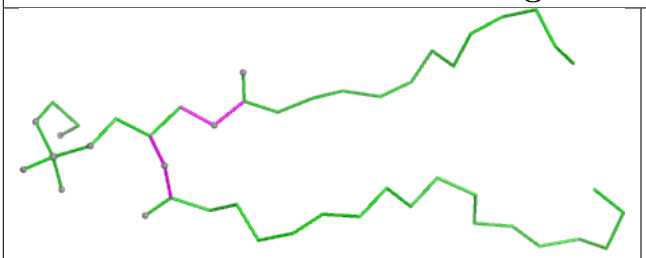
Ligand 3PE X 401



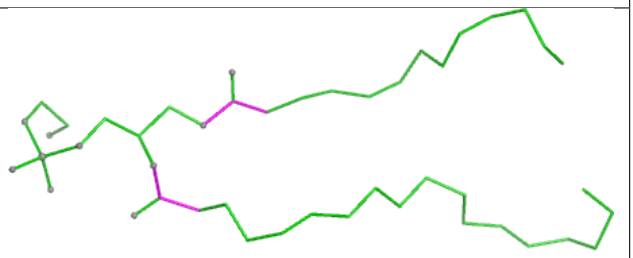
Ligand PC1 B 202



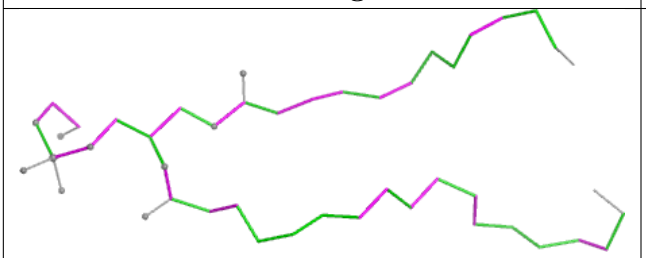
Ligand 3PE M 601



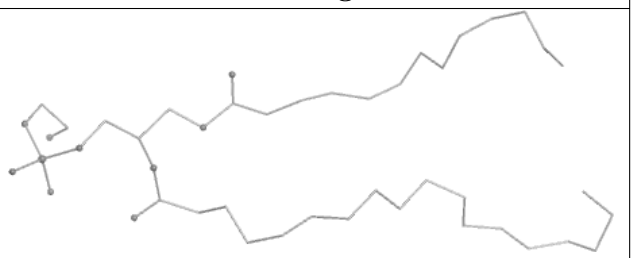
Bond lengths



Bond angles

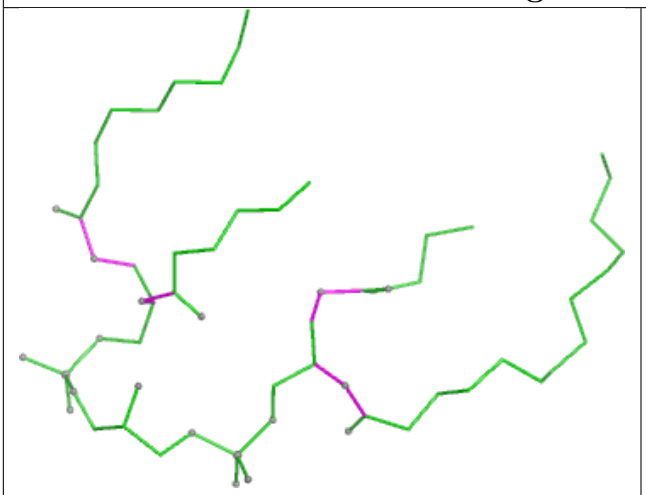


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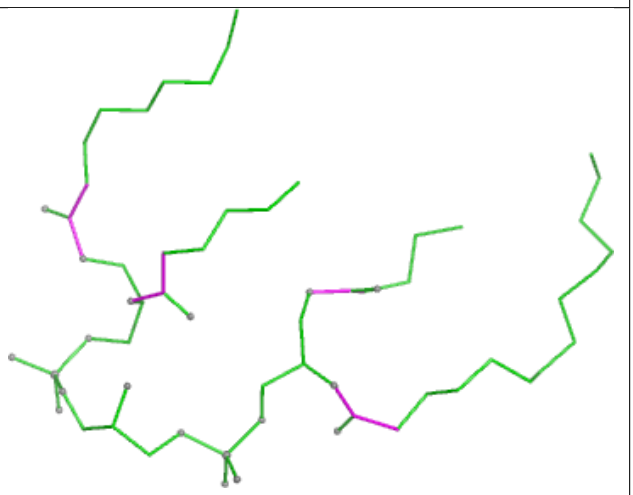


Rings

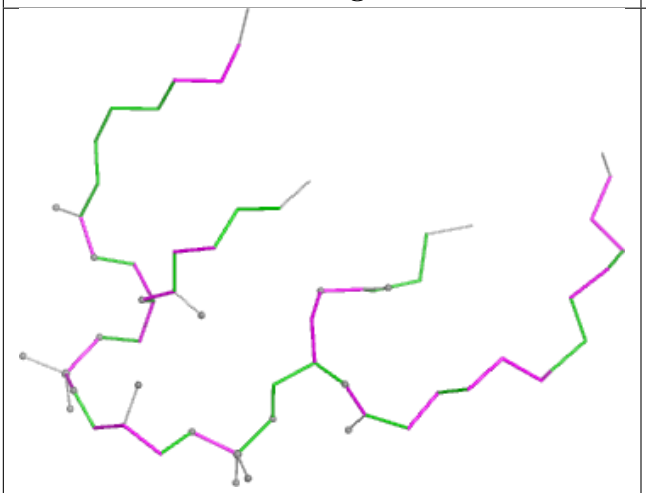
Ligand CDL L 702



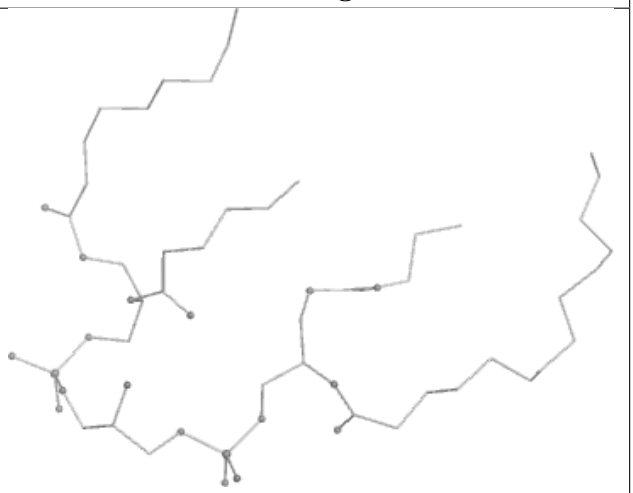
Bond lengths



Bond angles

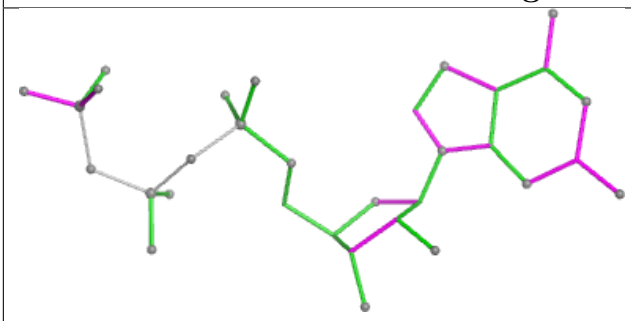


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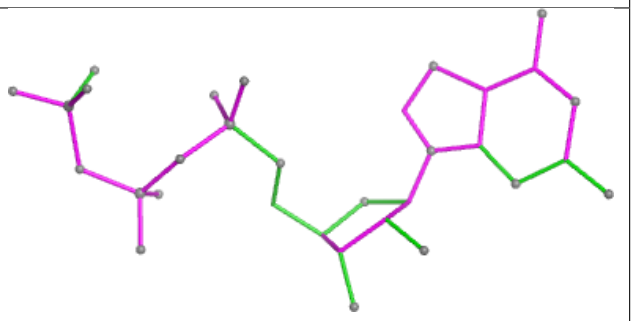


Rings

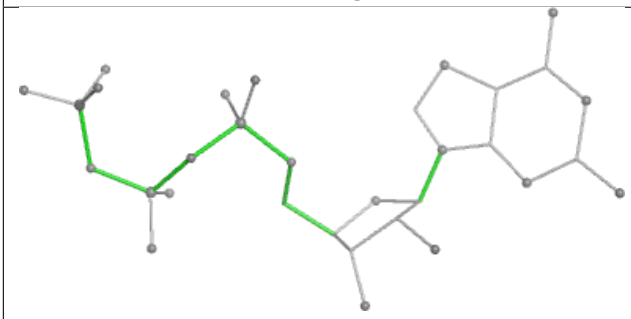
Ligand GTP O 401



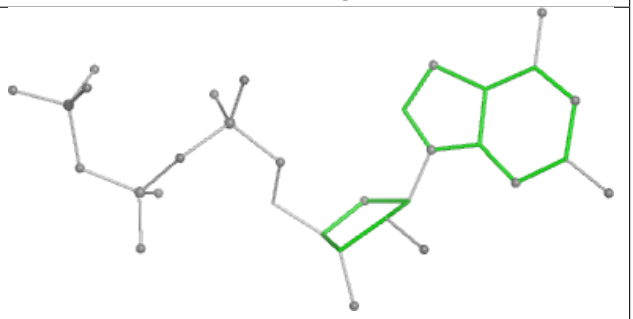
Bond lengths



Bond angles

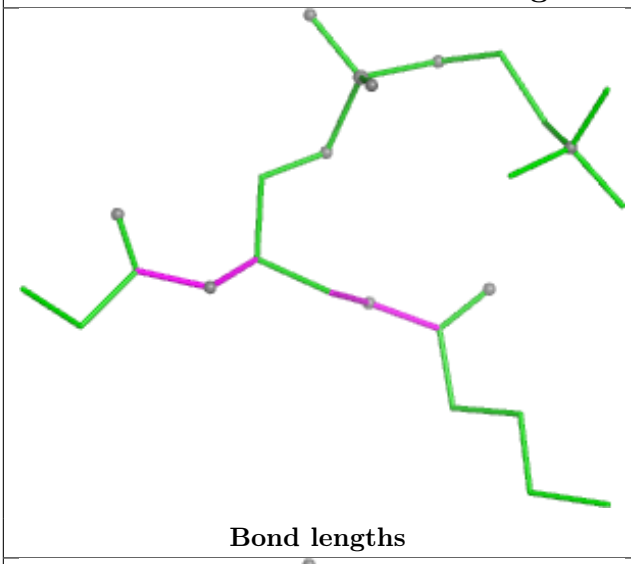


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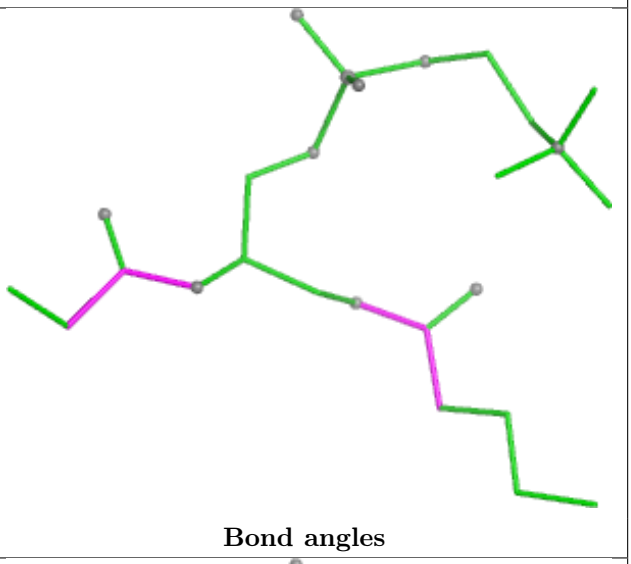


