



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 05:57 AM UTC

PDB ID : 5LNK / pdb_00005lnk
EMDB ID : EMD-4093
Title : Entire ovine respiratory complex I
Authors : Fiedorczuk, K.; Letts, J.A.; Kaszuba, K.; Sazanov, L.A.
Deposited on : 2016-08-04
Resolution : 3.90 Å(reported)
Based on initial model : 4HEA

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.49

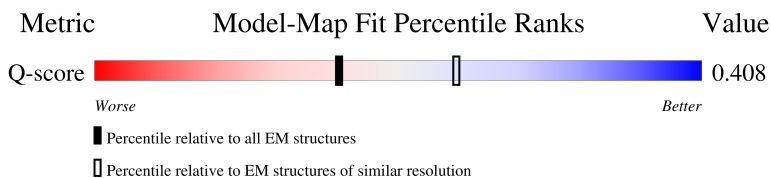
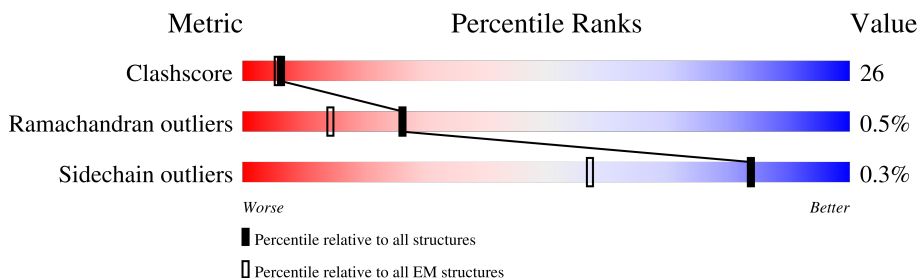
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	8855 (3.40 - 4.40)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	445	
2	2	217	
3	3	704	
4	4	412	

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Mol	Chain	Length	Quality of chain
5	5	228	
6	6	179	
7	9	176	
8	H	318	
9	N	347	
10	A	115	
11	M	459	
12	K	98	
13	L	599	
14	J	175	
15	a	75	
16	b	96	
17	c	133	
18	d	338	
19	e	98	
20	f	115	
21	g	127	
22	h	112	
23	i	145	
24	X	88	
24	j	88	
25	k	320	
26	l	105	
27	m	83	
28	n	97	

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Mol	Chain	Length	Quality of chain
29	o	120	
30	p	128	
31	q	143	
32	r	127	
33	s	136	
34	t	178	
35	u	72	
36	v	158	
37	w	125	
38	x	49	
39	y	57	
40	z	70	
41	Z	175	
42	Y	171	
43	W	143	
44	V	119	

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
45	SF4	1	500	-	-	X	-
45	SF4	6	300	-	-	X	-
45	SF4	9	502	-	-	X	-

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 63760 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 Mitochondrial complex I, 51 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	432	Total	C	N	O	S	0	0
			3328	2097	596	615	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	214	Total	C	N	O	S	0	0
			1655	1056	279	310	10		

- Molecule 3 is a protein called Mitochondrial complex I, 75 kDa subunit.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	387	Total	C	N	O	S	0	0
			3098	1974	535	565	24		

- Molecule 5 is a protein called Mitochondrial complex I, 30 kDa subunit.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	155	Total	C	N	O	S	0	0
			1241	792	224	211	14		

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

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

- Molecule 8 is a protein called Mitochondrial complex I, ND1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	318	Total	C	N	O	S	0	0
			2528	1704	384	421	19		

- Molecule 9 is a protein called Mitochondrial complex I, ND2 subunit.

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

- Molecule 10 is a protein called Mitochondrial complex I, ND3 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	115	Total	C	N	O	S	0	0
			922	621	133	161	7		

- Molecule 11 is a protein called Mitochondrial complex I, ND4 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	459	Total	C	N	O	S	0	0
			3645	2428	571	606	40		

- Molecule 12 is a protein called Mitochondrial complex I, ND4L subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	86	Total	C	N	O	S	0	0
			649	428	96	111	14		

- Molecule 13 is a protein called Mitochondrial complex I, ND5 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	599	Total	C	N	O	S	0	0
			4456	2926	714	777	39		

- Molecule 14 is a protein called Mitochondrial complex I, ND6 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	175	Total	C	N	O	S	0	0
			1188	780	184	214	10		

- Molecule 15 is a protein called Mitochondrial complex I, 10 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	a	41	Total	C	N	O	S	0	0
			343	213	61	68	1		

- Molecule 16 is a protein called Mitochondrial complex I, 13 kDa subunit.

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

- Molecule 17 is a protein called Mitochondrial complex I, 18 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	c	123	Total	C	N	O	S	0	0
			1000	631	178	188	3		

- Molecule 18 is a protein called Mitochondrial complex I, 39 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	d	314	Total	C	N	O	S	0	0
			2473	1585	448	435	5		

- Molecule 19 is a protein called Mitochondrial complex I, B8 subunit.

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

- Molecule 20 is a protein called Mitochondrial complex I, B13 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	f	112	Total	C	N	O	S	0	0
			909	589	152	166	2		

- Molecule 21 is a protein called Mitochondrial complex I, B14 subunit.

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

- Molecule 22 is a protein called Mitochondrial complex I, B14.5a subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	h	95	Total	C	N	O	S	0	0
			757	473	144	137	3		

- Molecule 23 is a protein called Mitochondrial complex I, B17.2 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	i	144	Total	C	N	O	S	0	0
			1200	772	214	209	5		

- Molecule 24 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	j	85	Total	C	N	O	S	0	0
			684	442	101	136	5		
24	X	88	Total	C	N	O	S	0	0
			707	454	104	144	5		

- Molecule 25 is a protein called Mitochondrial complex I, 42 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	k	320	Total	C	N	O	S	0	0
			2268	1430	394	435	9		

- Molecule 26 is a protein called Mitochondrial complex I, 15 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	l	95	Total	C	N	O	S	0	0
			792	503	146	137	6		

- Molecule 27 is a protein called Mitochondrial complex I, B9 subunit.

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

- Molecule 28 is a protein called Mitochondrial complex I, B12 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	n	74	Total	C	N	O	S	0	0
			578	378	100	98	2		

- Molecule 29 is a protein called Mitochondrial complex I, B14.5b subunit.

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

- Molecule 30 is a protein called Mitochondrial complex I, B15 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	p	112	Total	C	N	O	S	0	0
			841	526	162	152	1		

- Molecule 31 is a protein called Mitochondrial complex I, B16.6 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	q	140	Total	C	N	O	S	0	0
			1151	739	202	201	9		

- Molecule 32 is a protein called Mitochondrial complex I, B17 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	r	93	Total	C	N	O		0	0
			752	491	131	130			

- Molecule 33 is a protein called Mitochondrial complex I, B18 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	s	118	Total	C	N	O	S	0	0
			988	616	187	176	9		

- Molecule 34 is a protein called Mitochondrial complex I, B22 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	t	166	Total	C	N	O	S	0	0
			1434	916	265	247	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	u	66	Total	C	N	O	S	0	0
			563	372	94	96	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	v	143	Total	C	N	O	S	0	0
			861	544	155	158	4		

- Molecule 37 is a protein called Mitochondrial complex I, ESSS subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	w	86	Total	C	N	O	S	0	0
			715	462	119	130	4		

- Molecule 38 is a protein called Mitochondrial complex I, KFYI subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	x	48	Total	C	N	O	0	0
			403	266	69	68		

- Molecule 39 is a protein called Mitochondrial complex I, MNLL subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	y	53	Total	C	N	O	0	0
			457	301	80	76		

- Molecule 40 is a protein called Mitochondrial complex I, MWFE subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	z	69	Total	C	N	O	S	0	0
			568	364	105	95	4		

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

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

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

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

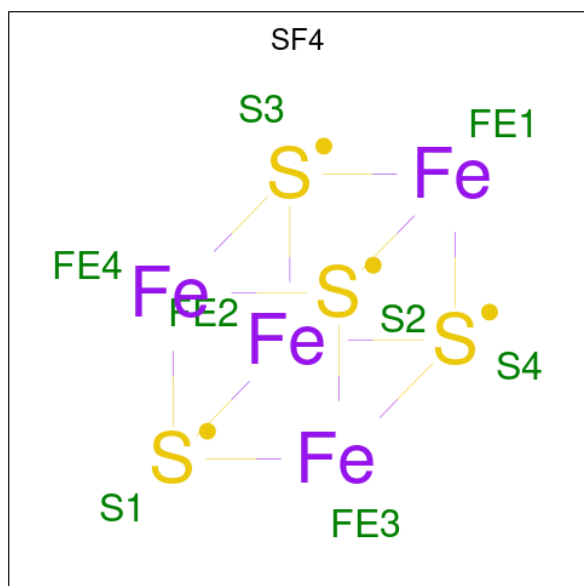
- Molecule 43 is a protein called Mitochondrial complex I, SGD1 subunit.

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

- Molecule 44 is a protein called Mitochondrial complex I, B14.7 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	V	119	Total	C	N	O	S	0	0
			595	357	119	119			

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



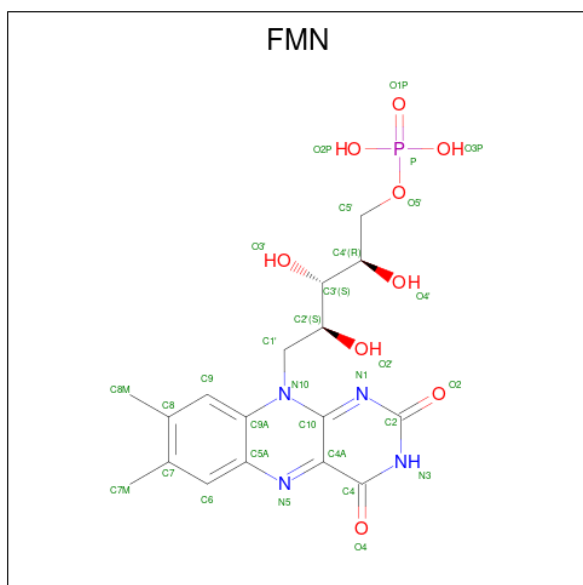
Mol	Chain	Residues	Atoms			AltConf
45	1	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	6	1	Total	Fe	S	0
			8	4	4	

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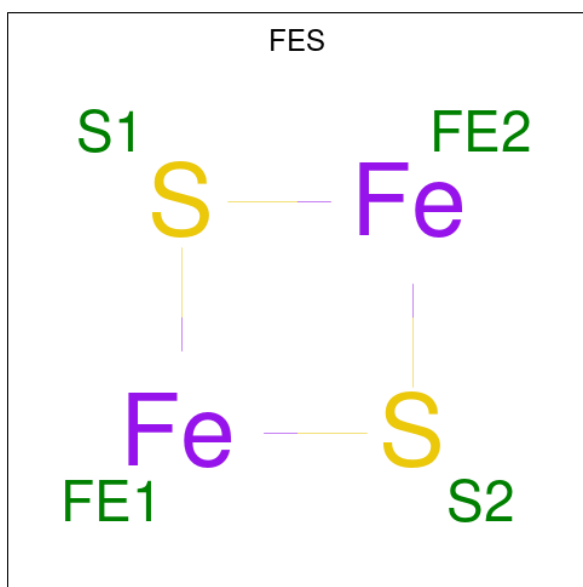
Mol	Chain	Residues	Atoms			AltConf
45	9	1	Total	Fe	S	0
			8	4	4	
45	9	1	Total	Fe	S	0
			8	4	4	

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



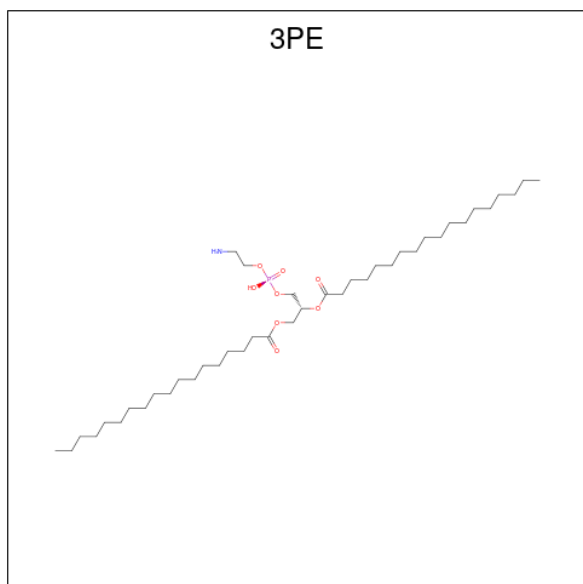
Mol	Chain	Residues	Atoms					AltConf
46	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
47	2	1	Total	Fe	S	0
			4	2	2	
47	3	1	Total	Fe	S	0
			4	2	2	

- Molecule 48 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



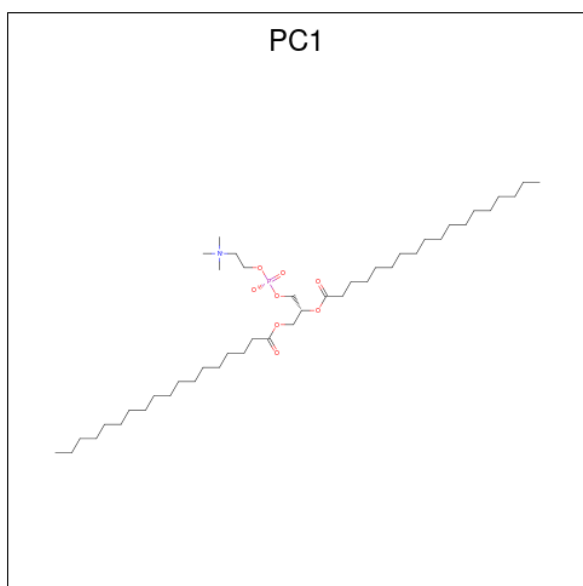
Mol	Chain	Residues	Atoms					AltConf
48	9	1	Total	C	N	O	P	0
			51	41	1	8	1	

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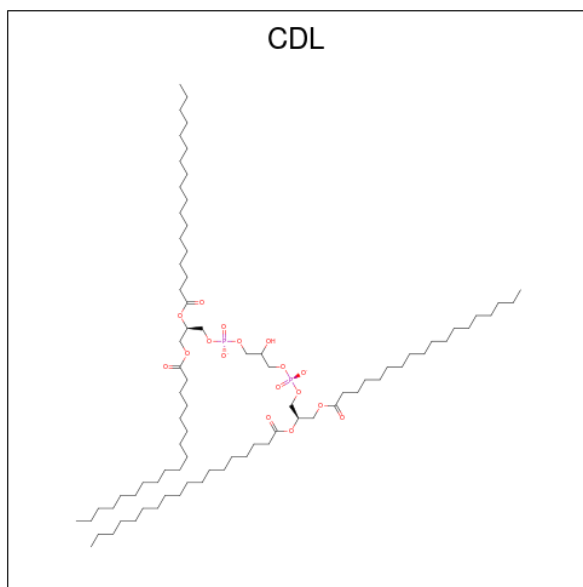
Mol	Chain	Residues	Atoms					AltConf
48	J	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	o	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	o	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 49 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
49	N	1	Total	C	N	O	P	0
			46	36	1	8	1	
49	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
49	M	1	Total	C	N	O	P	0
			46	36	1	8	1	
49	o	1	Total	C	N	O	P	0
			39	29	1	8	1	

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

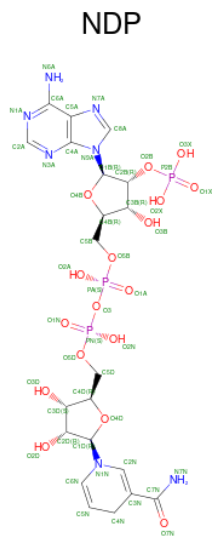


Mol	Chain	Residues	Atoms				AltConf
50	M	1	Total	C	O	P	0
			82	63	17	2	
50	L	1	Total	C	O	P	0
			84	65	17	2	
50	J	1	Total	C	O	P	0
			79	60	17	2	
50	i	1	Total	C	O	P	0
			58	39	17	2	

- Molecule 51 is ZINC ION (CCD ID: ZN) (formula: Zn).

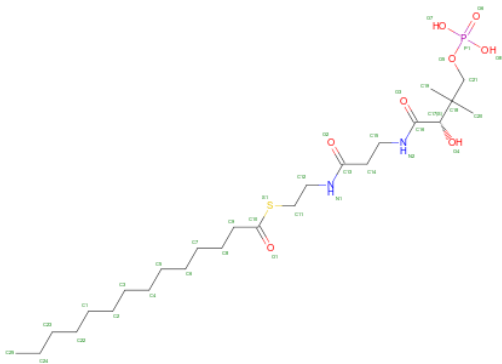
Mol	Chain	Residues	Atoms		AltConf
51	b	1	Total	Zn	0
			1	1	

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



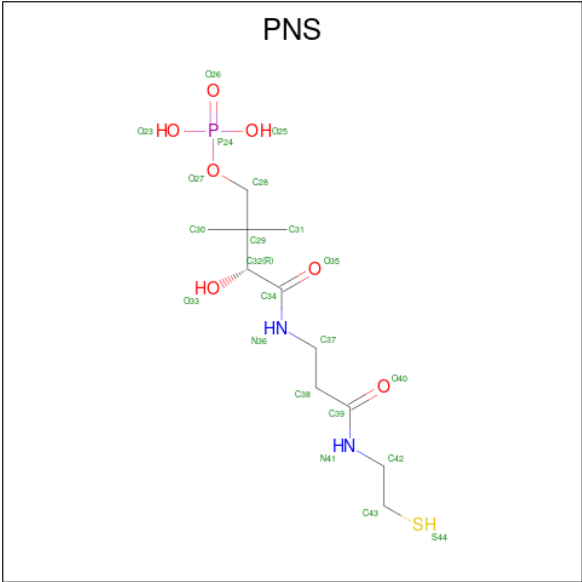
Mol	Chain	Residues	Atoms					AltConf
52	d	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 53 is S-[2-($\{N-[(2S)-2\text{-hydroxy-}3,3\text{-dimethyl-}4\text{-(phosphonooxy)butanoyl}]\text{-beta-alanyl}\}$ amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



Mol	Chain	Residues	Atoms					AltConf	
53	j	1	Total 34	C 23	N 2	O 7	P 1	S 1	0

- Molecule 54 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: $\text{C}_{11}\text{H}_{23}\text{N}_2\text{O}_7\text{PS}$).

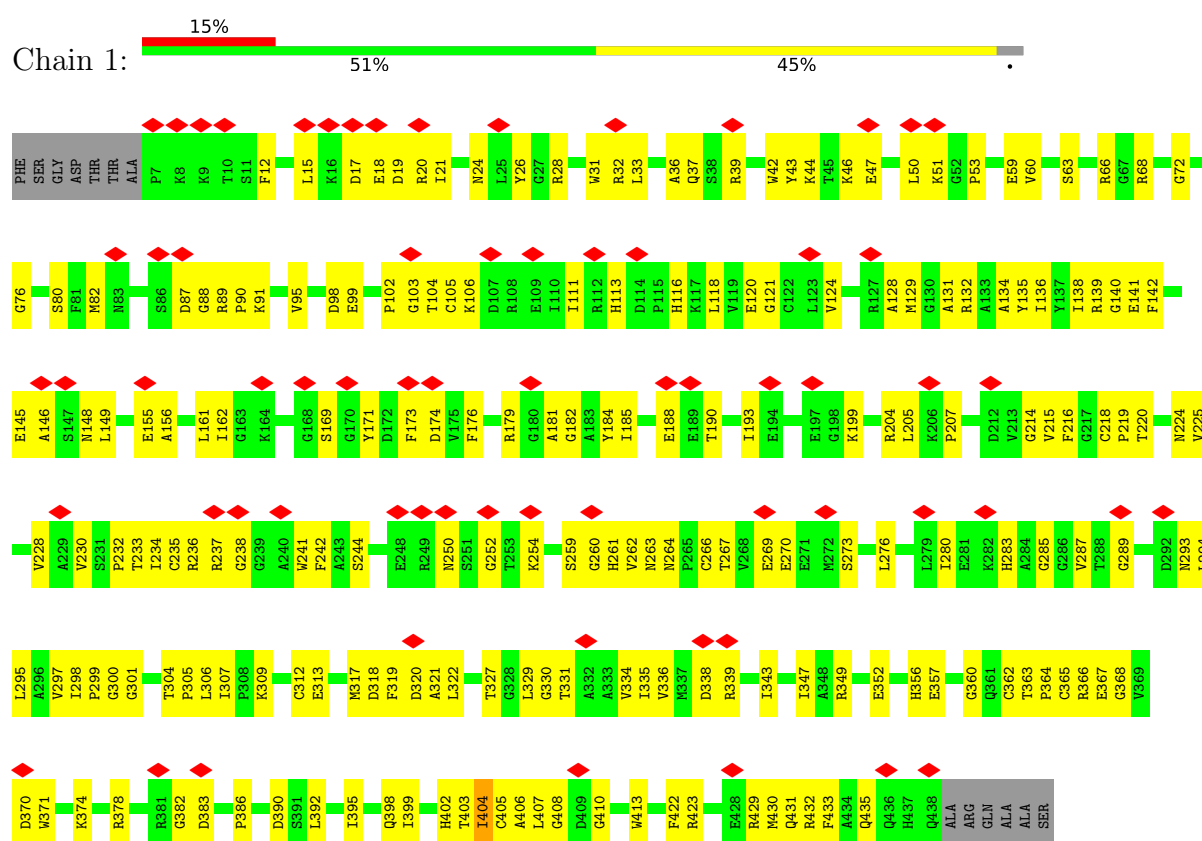


Mol	Chain	Residues	Atoms						AltConf
54	X	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	

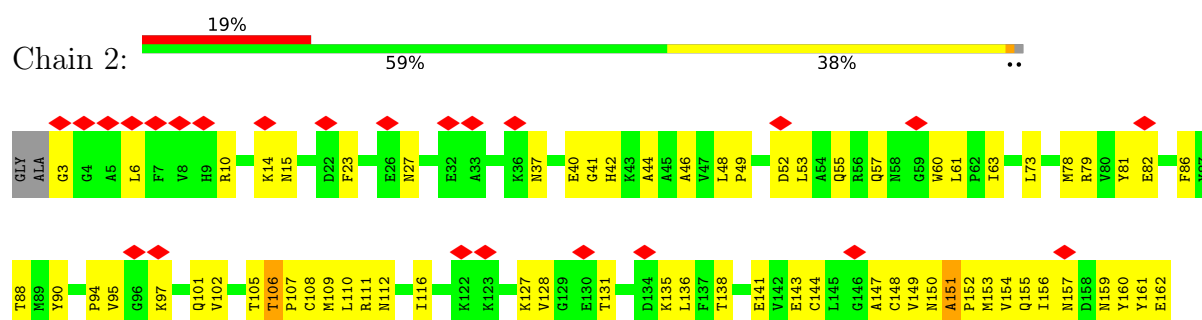
3 Residue-property plots

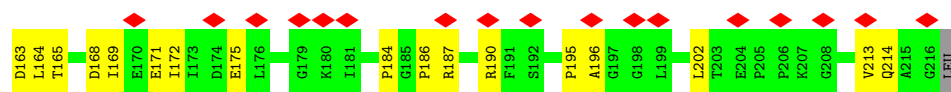
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Mitochondrial complex I, 51 kDa subunit