Rings

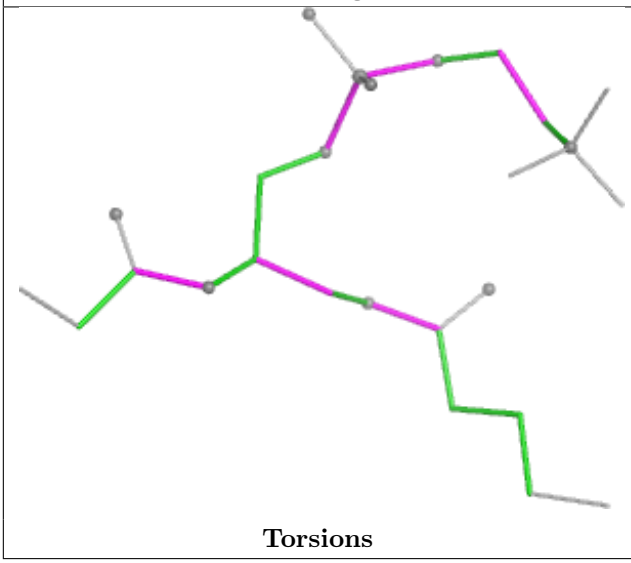
Ligand PC1 d 501



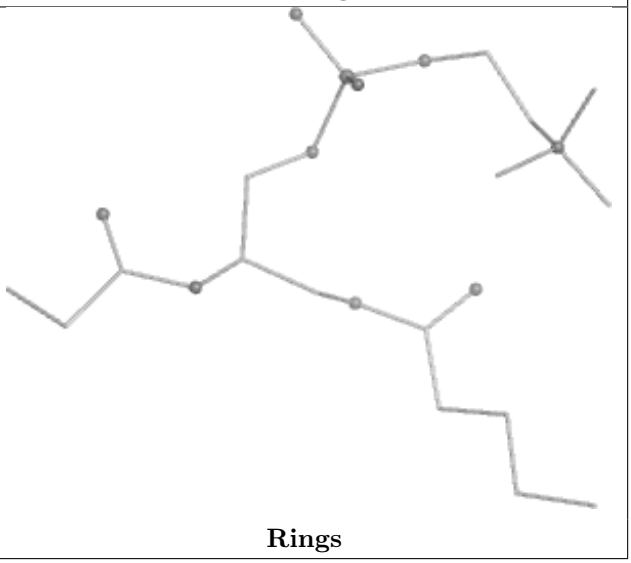
Bond lengths



Bond angles



Torsions

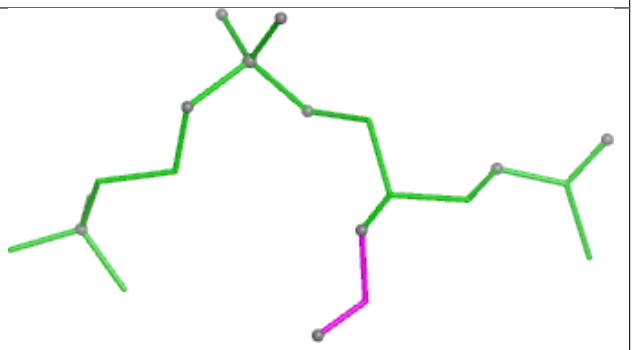


Rings

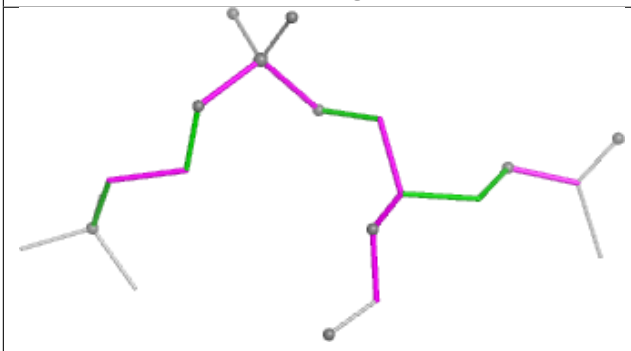
Ligand PC1 A 701



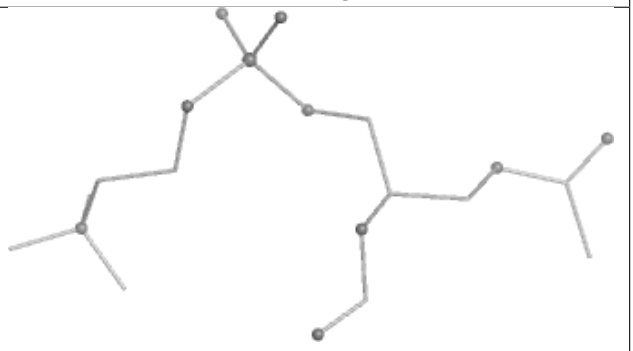
Bond lengths



Bond angles

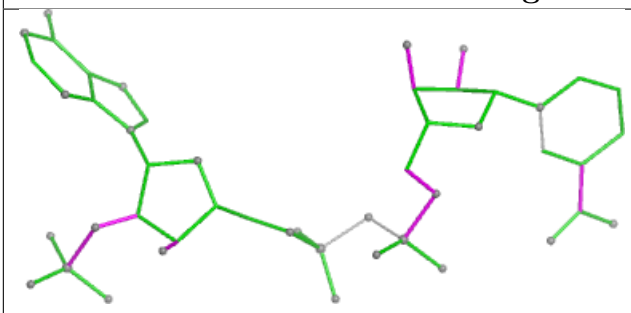


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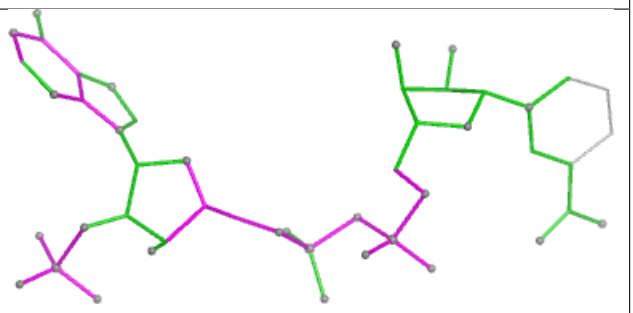


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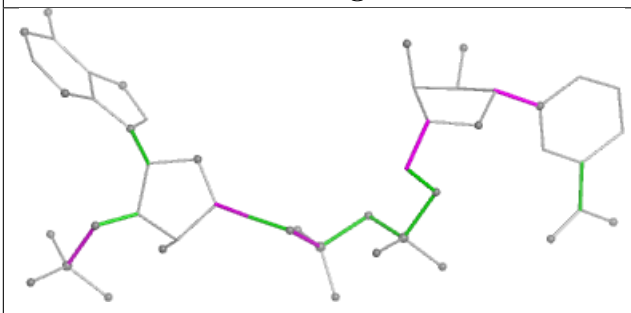
Ligand NDP P 501



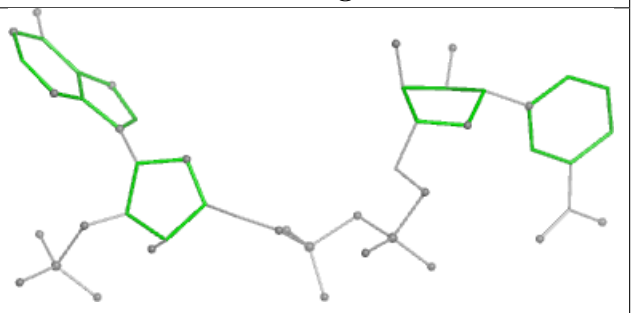
Bond lengths



Bond angles

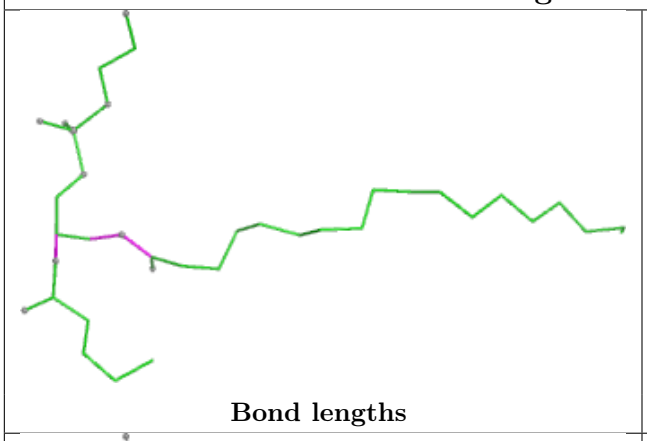


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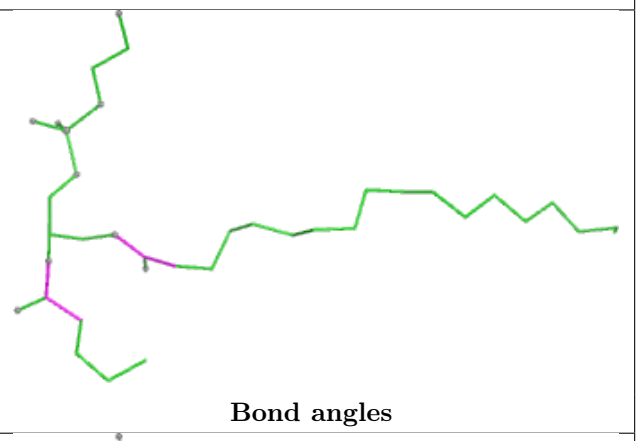


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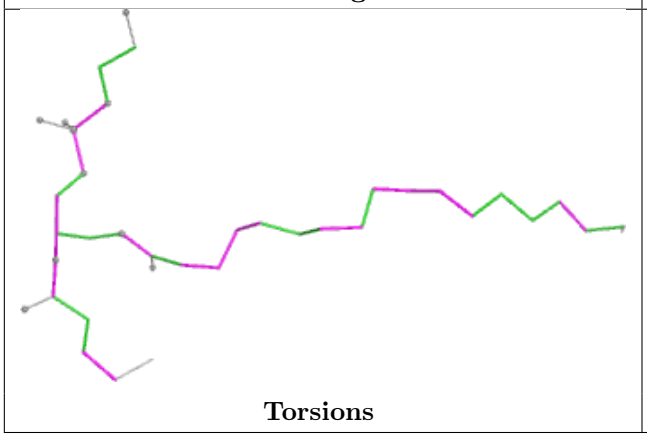
Ligand 3PE c 301



Bond lengths



Bond angles

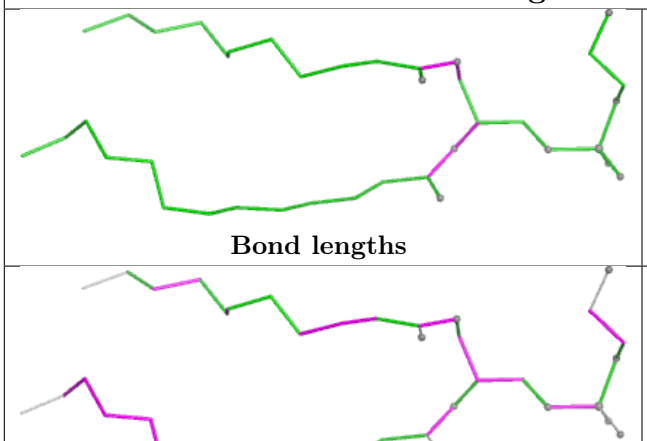


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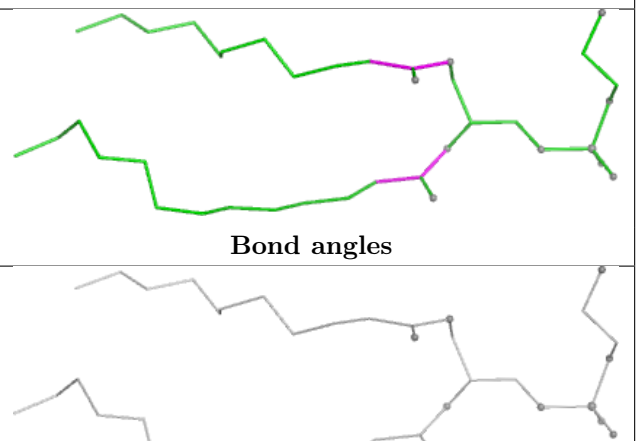