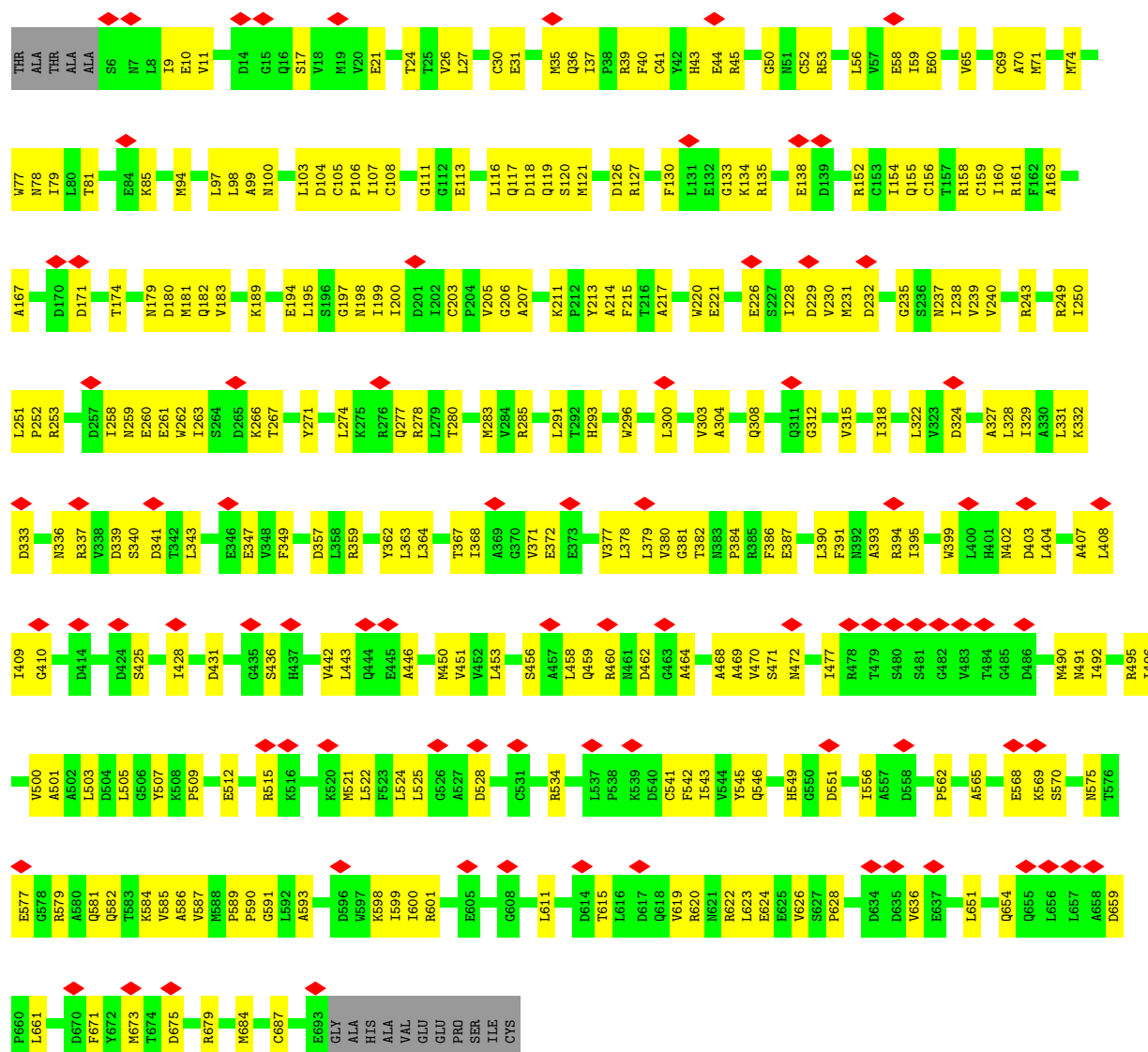


- Molecule 2: Mitochondrial complex I, 24 kDa subunit

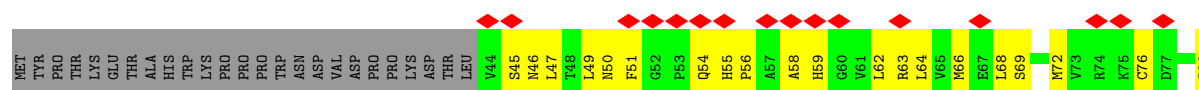


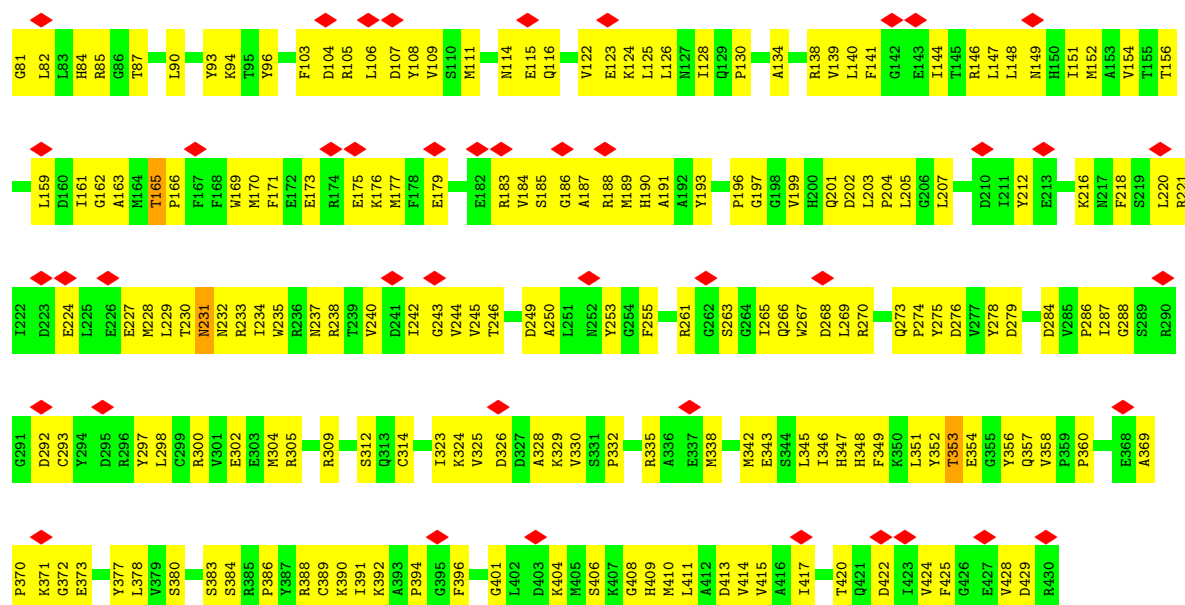


• Molecule 3: Mitochondrial complex I, 75 kDa subunit

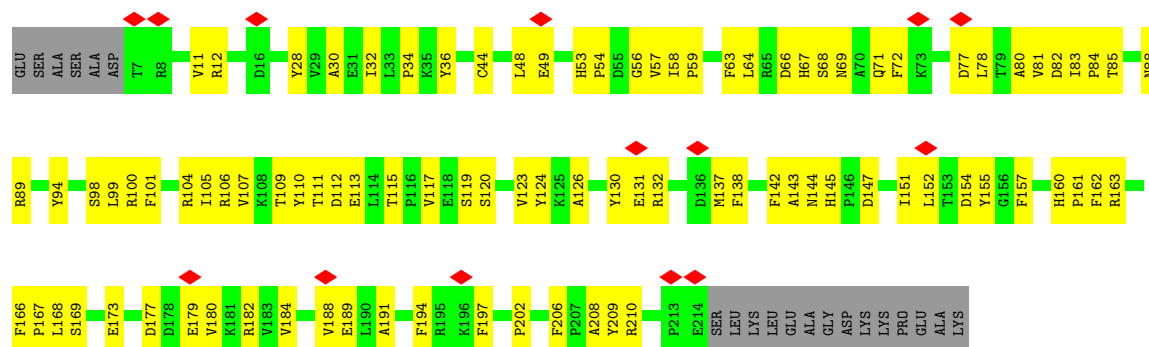


• Molecule 4: Mitochondrial complex I, 49 kDa subunit

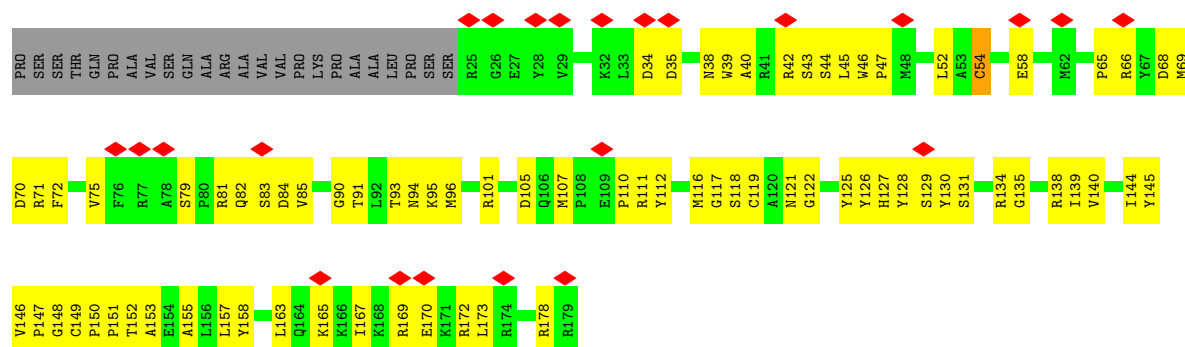




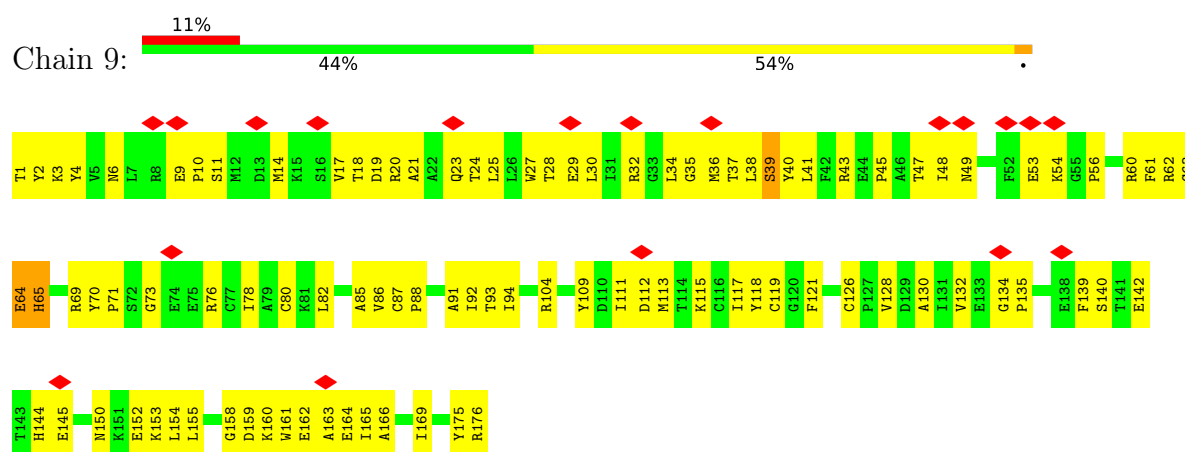
• Molecule 5: Mitochondrial complex I, 30 kDa subunit



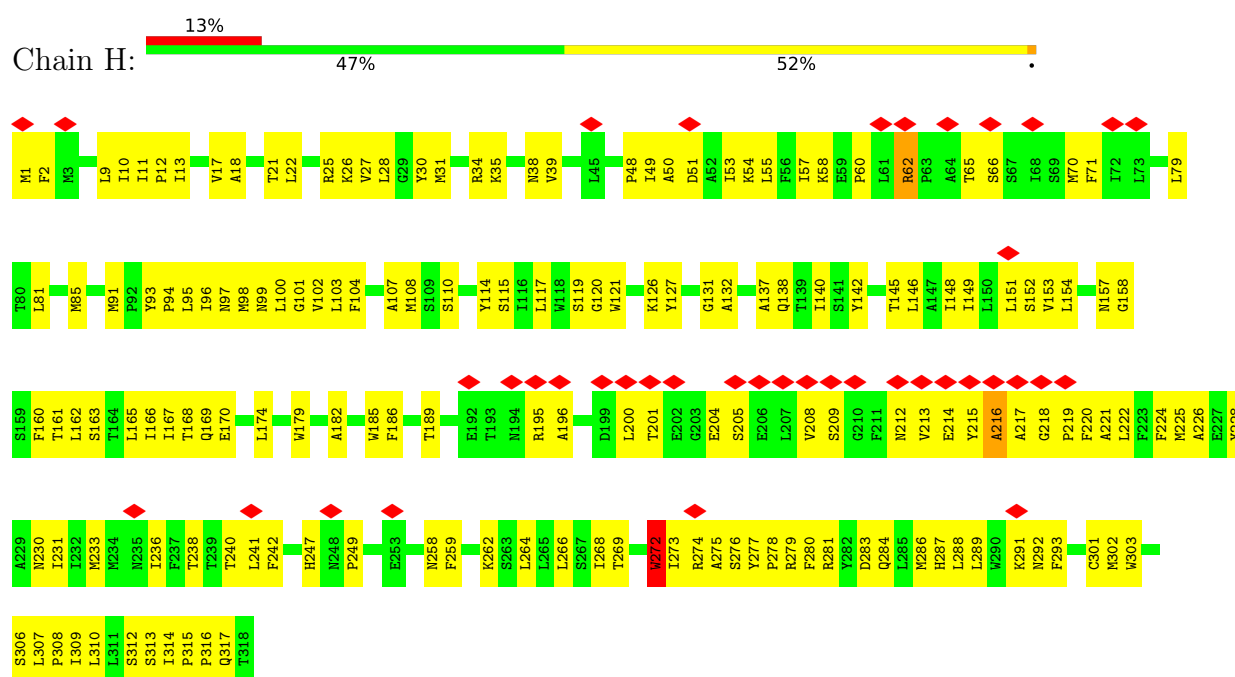
• Molecule 6: Mitochondrial complex I, PSST subunit



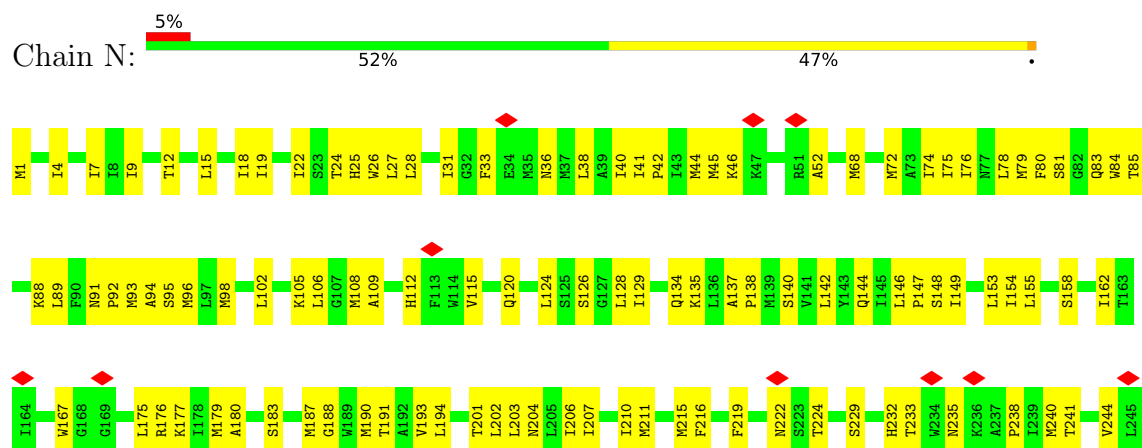
• Molecule 7: Mitochondrial complex I, TYKY subunit

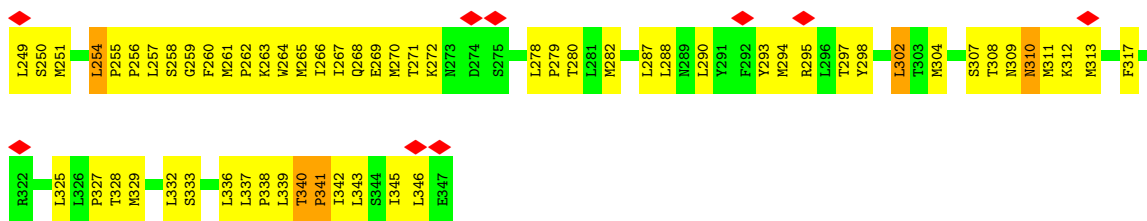


• Molecule 8: Mitochondrial complex I, ND1 subunit

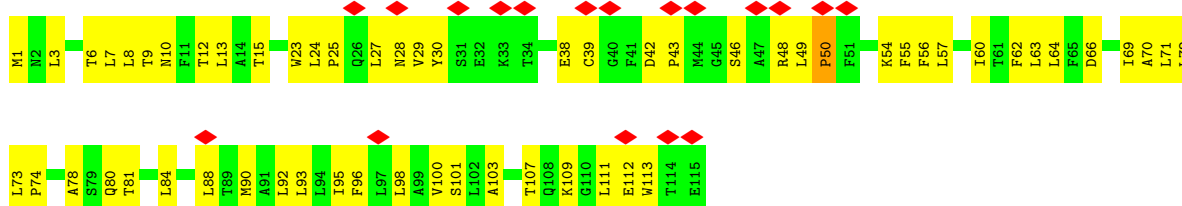


• Molecule 9: Mitochondrial complex I, ND2 subunit

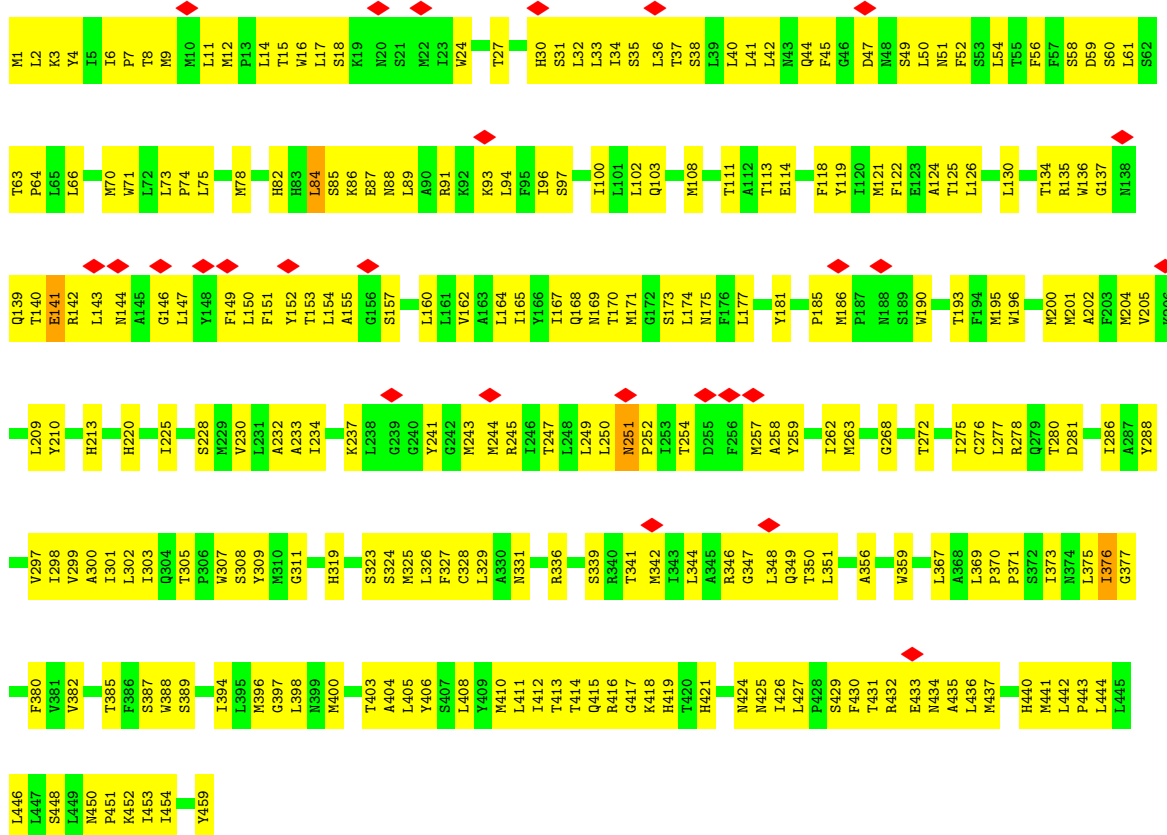




• Molecule 10: Mitochondrial complex I, ND3 subunit



• Molecule 11: Mitochondrial complex I, ND4 subunit

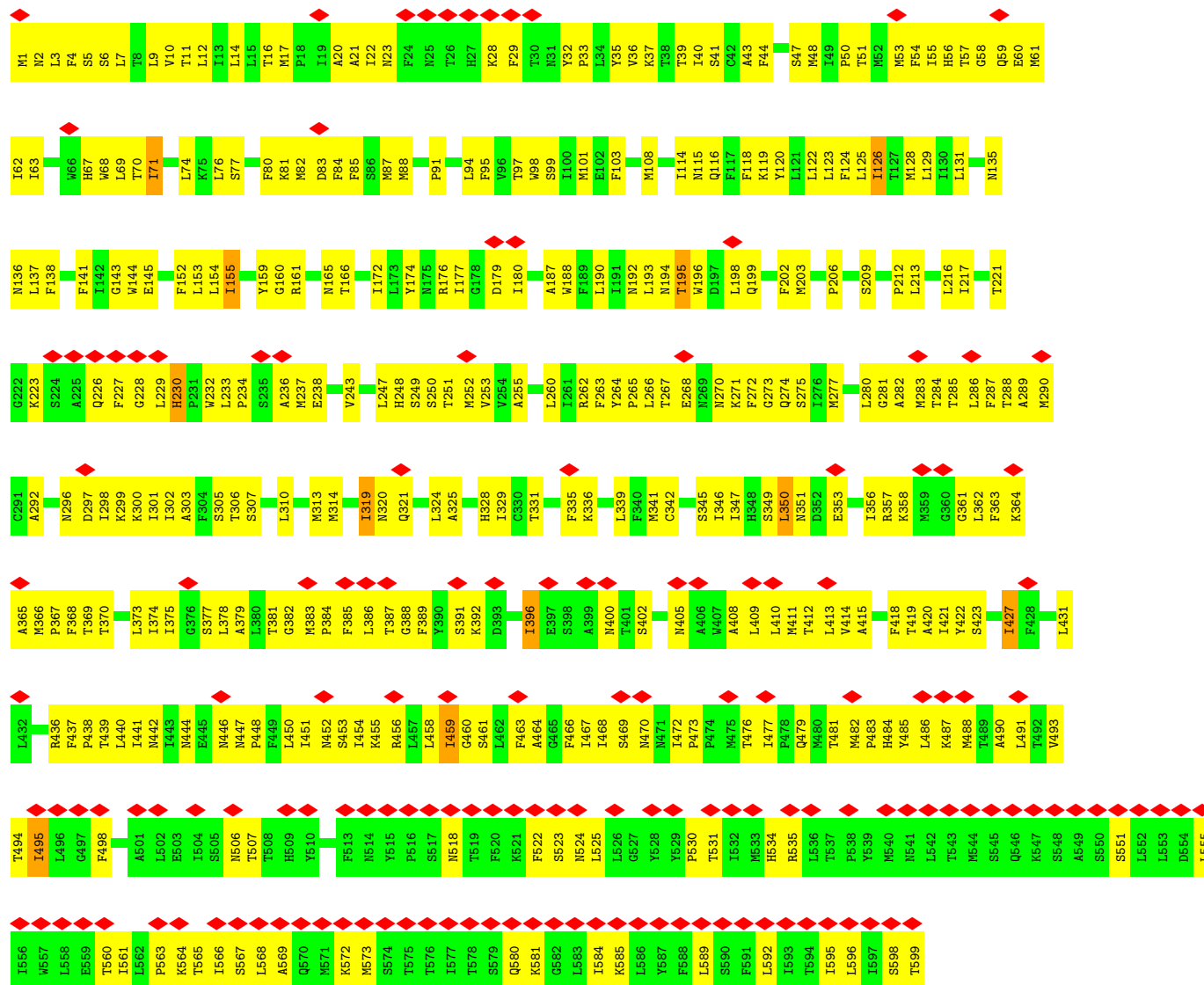


• Molecule 12: Mitochondrial complex I, ND4L subunit

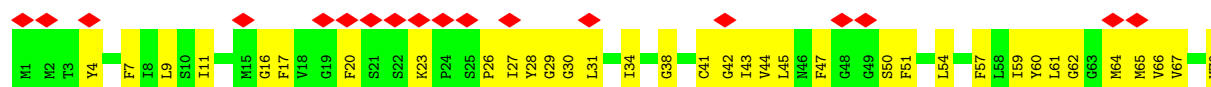


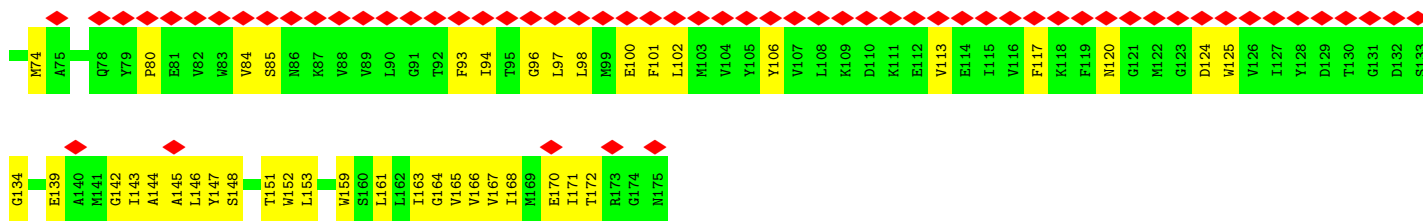


• Molecule 13: Mitochondrial complex I, ND5 subunit

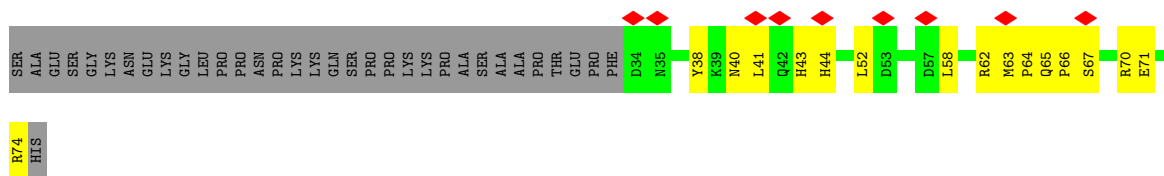
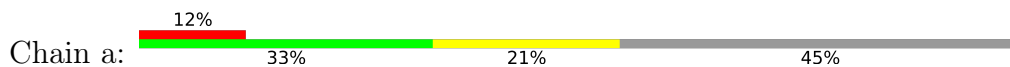


• Molecule 14: Mitochondrial complex I, ND6 subunit

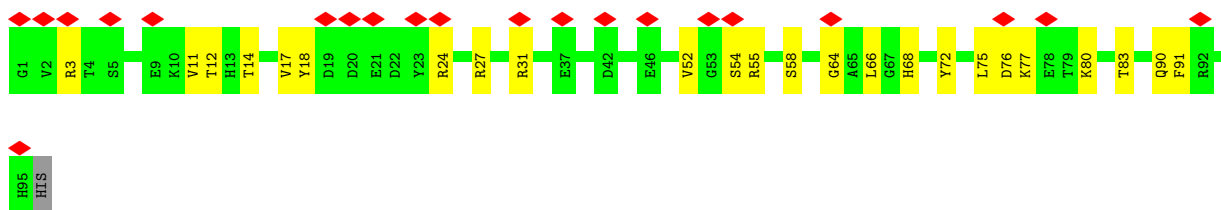
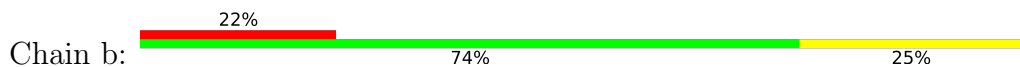