Rings

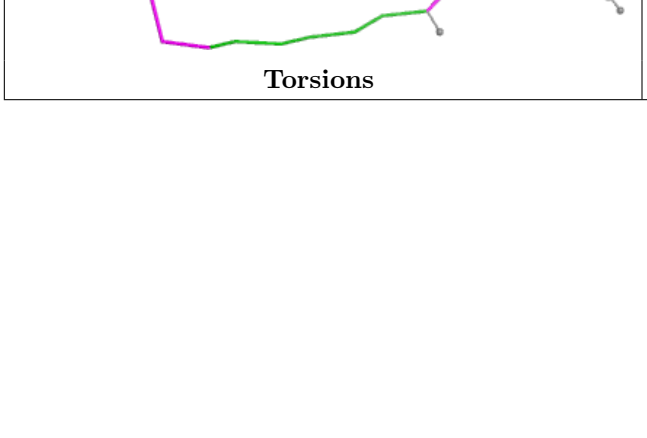
Ligand 3PE K 101



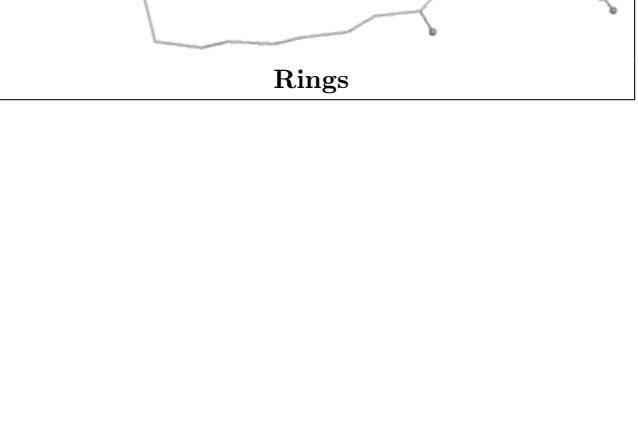
Bond lengths



Bond angles

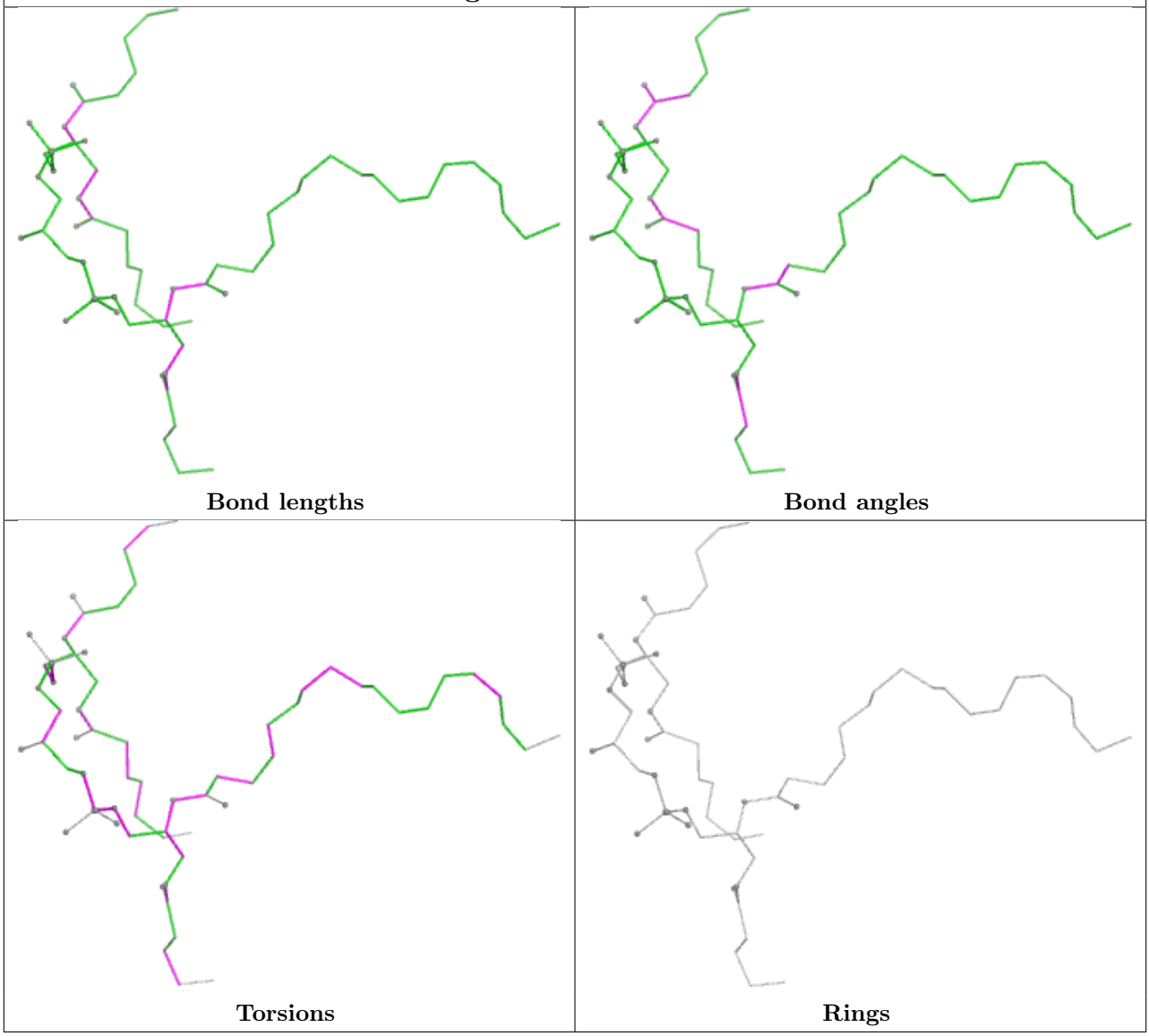


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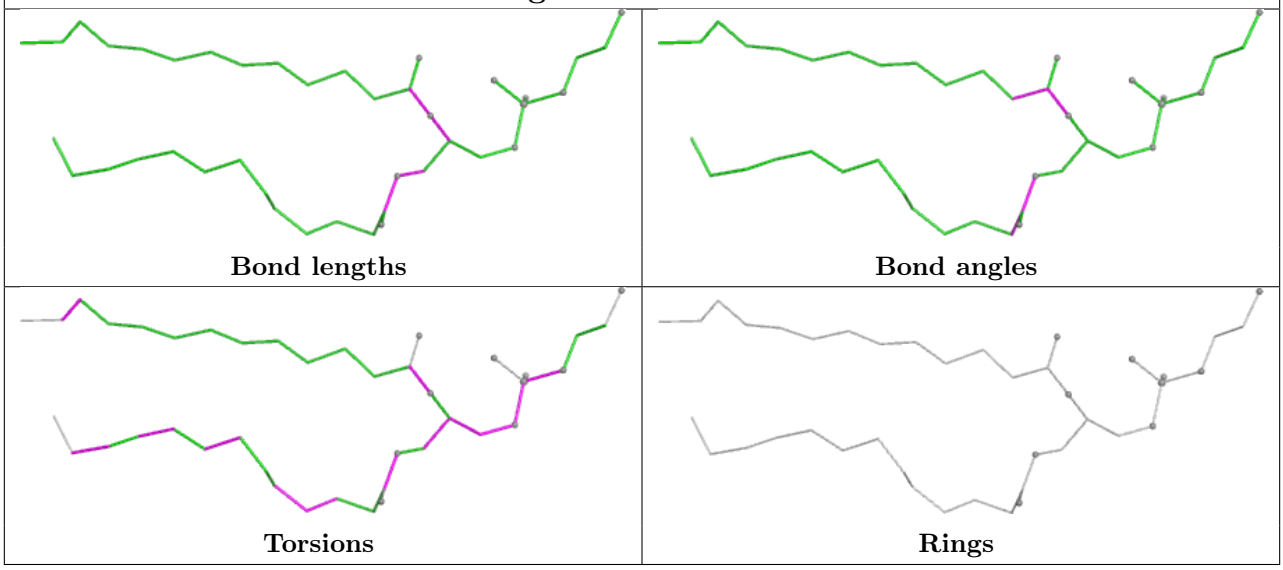


Rings

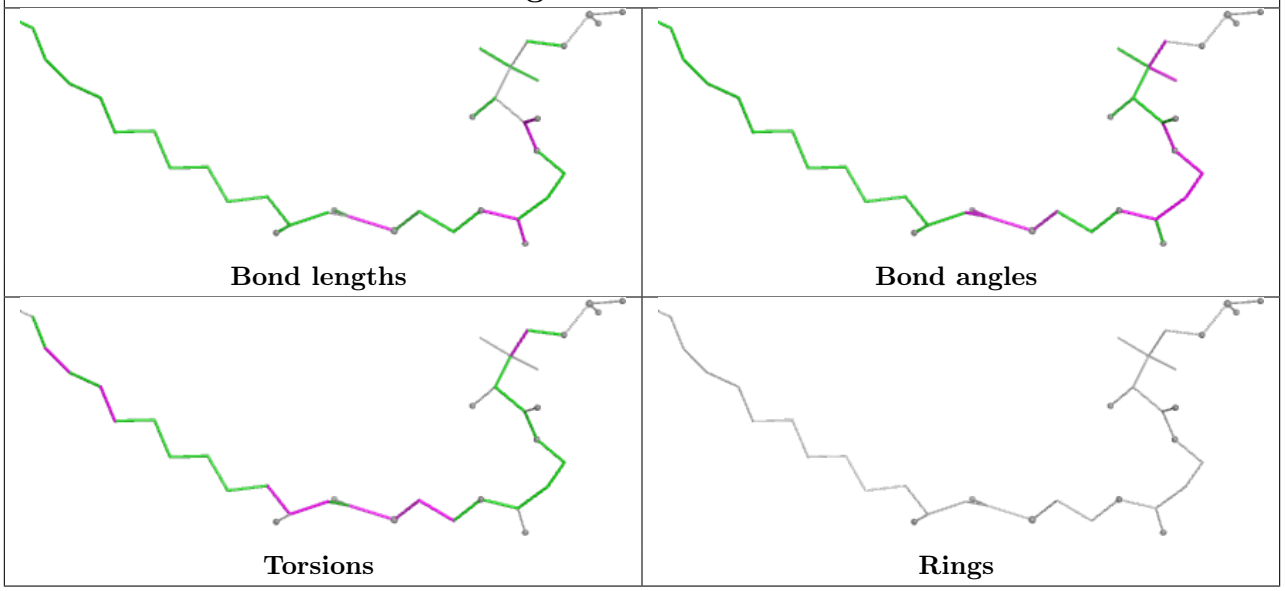
Ligand CDL h 1001



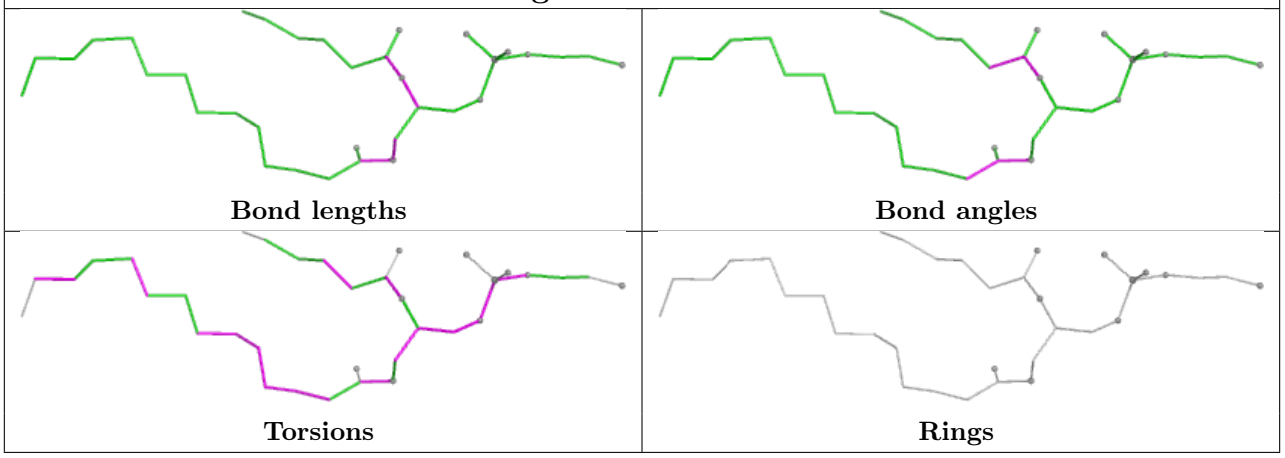
Ligand 3PE N 903



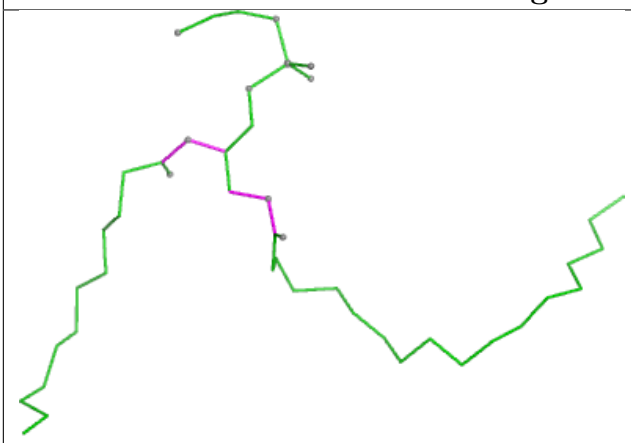
Ligand EHZ T 101



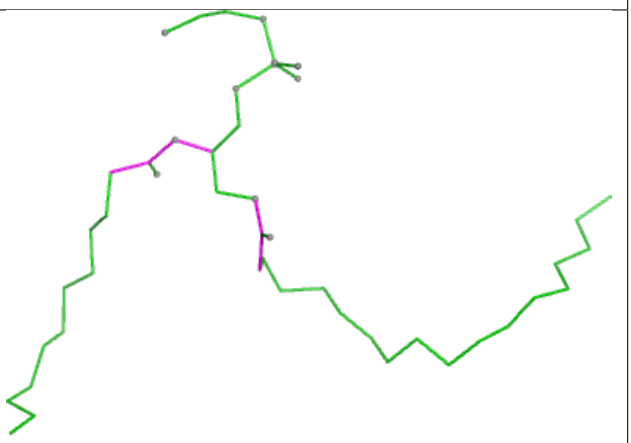
Ligand 3PE L 704



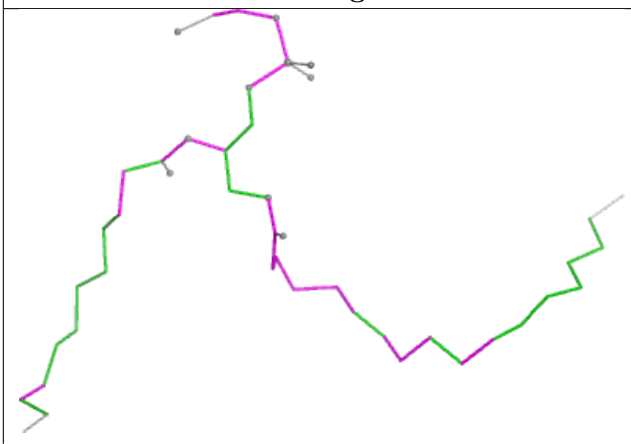
Ligand 3PE L 703



Bond lengths



Bond angles

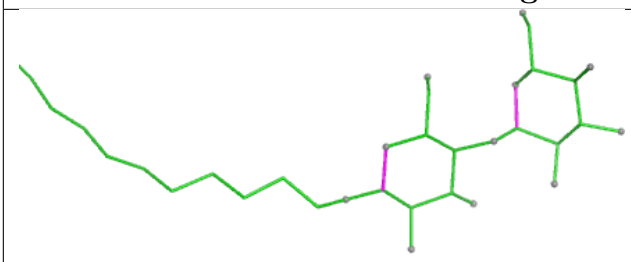


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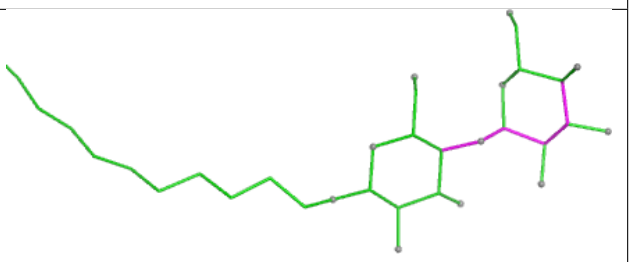


Rings

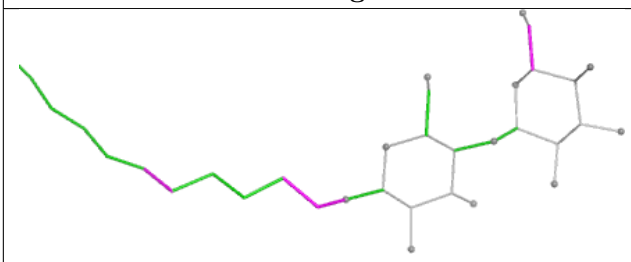
Ligand LMT N 901



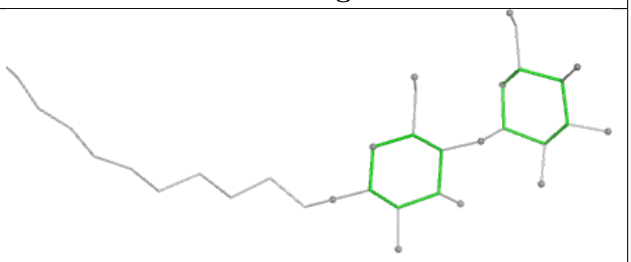
Bond lengths



Bond angles

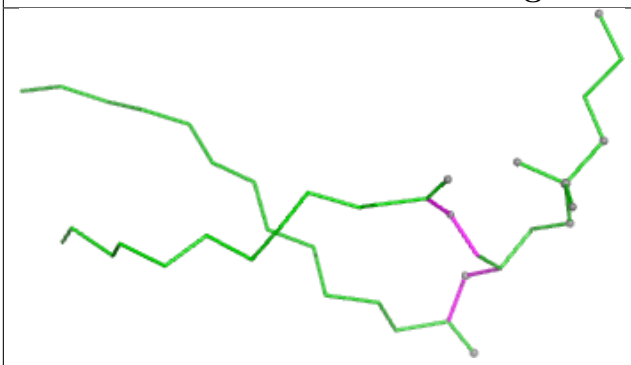


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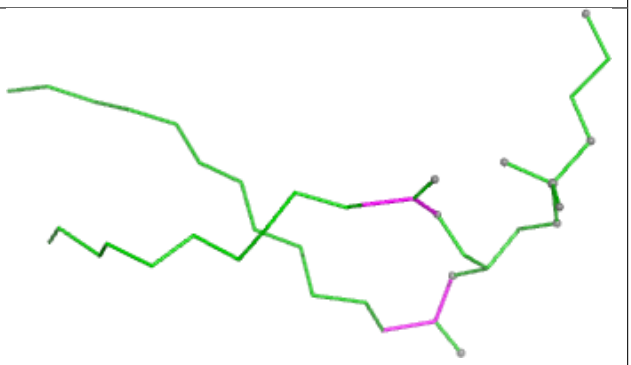


Rings

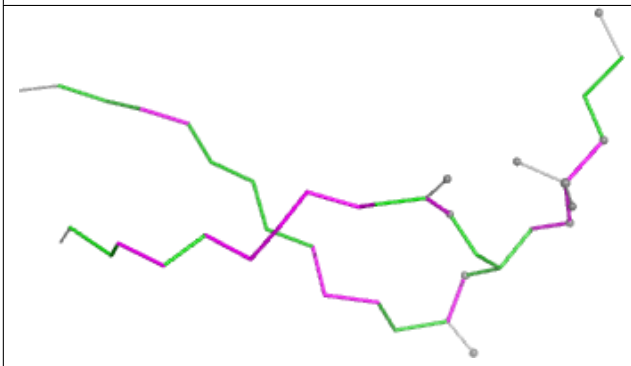
Ligand 3PE M 603



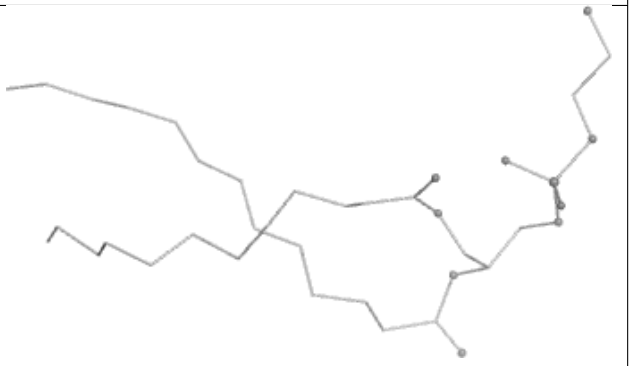
Bond lengths



Bond angles

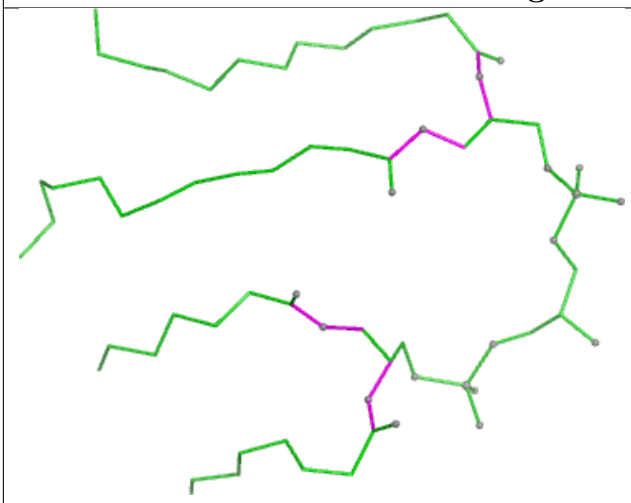


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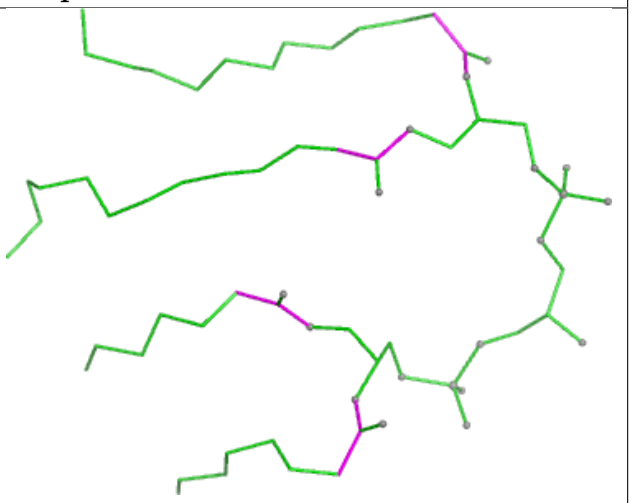