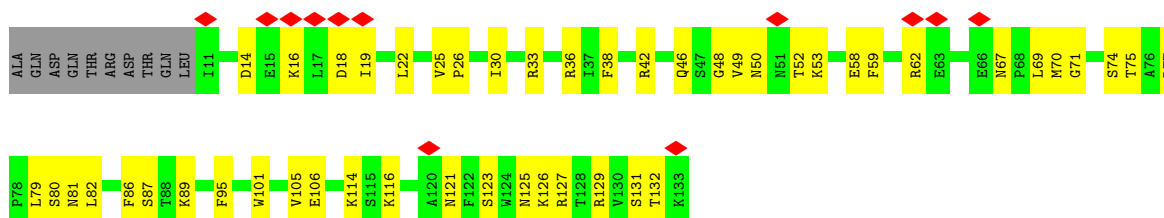
• Molecule 15: Mitochondrial complex I, 10 kDa subunit



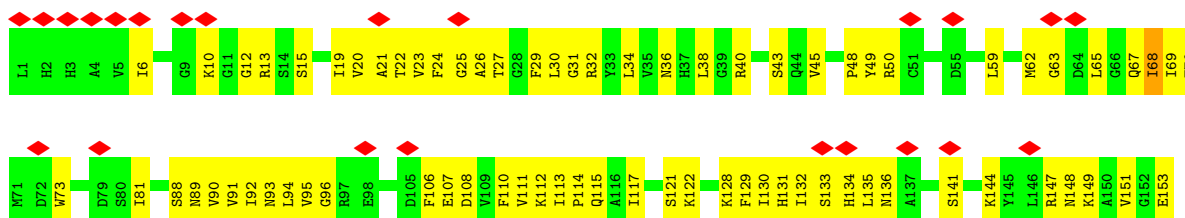
• Molecule 16: Mitochondrial complex I, 13 kDa subunit

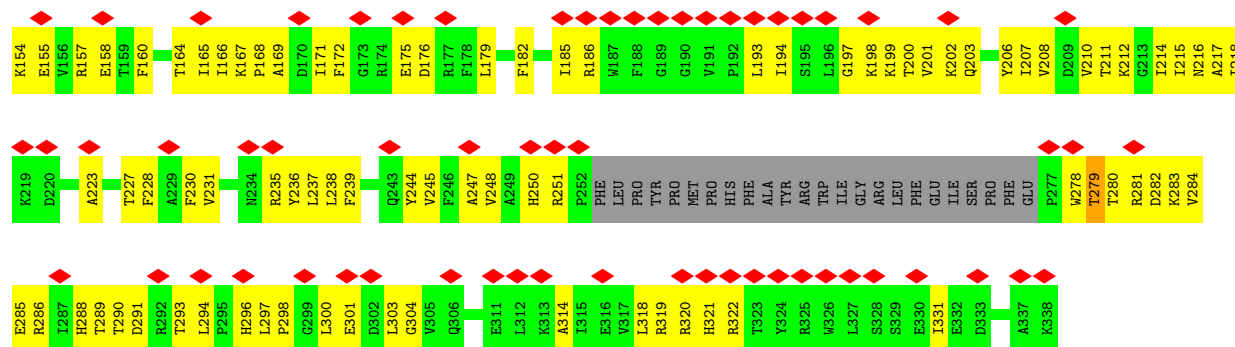


• Molecule 17: Mitochondrial complex I, 18 kDa subunit

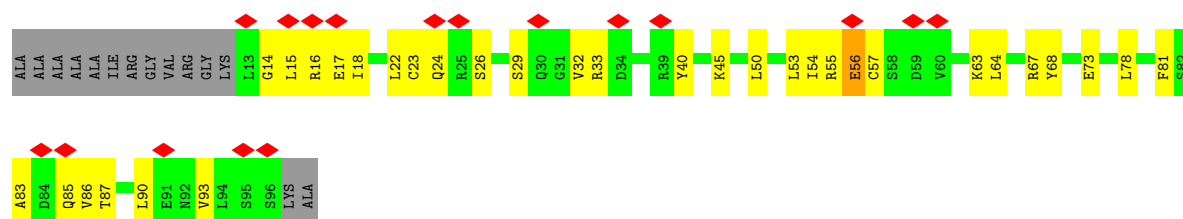


• Molecule 18: Mitochondrial complex I, 39 kDa subunit

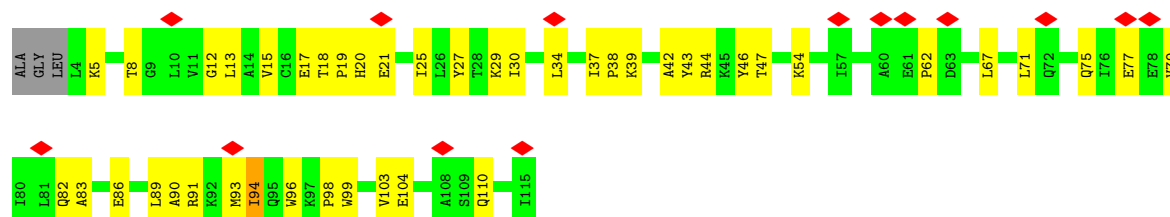




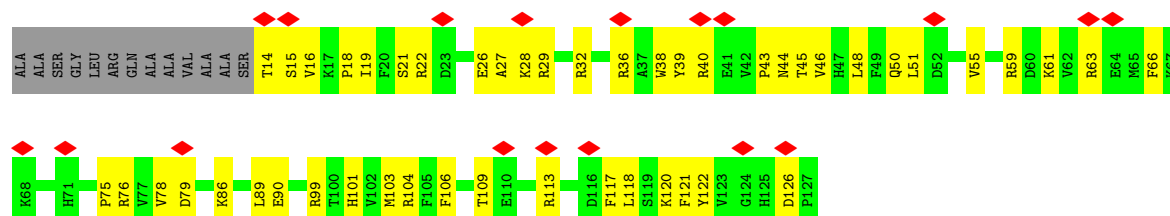
• Molecule 19: Mitochondrial complex I, B8 subunit



• Molecule 20: Mitochondrial complex I, B13 subunit

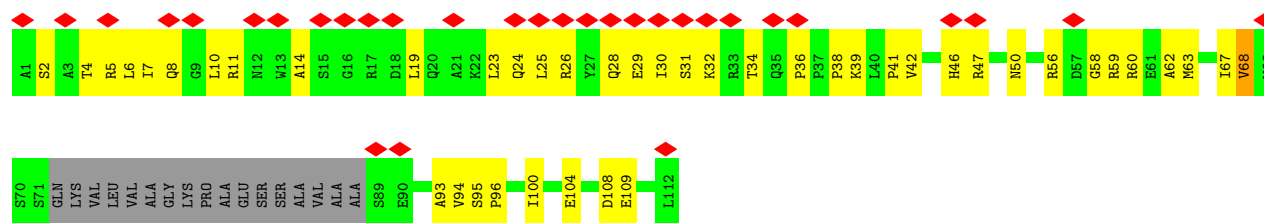


• Molecule 21: Mitochondrial complex I, B14 subunit

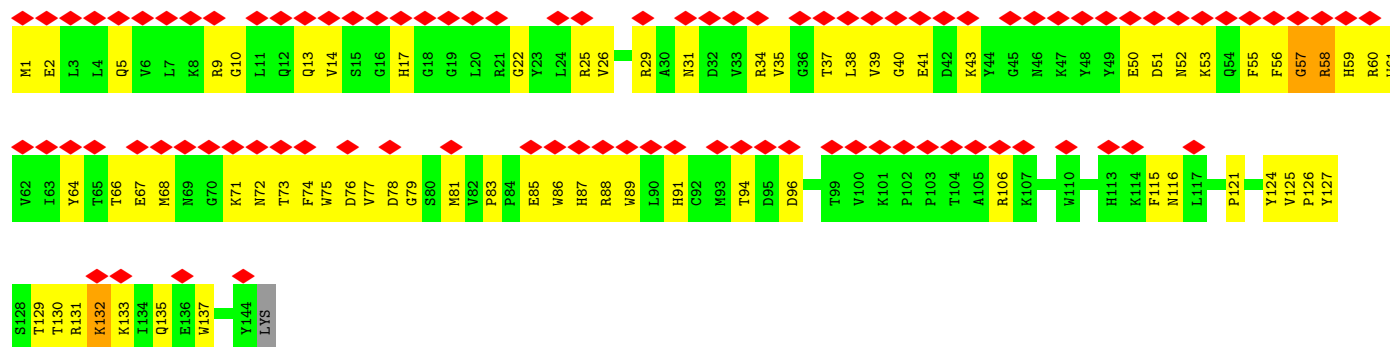


• Molecule 22: Mitochondrial complex I, B14.5a subunit

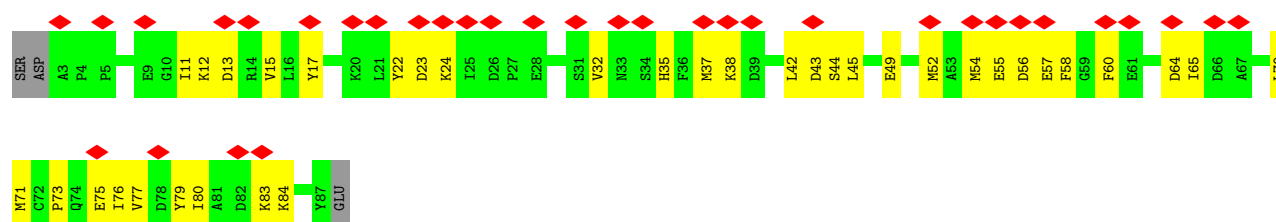
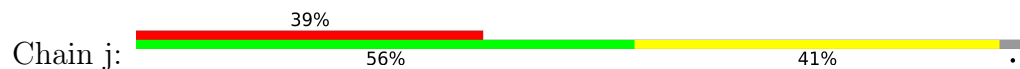




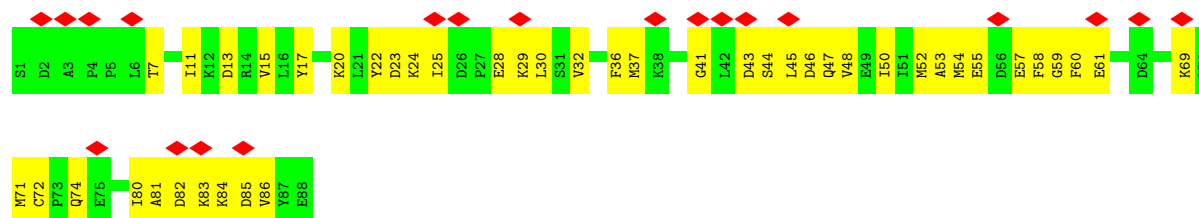
• Molecule 23: Mitochondrial complex I, B17.2 subunit



• Molecule 24: Acyl carrier protein

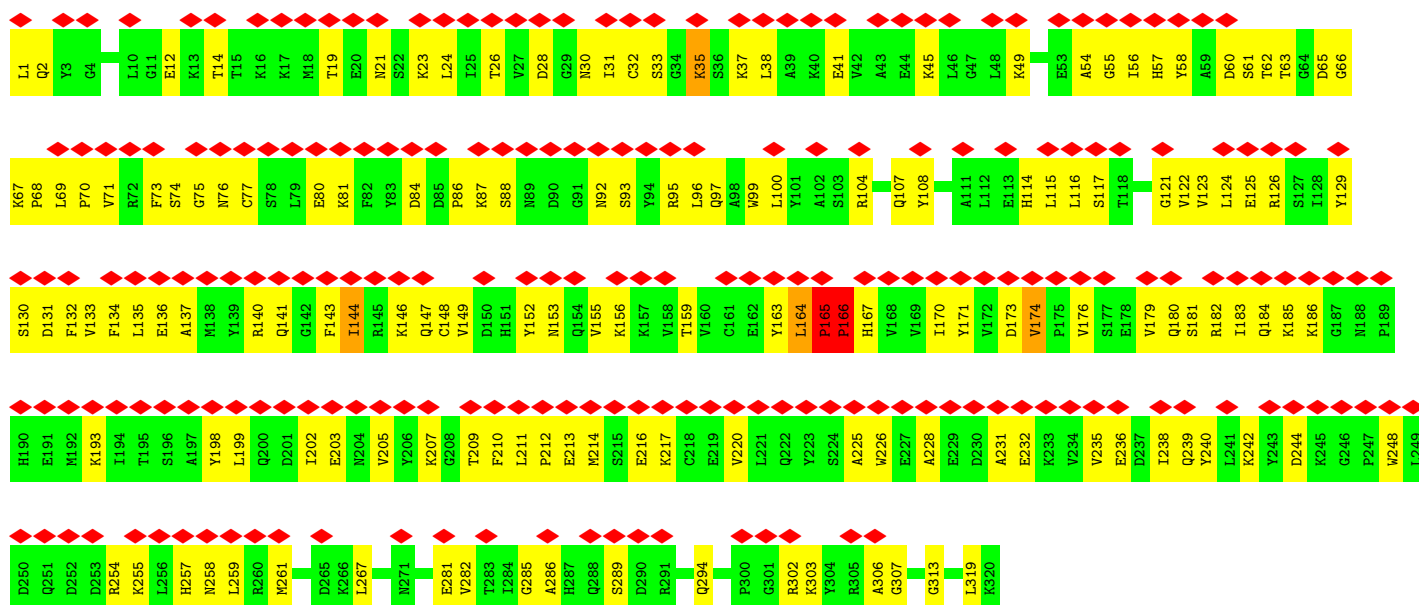


• Molecule 24: Acyl carrier protein

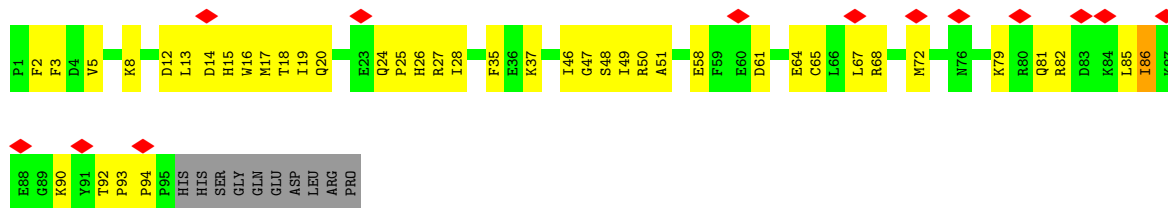


• Molecule 25: Mitochondrial complex I, 42 kDa subunit

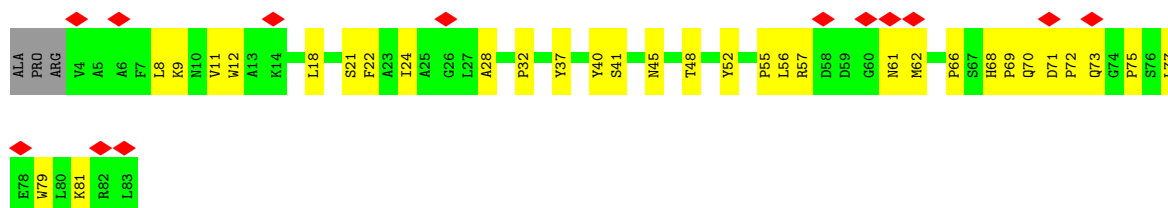




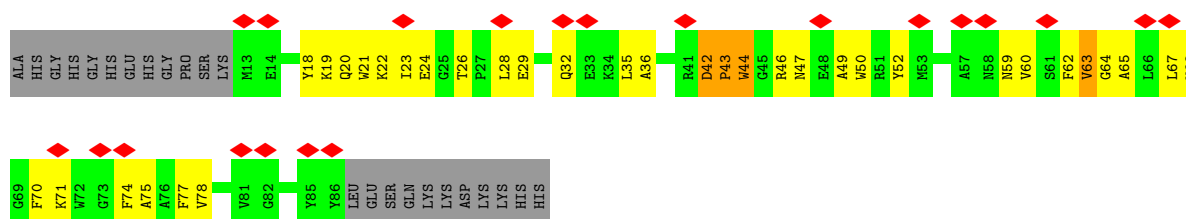
• Molecule 26: Mitochondrial complex I, 15 kDa subunit



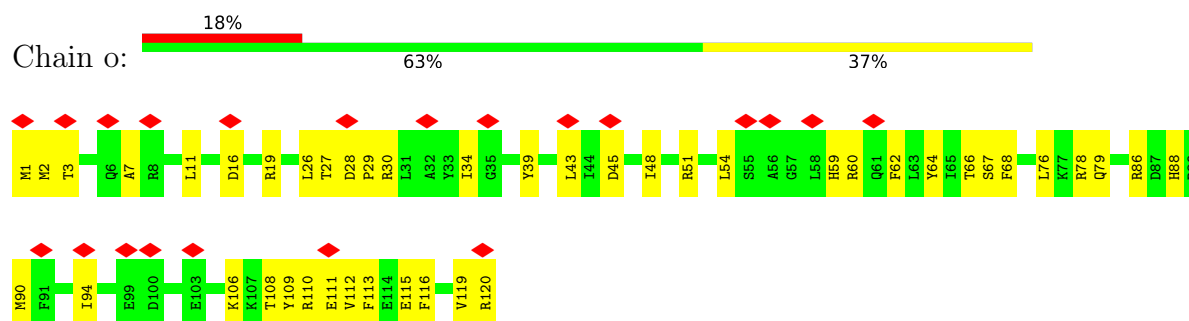
• Molecule 27: Mitochondrial complex I, B9 subunit



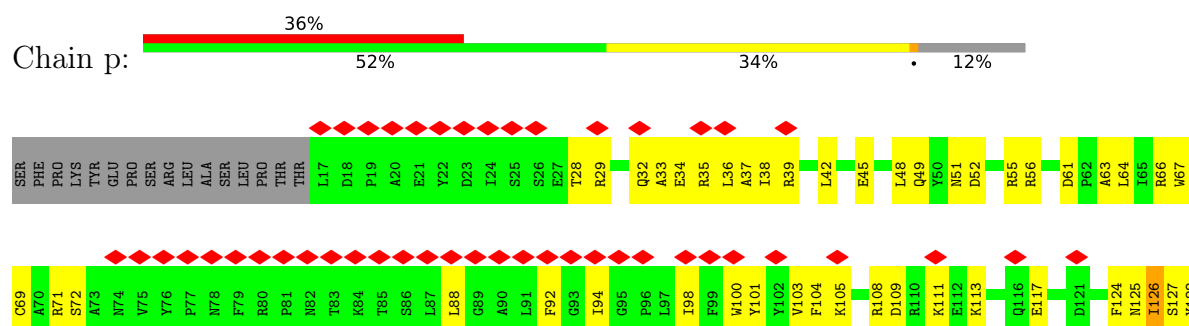
• Molecule 28: Mitochondrial complex I, B12 subunit



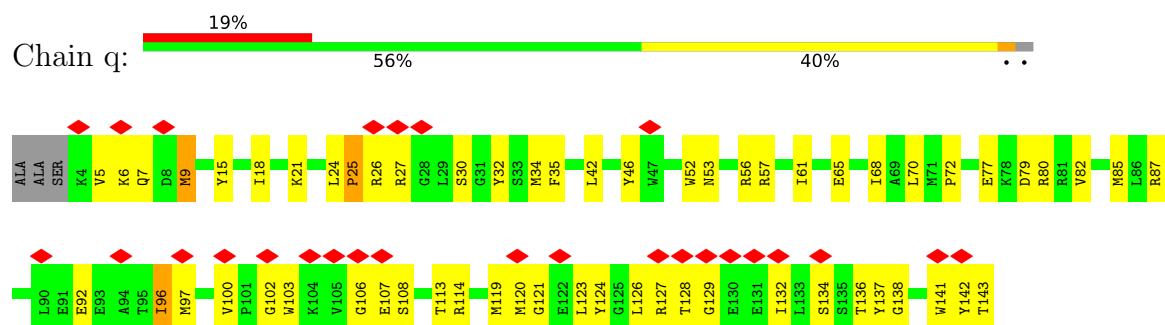
- Molecule 29: Mitochondrial complex I, B14.5b subunit



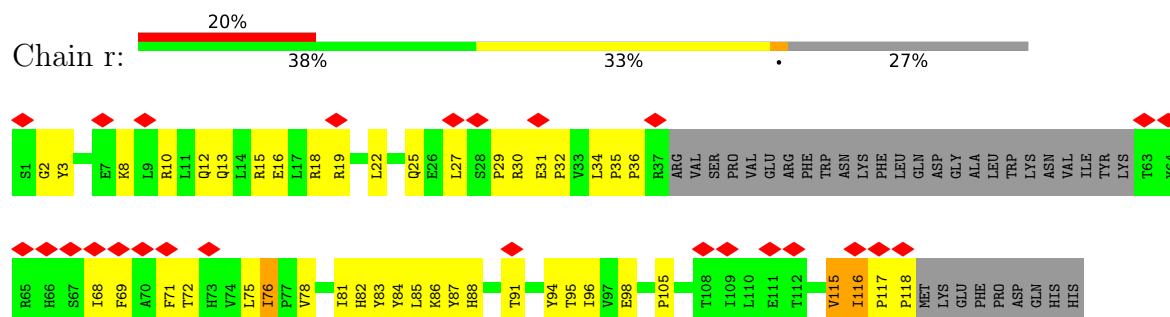
- Molecule 30: Mitochondrial complex I, B15 subunit



- Molecule 31: Mitochondrial complex I, B16.6 subunit

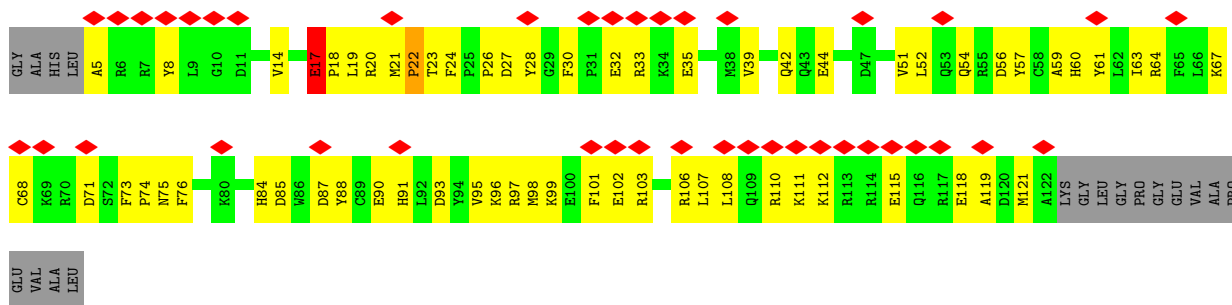


- Molecule 32: Mitochondrial complex I, B17 subunit

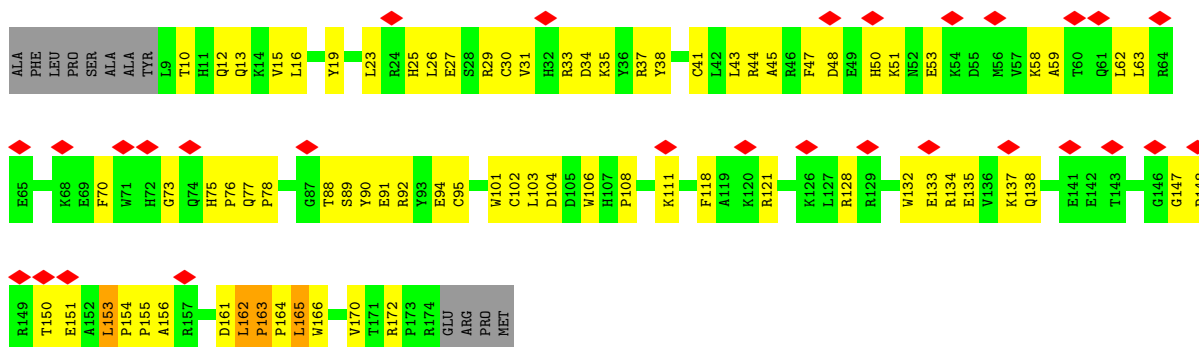


- Molecule 33: Mitochondrial complex I, B18 subunit

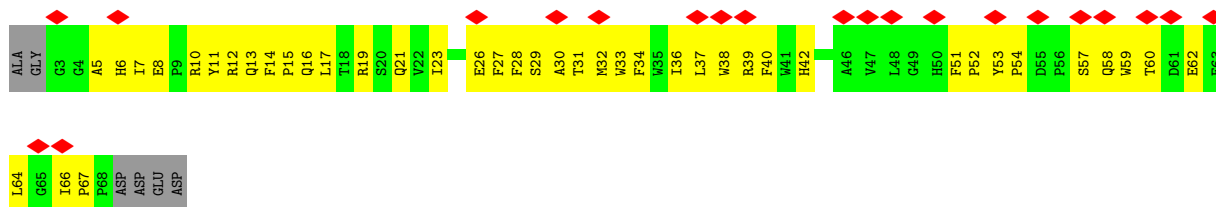




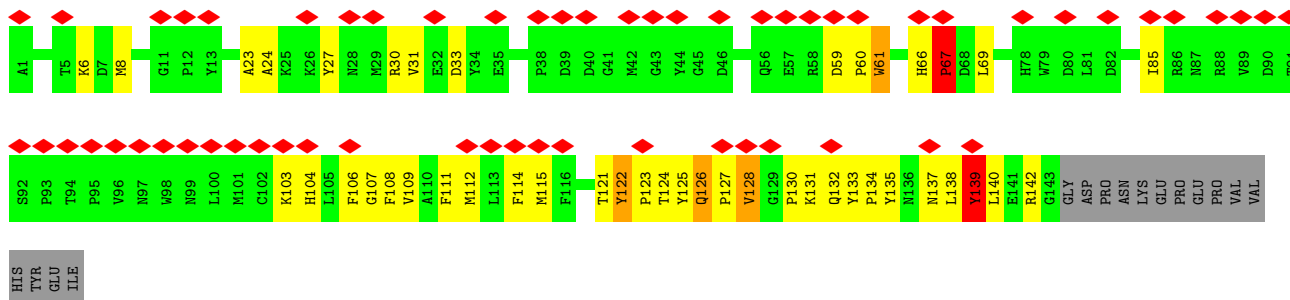
• Molecule 34: Mitochondrial complex I, B22 subunit