Rings

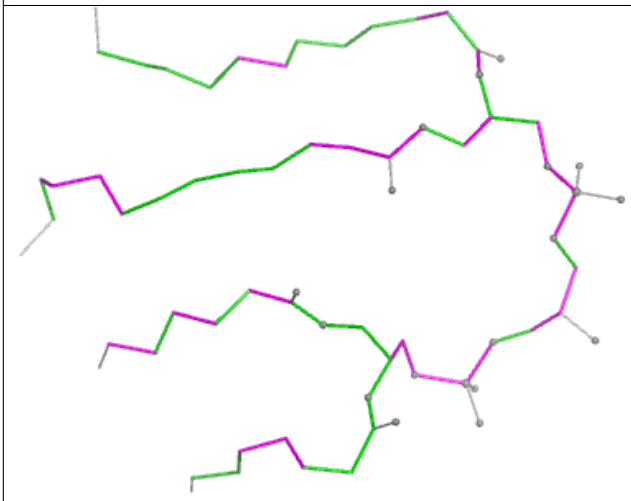
Ligand CDL q 201



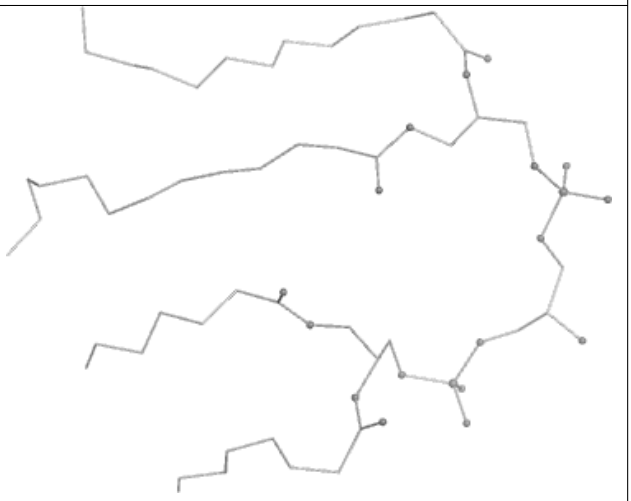
Bond lengths



Bond angles

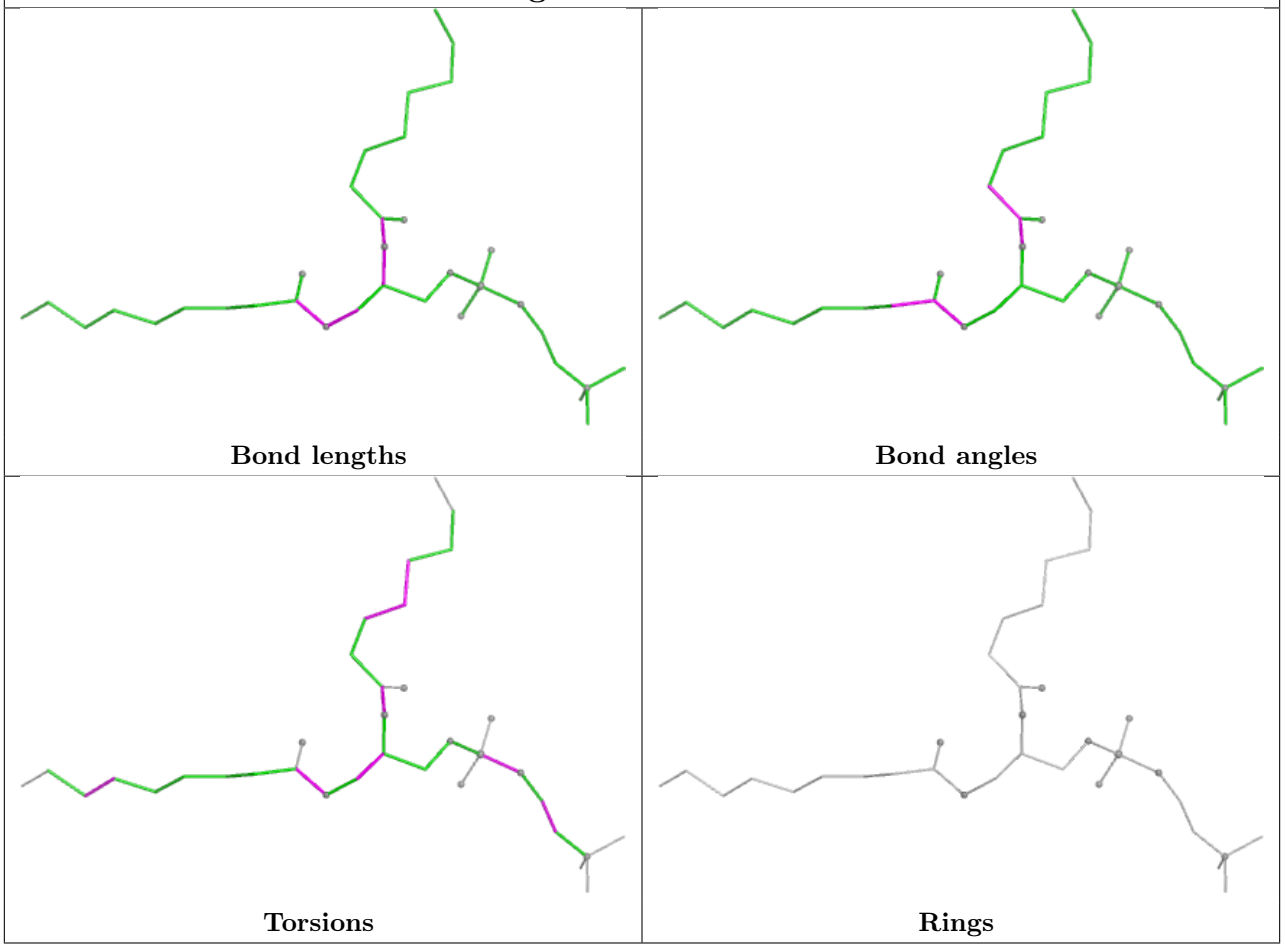


Torsions



Rings

Ligand PC1 B 203



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

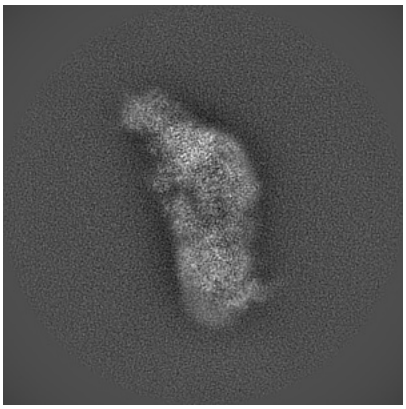
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14127. These allow visual inspection of the internal detail of the map and identification of artifacts.

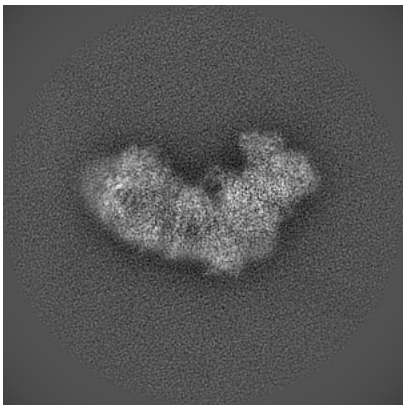
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

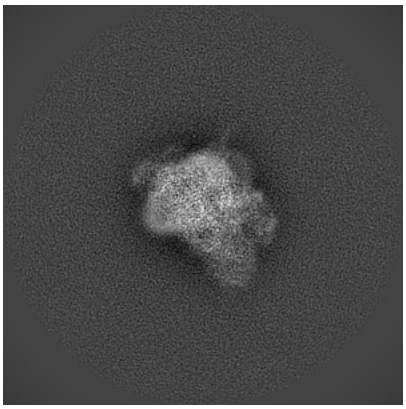
6.1.1 Primary map



X

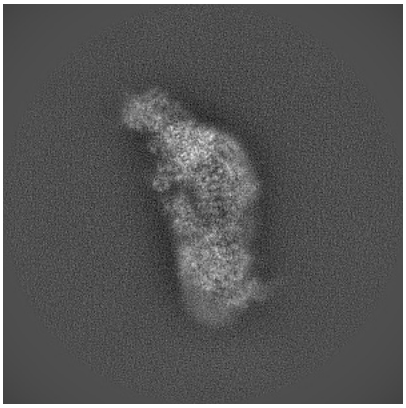


Y

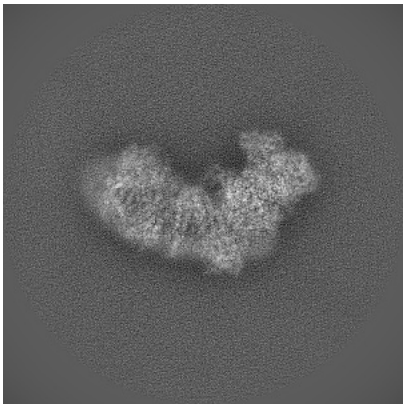


Z

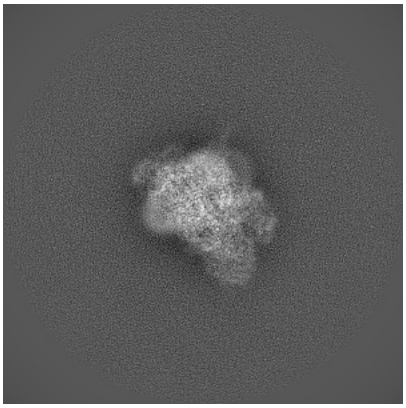
6.1.2 Raw map



X



Y

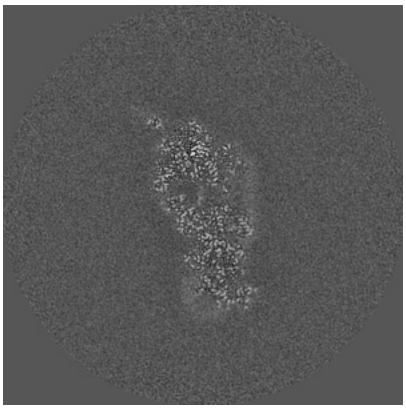


Z

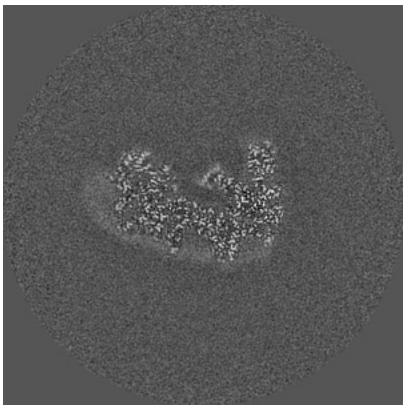
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

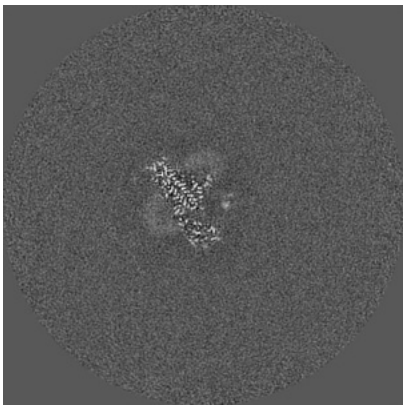
6.2.1 Primary map



X Index: 225

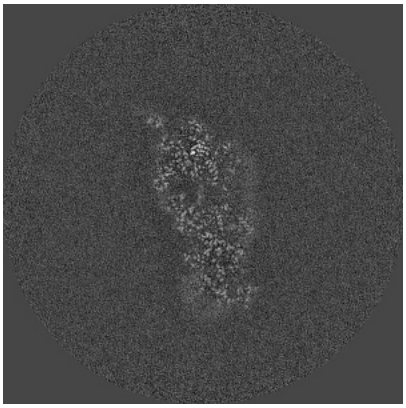


Y Index: 225

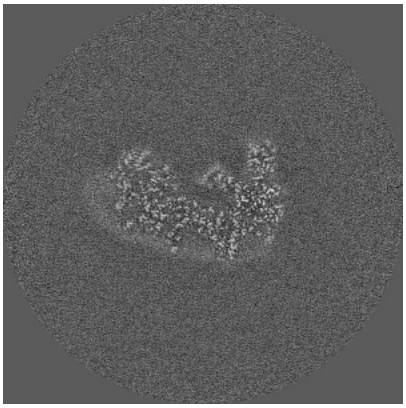


Z Index: 225

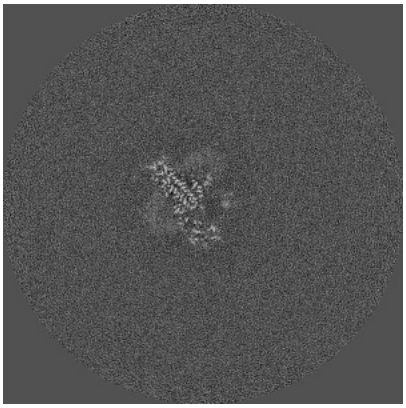
6.2.2 Raw map



X Index: 225



Y Index: 225

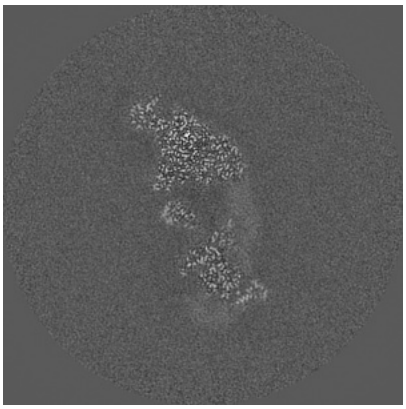


Z Index: 225

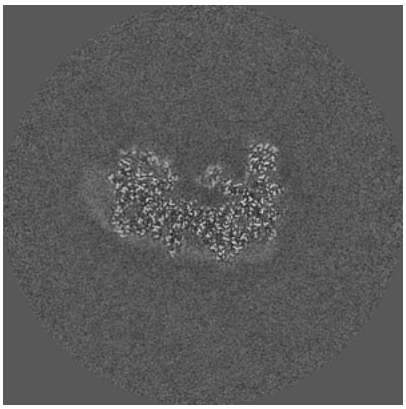
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