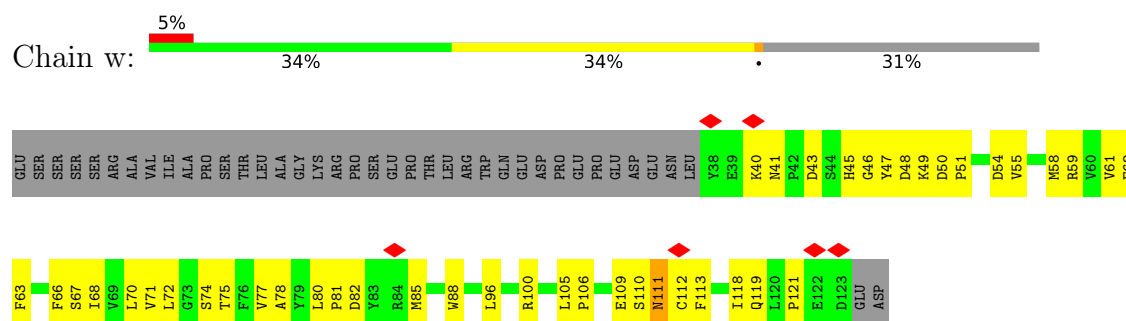
• Molecule 35: Mitochondrial complex I, AGGG subunit



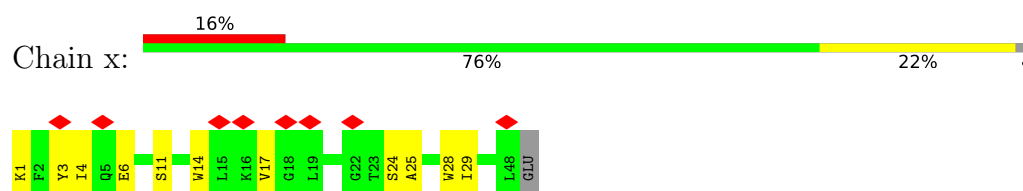
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



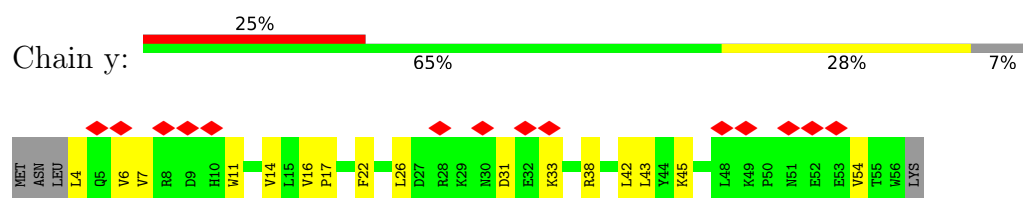
- Molecule 37: Mitochondrial complex I, ESSS subunit



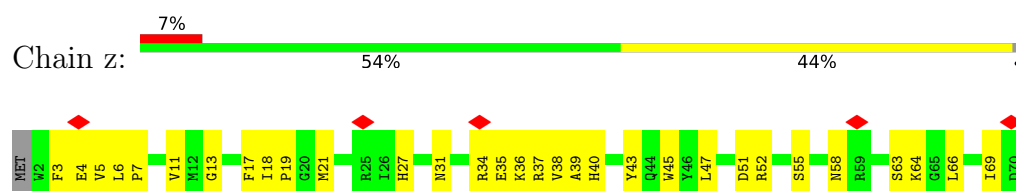
- Molecule 38: Mitochondrial complex I, KFYI subunit



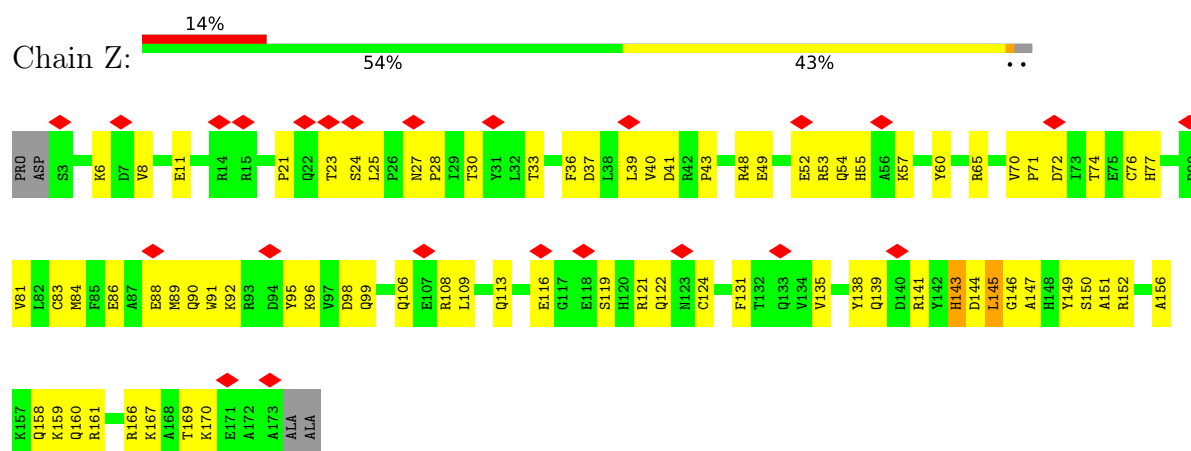
- Molecule 39: Mitochondrial complex I, MNLL subunit



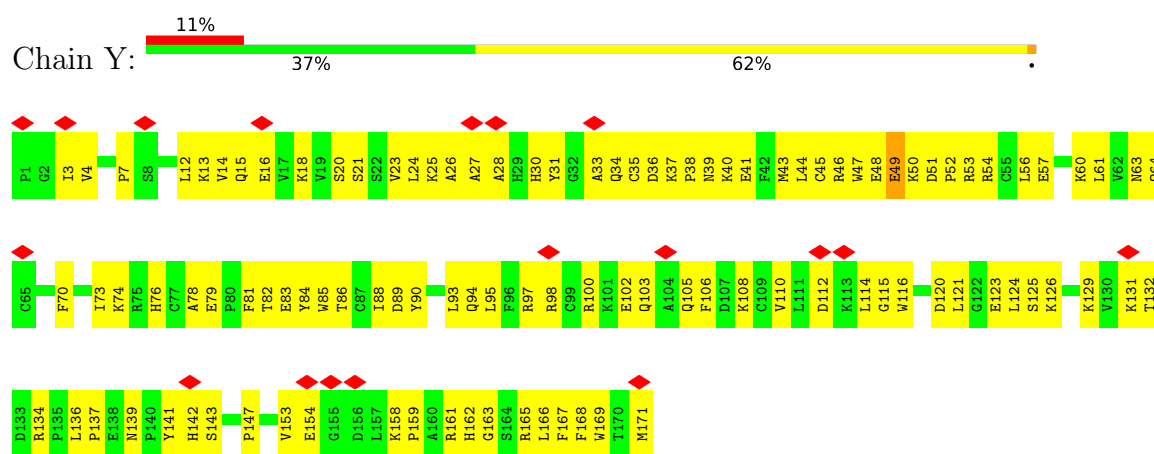
- Molecule 40: Mitochondrial complex I, MWFE subunit



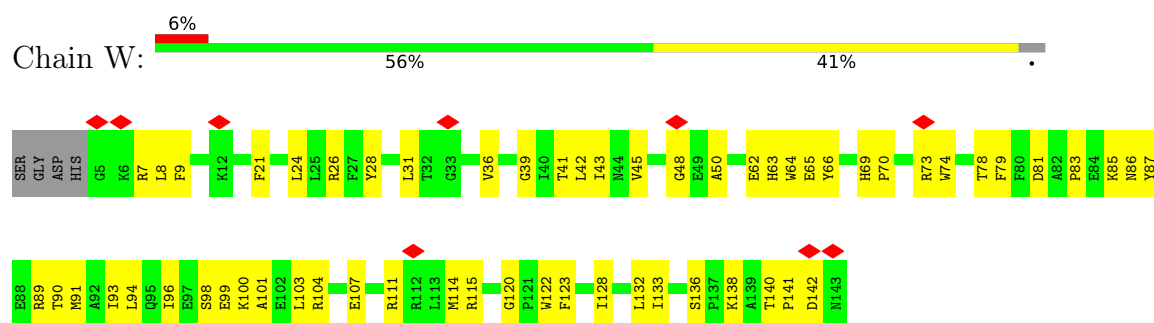
- Molecule 41: Mitochondrial complex I, PDSW subunit



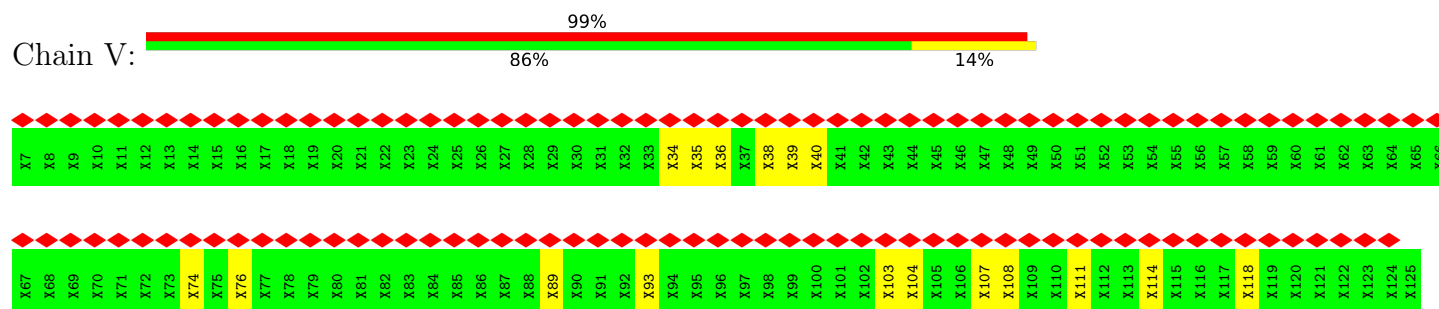
- Molecule 42: Mitochondrial complex I, PGIV subunit



• Molecule 43: Mitochondrial complex I, SGD1 subunit



• Molecule 44: Mitochondrial complex I, B14.7 subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82000	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 ($e^-/\text{\AA}^2$)	26	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	100720	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.314	Depositor
Minimum map value	-0.549	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	179.31, 195.99, 290.51	wwPDB
Map dimensions	209, 141, 129	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.3900001	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, PNS, ZN, 3PE, NDP, CDL, FMN, SF4, FES, ZMP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1	0.24	0/3403	0.48	0/4597
2	2	0.25	0/1695	0.54	0/2305
3	3	0.26	0/5362	0.48	0/7266
4	4	0.32	0/3172	0.57	1/4288 (0.0%)
5	5	0.30	0/1776	0.50	0/2417
6	6	0.33	0/1272	0.56	0/1720
7	9	0.36	0/1445	0.69	3/1956 (0.2%)
8	H	0.36	0/2603	0.65	2/3561 (0.1%)
9	N	0.38	1/2787 (0.0%)	0.64	3/3795 (0.1%)
10	A	0.35	0/947	0.59	0/1296
11	M	0.34	0/3739	0.61	0/5095
12	K	0.34	0/658	0.54	0/888
13	L	0.32	0/4563	0.63	0/6227
14	J	0.31	0/1212	0.64	2/1652 (0.1%)
15	a	0.18	0/352	0.59	0/476
16	b	0.30	0/749	0.46	0/1009
17	c	0.29	0/1023	0.53	0/1382
18	d	0.25	0/2532	0.61	0/3430
19	e	0.36	1/688 (0.1%)	0.52	0/927
20	f	0.23	0/929	0.52	0/1260
21	g	0.26	0/993	0.49	0/1336
22	h	0.23	0/775	0.61	0/1048
23	i	0.21	0/1241	0.54	0/1687
24	X	0.24	0/719	0.58	1/971 (0.1%)
24	j	0.20	0/696	0.46	0/940
25	k	0.25	1/2309 (0.0%)	0.75	6/3141 (0.2%)
26	l	0.29	0/811	0.58	0/1085
27	m	0.25	0/647	0.45	0/890
28	n	0.25	0/595	0.72	0/805
29	o	0.27	0/1035	0.54	0/1398
30	p	0.23	0/855	0.59	0/1155
31	q	0.28	0/1180	0.69	0/1590