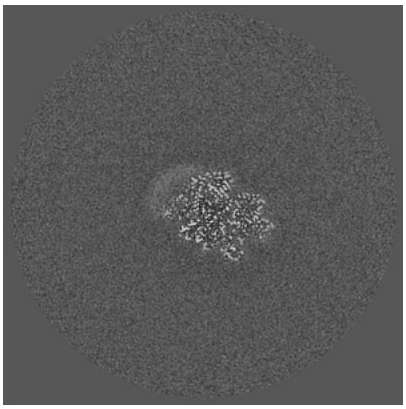
6.3.1 Primary map



X Index: 238

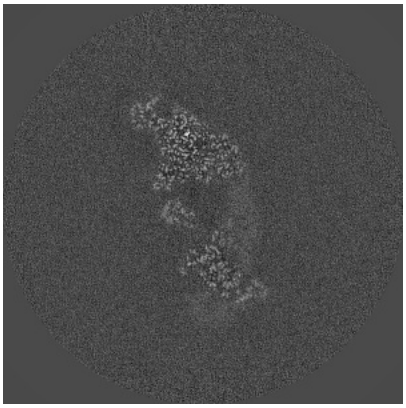


Y Index: 229

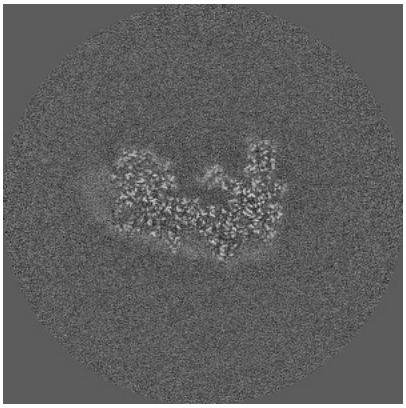


Z Index: 290

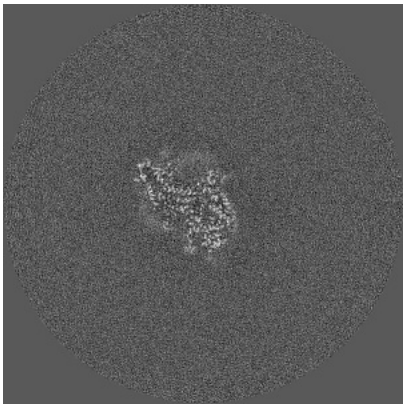
6.3.2 Raw map



X Index: 238



Y Index: 227

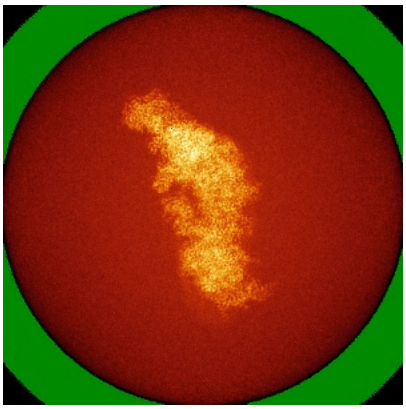


Z Index: 254

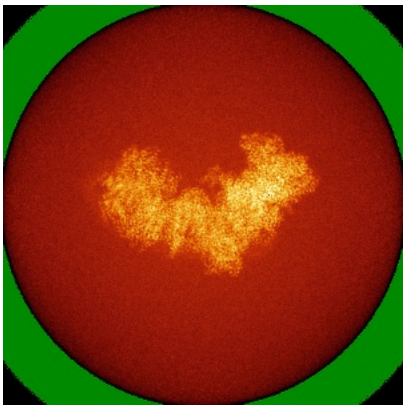
The images above show the largest variance slices of the map in three orthogonal directions.

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

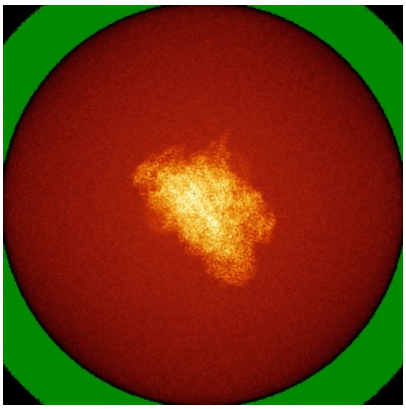
6.4.1 Primary map



X

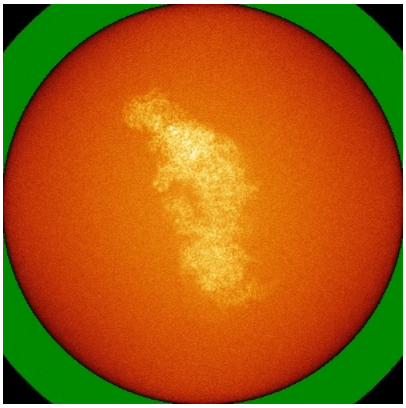


Y

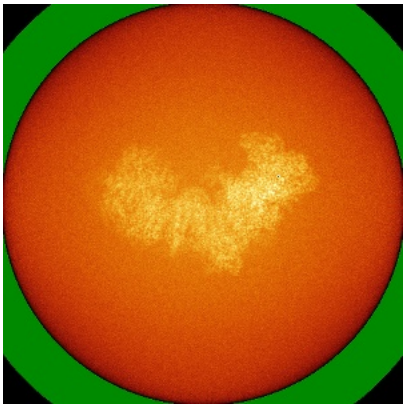


Z

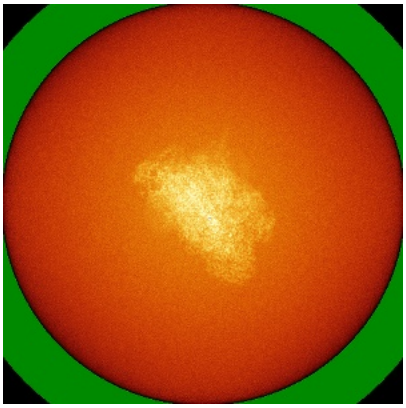
6.4.2 Raw map



X



Y

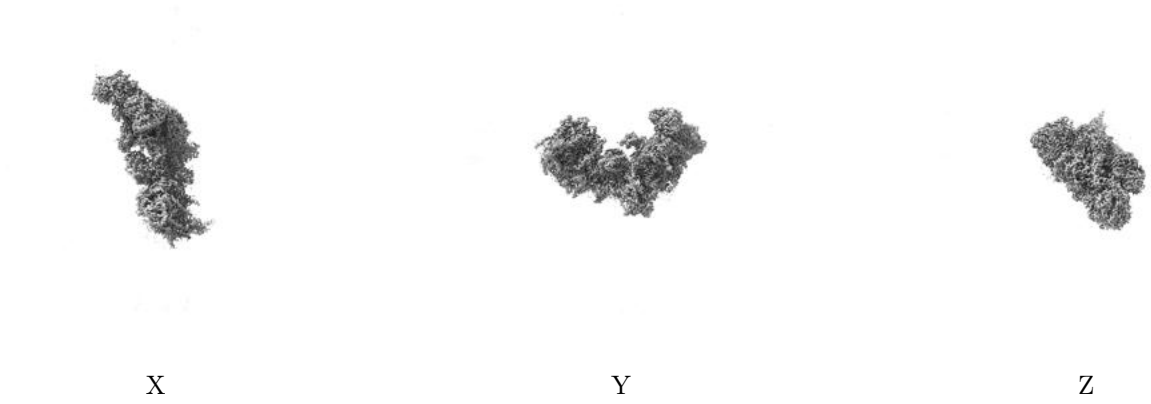


Z

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

6.5 Orthogonal surface views (i)

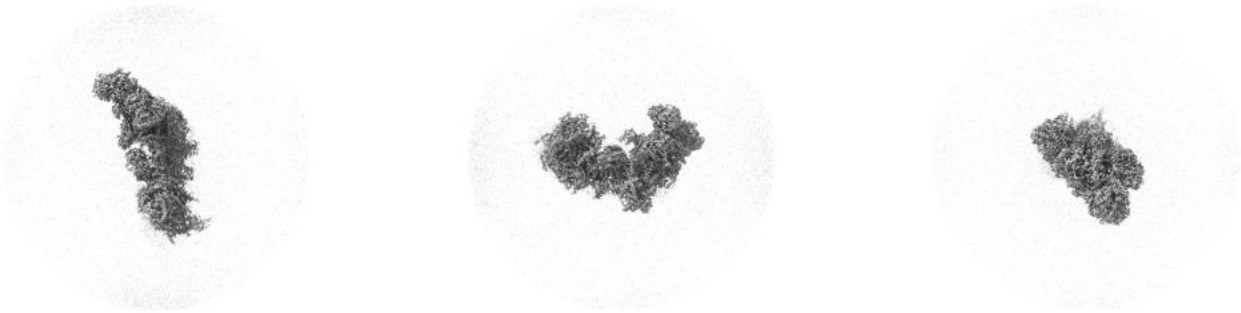
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 5.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

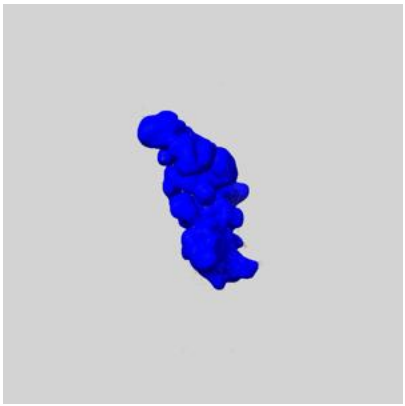
6.6 Mask visualisation (i)

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

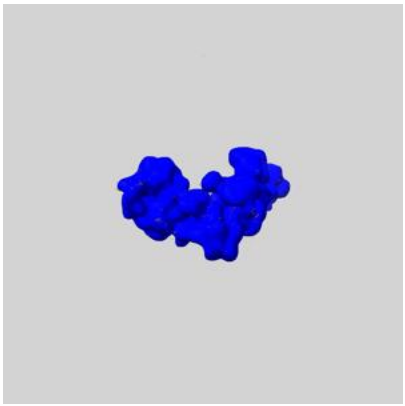
A mask typically either:

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

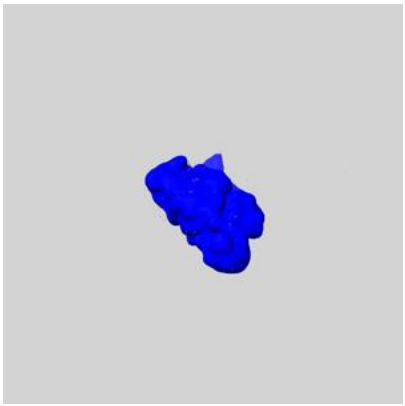
6.6.1 emd_14127_msk_1.map (i)



X



Y

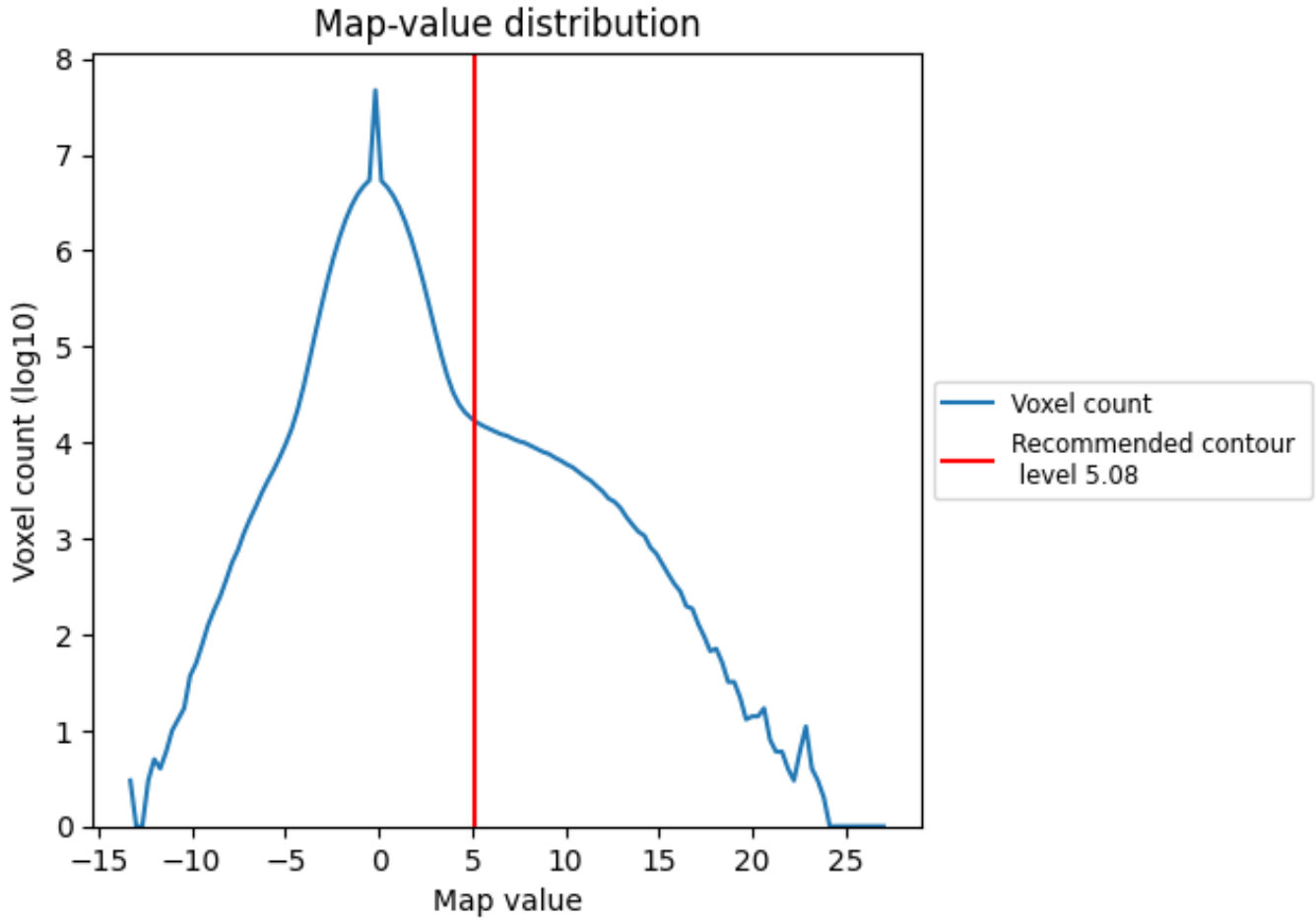


Z

7 Map analysis

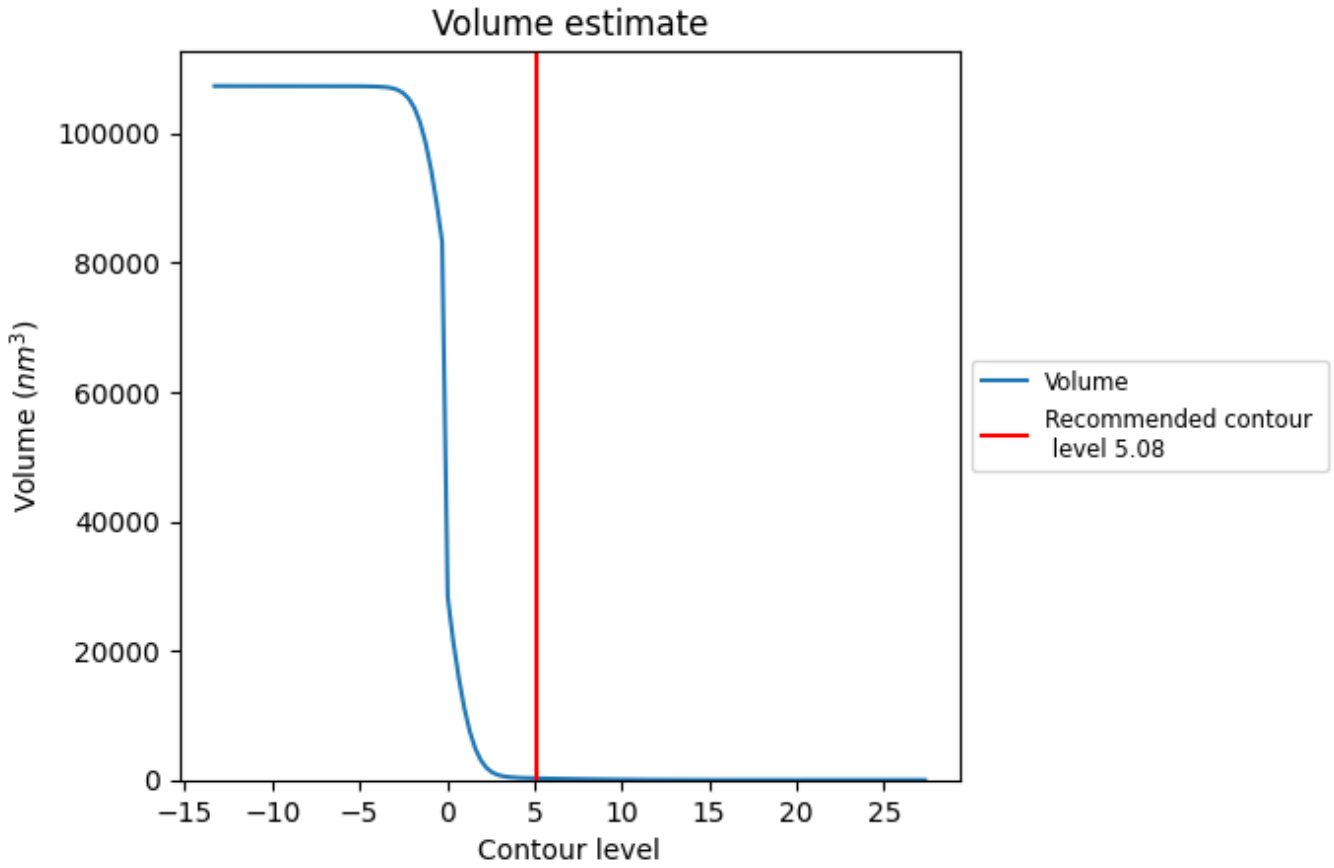
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

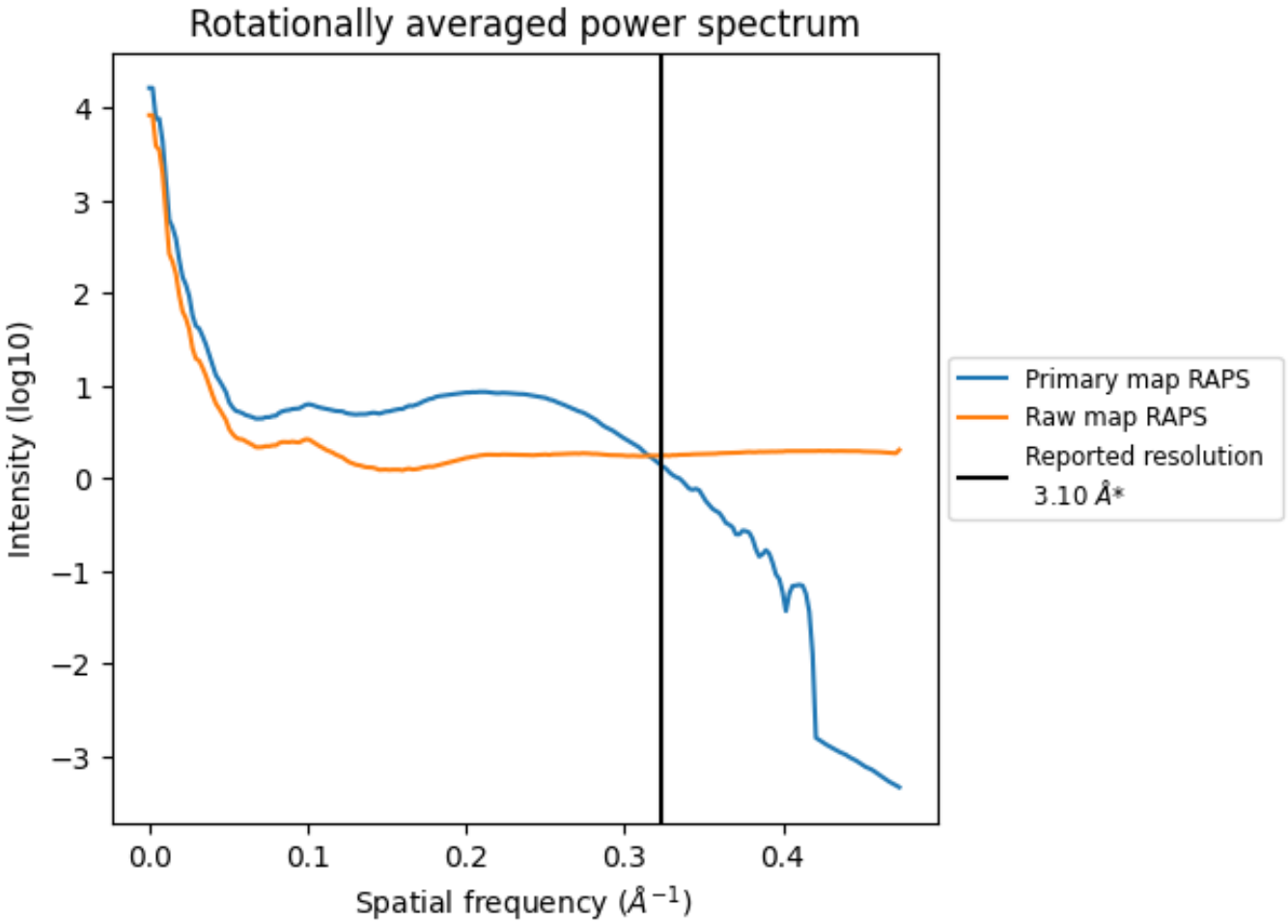
7.2 Volume estimate (i)



The volume at the recommended contour level is 257 nm^3; this corresponds to an approximate mass of 232 kDa.

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

7.3 Rotationally averaged power spectrum (i)

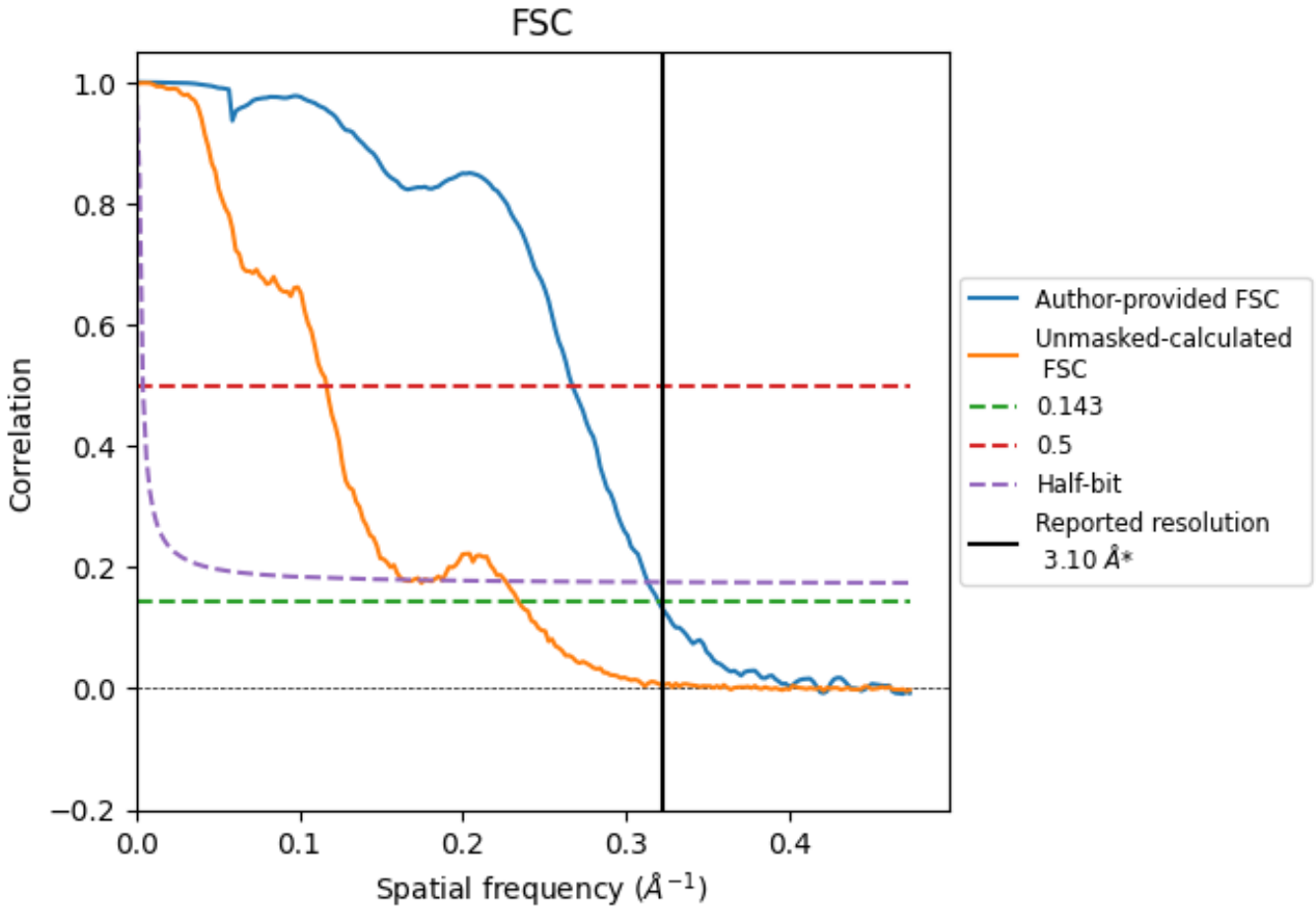


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8.2 Resolution estimates (i)

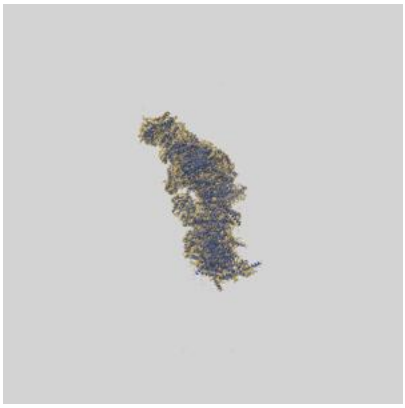
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.13	3.75	3.19
Unmasked-calculated*	4.27	8.58	6.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.27 differs from the reported value 3.1 by more than 10 %

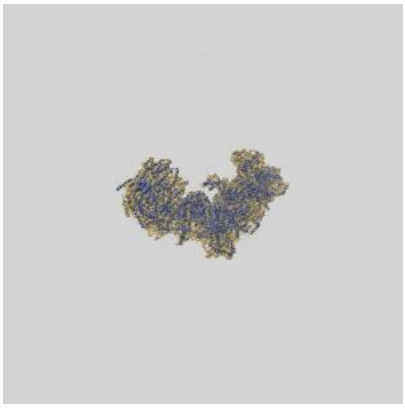
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14127 and PDB model 7QSD. Per-residue inclusion information can be found in section 3 on page 20.

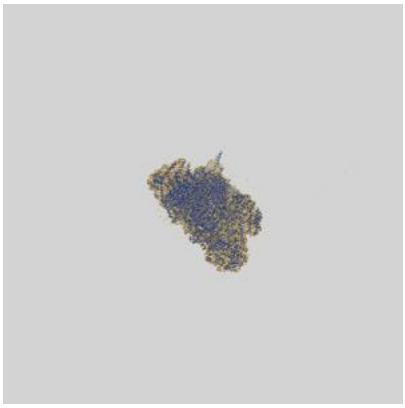
9.1 Map-model overlay



X



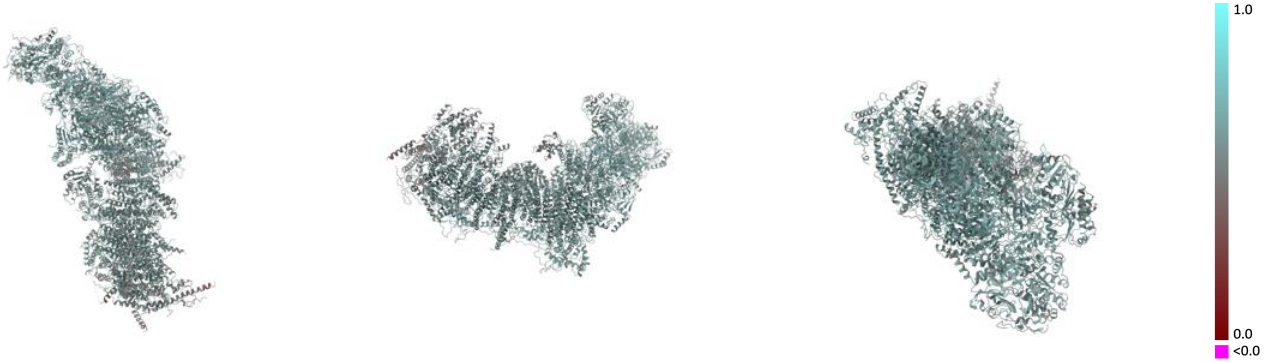
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.08 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.

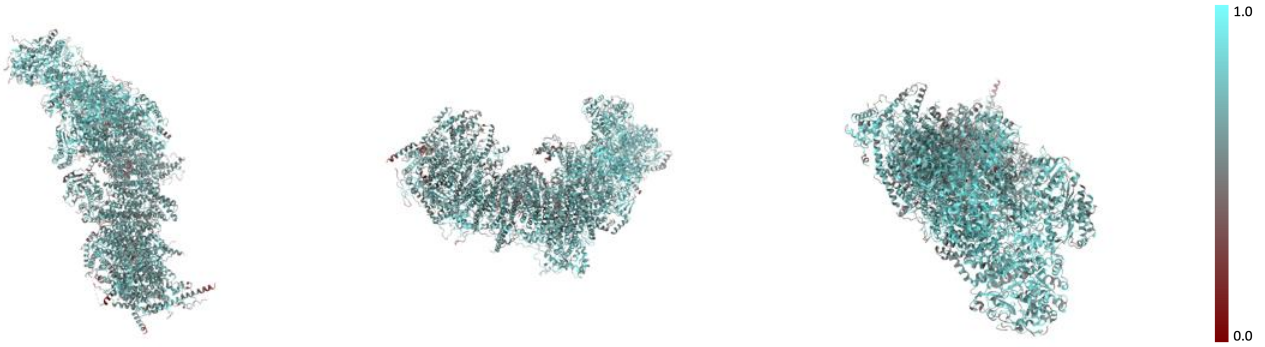
9.2 Q-score mapped to coordinate model (i)



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.

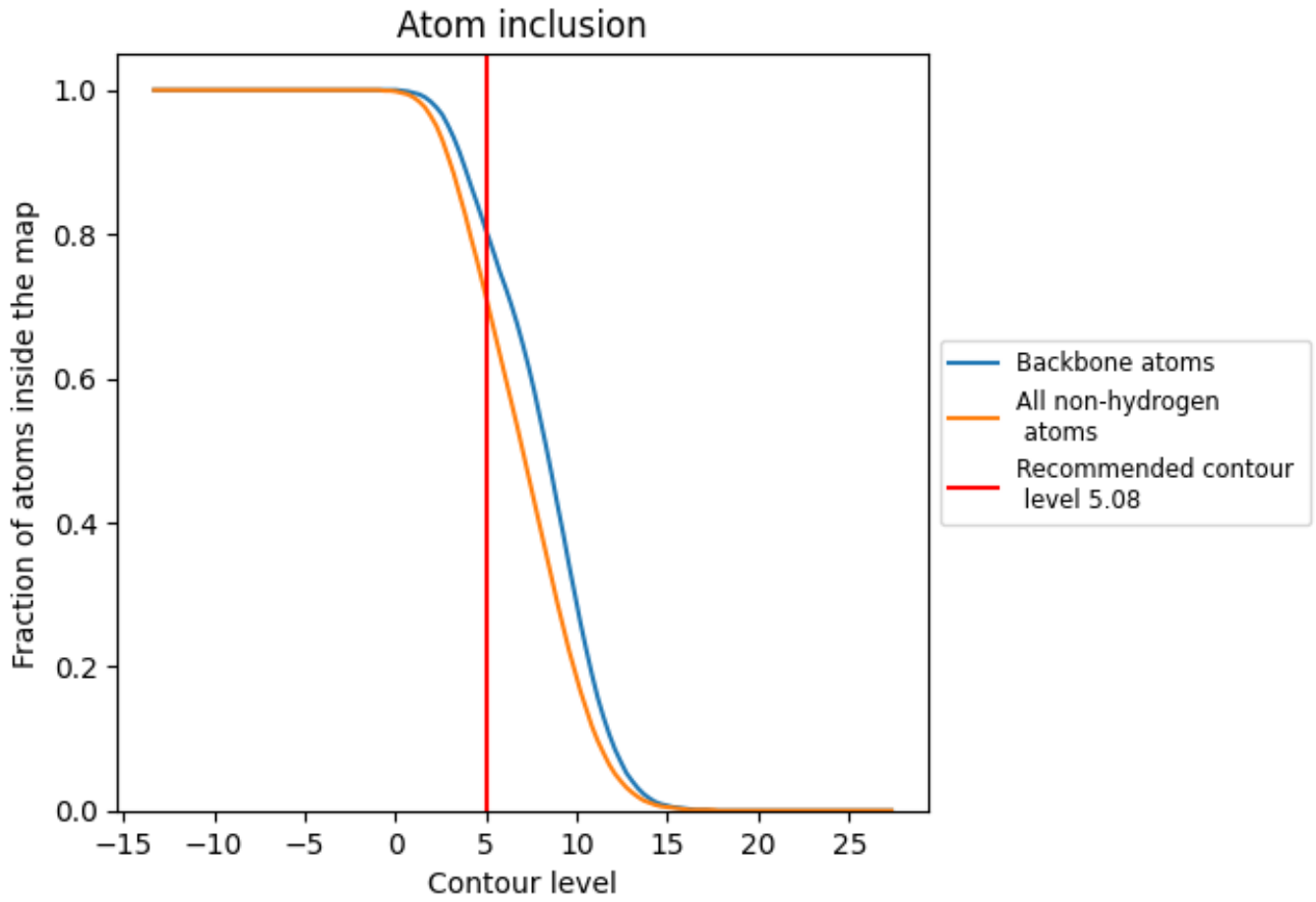
9.3 Atom inclusion mapped to coordinate model (i)



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 (5.08).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (5.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7050	0.5850
A	0.6560	0.6000
B	0.8020	0.6320
C	0.8130	0.6290
D	0.7960	0.6240
E	0.7060	0.5780
F	0.7350	0.5800
G	0.7550	0.6010
H	0.7600	0.6190
I	0.8280	0.6280
J	0.6710	0.5910
K	0.7290	0.6090
L	0.6540	0.5670
M	0.7200	0.6070
N	0.7340	0.6140
O	0.6700	0.5660
P	0.7400	0.5960
Q	0.7260	0.6120
R	0.7290	0.6020
S	0.6780	0.5550
T	0.5030	0.4900
U	0.5770	0.5180
V	0.6660	0.5880
W	0.6810	0.5940
X	0.6940	0.5780
Y	0.5820	0.5510
Z	0.7110	0.5910
a	0.7320	0.5980
b	0.6580	0.5660
c	0.5590	0.5550
d	0.6750	0.5830
e	0.6900	0.5810
f	0.5900	0.5460
g	0.6540	0.5720
h	0.7050	0.5920



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.5530	0.5260
j	0.6450	0.4950
k	0.5800	0.4990
l	0.6750	0.5440
m	0.6390	0.5500
n	0.6750	0.5500
o	0.5890	0.4930
p	0.6780	0.5610
q	0.7310	0.6020
r	0.7320	0.6020
s	0.6550	0.5530