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	r	0.31	0/774	0.68	0/1058
33	s	0.25	0/1011	0.66	0/1356
34	t	0.32	1/1483 (0.1%)	0.62	0/2006
35	u	0.27	0/590	0.61	0/809
36	v	0.25	0/877	0.82	1/1208 (0.1%)
37	w	0.29	0/737	0.60	0/999
38	x	0.19	0/416	0.40	0/564
39	y	0.25	0/470	0.50	0/636
40	z	0.28	0/583	0.55	0/785
41	Z	0.29	0/1475	0.58	0/1989
42	Y	0.31	0/1440	0.70	0/1942
43	W	0.30	0/1188	0.56	0/1607
All	All	0.29	4/63807 (0.0%)	0.59	19/86552 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2	0	1
4	4	0	1
7	9	0	1
8	H	0	3
9	N	0	3
10	A	0	2
13	L	0	6
17	c	0	1
19	e	0	1
20	f	0	1
23	i	0	1
25	k	0	3
29	o	0	1
31	q	0	2
33	s	0	2
34	t	0	1
36	v	0	7
42	Y	0	1
All	All	0	38

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	e	50	LEU	C-N	-7.86	1.15	1.33
34	t	163	PRO	C-N	7.55	1.51	1.33
25	k	174	VAL	C-N	-6.77	1.18	1.33
9	N	304	MET	C-N	-5.64	1.16	1.33

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	k	164	LEU	CA-C-N	17.32	138.22	120.38
25	k	164	LEU	C-N-CA	17.32	138.22	120.38
25	k	165	PRO	N-CA-C	7.07	119.33	110.70
25	k	165	PRO	CA-C-N	6.76	128.29	119.84
25	k	165	PRO	C-N-CA	6.76	128.29	119.84

There are no chirality outliers.

5 of 38 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	151	ALA	Peptide
4	4	54	GLN	Peptide
7	9	64	GLU	Peptide
8	H	216	ALA	Peptide
8	H	62	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3328	0	3287	175	0
2	2	1655	0	1663	85	0
3	3	5275	0	5300	246	0
4	4	3098	0	3068	217	0
5	5	1726	0	1676	104	0
6	6	1241	0	1251	88	0
7	9	1414	0	1370	120	0
8	H	2528	0	2641	180	0
9	N	2723	0	2930	170	0
10	A	922	0	953	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	M	3645	0	3850	247	0
12	K	649	0	699	45	0
13	L	4456	0	4298	351	0
14	J	1188	0	1068	82	0
15	a	343	0	320	17	0
16	b	737	0	710	22	0
17	c	1000	0	997	61	0
18	d	2473	0	2461	156	0
19	e	677	0	686	30	0
20	f	909	0	947	41	0
21	g	969	0	980	45	0
22	h	757	0	771	54	0
23	i	1200	0	1169	70	0
24	X	707	0	700	35	0
24	j	684	0	682	26	0
25	k	2268	0	1995	125	0
26	l	792	0	798	55	0
27	m	626	0	635	31	0
28	n	578	0	558	40	0
29	o	1004	0	995	55	0
30	p	841	0	760	56	0
31	q	1151	0	1150	69	0
32	r	752	0	752	60	0
33	s	988	0	930	79	0
34	t	1434	0	1392	91	0
35	u	563	0	511	56	0
36	v	861	0	557	36	0
37	w	715	0	679	51	0
38	x	403	0	405	10	0
39	y	457	0	459	10	0
40	z	568	0	558	34	0
41	Z	1441	0	1416	82	0
42	Y	1403	0	1384	123	0
43	W	1155	0	1177	67	0
44	V	595	0	127	9	0
45	1	8	0	0	2	0
45	3	16	0	0	2	0
45	6	8	0	0	2	0
45	9	16	0	0	4	0
46	1	31	0	19	8	0
47	2	4	0	0	0	0
47	3	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	9	51	0	82	10	0
48	J	51	0	82	6	0
48	o	87	0	128	8	0
49	A	47	0	71	5	0
49	M	46	0	66	2	0
49	N	46	0	66	3	0
49	o	39	0	55	3	0
50	J	79	0	108	1	0
50	L	84	0	118	13	0
50	M	82	0	114	3	0
50	i	58	0	60	1	0
51	b	1	0	0	0	0
52	d	48	0	26	8	0
53	j	34	0	40	3	0
54	X	21	0	21	8	0
All	All	63760	0	62771	3237	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 26.

The worst 5 of 3237 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:451:ILE:O	13:L:455:LYS:HB2	1.43	1.15
37:w:68:ILE:O	37:w:72:LEU:HB2	1.51	1.10
13:L:374:ILE:O	13:L:378:LEU:HB3	1.62	0.98
31:q:134:SER:O	31:q:138:GLY:HA3	1.64	0.98
11:M:254:THR:O	11:M:258:ALA:HB2	1.64	0.97

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	430/445 (97%)	405 (94%)	24 (6%)	1 (0%)	43	74
2	2	212/217 (98%)	189 (89%)	22 (10%)	1 (0%)	24	59
3	3	686/704 (97%)	616 (90%)	70 (10%)	0	100	100
4	4	385/412 (93%)	337 (88%)	46 (12%)	2 (0%)	24	59
5	5	206/228 (90%)	183 (89%)	23 (11%)	0	100	100
6	6	153/179 (86%)	138 (90%)	15 (10%)	0	100	100
7	9	174/176 (99%)	150 (86%)	24 (14%)	0	100	100
8	H	316/318 (99%)	278 (88%)	37 (12%)	1 (0%)	36	69
9	N	345/347 (99%)	315 (91%)	30 (9%)	0	100	100
10	A	113/115 (98%)	97 (86%)	15 (13%)	1 (1%)	14	47
11	M	457/459 (100%)	392 (86%)	64 (14%)	1 (0%)	43	74
12	K	84/98 (86%)	72 (86%)	12 (14%)	0	100	100
13	L	597/599 (100%)	518 (87%)	75 (13%)	4 (1%)	18	53
14	J	173/175 (99%)	142 (82%)	29 (17%)	2 (1%)	10	41
15	a	39/75 (52%)	33 (85%)	6 (15%)	0	100	100
16	b	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
17	c	121/133 (91%)	109 (90%)	12 (10%)	0	100	100
18	d	310/338 (92%)	253 (82%)	56 (18%)	1 (0%)	36	69
19	e	82/98 (84%)	74 (90%)	8 (10%)	0	100	100
20	f	110/115 (96%)	95 (86%)	15 (14%)	0	100	100
21	g	112/127 (88%)	102 (91%)	10 (9%)	0	100	100
22	h	91/112 (81%)	73 (80%)	17 (19%)	1 (1%)	11	43
23	i	142/145 (98%)	116 (82%)	24 (17%)	2 (1%)	9	38
24	X	86/88 (98%)	77 (90%)	9 (10%)	0	100	100
24	j	83/88 (94%)	70 (84%)	13 (16%)	0	100	100
25	k	318/320 (99%)	263 (83%)	50 (16%)	5 (2%)	7	36
26	l	93/105 (89%)	83 (89%)	10 (11%)	0	100	100
27	m	78/83 (94%)	72 (92%)	6 (8%)	0	100	100
28	n	72/97 (74%)	50 (69%)	18 (25%)	4 (6%)	1	16
29	o	118/120 (98%)	105 (89%)	13 (11%)	0	100	100
30	p	110/128 (86%)	83 (76%)	26 (24%)	1 (1%)	14	47
31	q	138/143 (96%)	126 (91%)	12 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	r	89/127 (70%)	75 (84%)	12 (14%)	2 (2%)	5	31
33	s	116/136 (85%)	93 (80%)	21 (18%)	2 (2%)	7	35
34	t	164/178 (92%)	142 (87%)	22 (13%)	0	100	100
35	u	64/72 (89%)	58 (91%)	6 (9%)	0	100	100
36	v	141/158 (89%)	103 (73%)	33 (23%)	5 (4%)	3	23
37	w	84/125 (67%)	67 (80%)	15 (18%)	2 (2%)	4	29
38	x	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
39	y	51/57 (90%)	50 (98%)	1 (2%)	0	100	100
40	z	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
41	Z	169/175 (97%)	147 (87%)	21 (12%)	1 (1%)	21	55
42	Y	169/171 (99%)	137 (81%)	32 (19%)	0	100	100
43	W	137/143 (96%)	115 (84%)	21 (15%)	1 (1%)	18	53
All	All	7824/8344 (94%)	6800 (87%)	984 (13%)	40 (0%)	26	59

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	106	THR
28	n	63	VAL
33	s	14	VAL
13	L	71	ILE
13	L	319	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	346/354 (98%)	346 (100%)	0	100	100
2	2	182/183 (100%)	182 (100%)	0	100	100
3	3	578/588 (98%)	578 (100%)	0	100	100
4	4	334/358 (93%)	334 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	5	189/204 (93%)	189 (100%)	0	100	100
6	6	131/150 (87%)	130 (99%)	1 (1%)	73	77
7	9	151/151 (100%)	150 (99%)	1 (1%)	76	78
8	H	278/278 (100%)	278 (100%)	0	100	100
9	N	315/315 (100%)	315 (100%)	0	100	100
10	A	103/103 (100%)	103 (100%)	0	100	100
11	M	412/412 (100%)	408 (99%)	4 (1%)	68	75
12	K	75/87 (86%)	75 (100%)	0	100	100
13	L	445/532 (84%)	439 (99%)	6 (1%)	61	71
14	J	101/144 (70%)	101 (100%)	0	100	100
15	a	40/68 (59%)	40 (100%)	0	100	100
16	b	79/80 (99%)	79 (100%)	0	100	100
17	c	110/119 (92%)	110 (100%)	0	100	100
18	d	257/292 (88%)	256 (100%)	1 (0%)	84	83
19	e	75/81 (93%)	75 (100%)	0	100	100
20	f	100/101 (99%)	99 (99%)	1 (1%)	68	75
21	g	107/113 (95%)	107 (100%)	0	100	100
22	h	83/94 (88%)	83 (100%)	0	100	100
23	i	130/131 (99%)	130 (100%)	0	100	100
24	X	81/81 (100%)	81 (100%)	0	100	100
24	j	78/81 (96%)	78 (100%)	0	100	100
25	k	199/284 (70%)	199 (100%)	0	100	100
26	l	85/94 (90%)	84 (99%)	1 (1%)	63	72
27	m	69/71 (97%)	69 (100%)	0	100	100
28	n	53/75 (71%)	53 (100%)	0	100	100
29	o	107/107 (100%)	107 (100%)	0	100	100
30	p	71/114 (62%)	71 (100%)	0	100	100
31	q	120/121 (99%)	119 (99%)	1 (1%)	73	77
32	r	80/121 (66%)	78 (98%)	2 (2%)	42	62
33	s	100/119 (84%)	100 (100%)	0	100	100
34	t	151/160 (94%)	149 (99%)	2 (1%)	61	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	u	58/62 (94%)	58 (100%)	0	100	100
36	v	38/142 (27%)	38 (100%)	0	100	100
37	w	77/112 (69%)	77 (100%)	0	100	100
38	x	43/44 (98%)	43 (100%)	0	100	100
39	y	49/53 (92%)	49 (100%)	0	100	100
40	z	58/59 (98%)	58 (100%)	0	100	100
41	Z	155/157 (99%)	154 (99%)	1 (1%)	78	80
42	Y	154/154 (100%)	154 (100%)	0	100	100
43	W	122/125 (98%)	122 (100%)	0	100	100
All	All	6569/7274 (90%)	6548 (100%)	21 (0%)	84	85

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	l	86	ILE
32	r	76	ILE
41	Z	145	LEU
34	t	153	LEU
32	r	34	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
19	e	75	ASN
26	l	24	GLN
41	Z	113	GLN
20	f	82	GLN
25	k	50	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 1 is monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
48	3PE	o	202	-	40,40,50	0.36	0	43,45,55	0.36	0
45	SF4	1	500	1	0,12,12	-	-	-		
48	3PE	J	301	-	50,50,50	0.31	0	53,55,55	0.33	0
45	SF4	3	802	3	0,12,12	-	-	-		
49	PC1	A	200	-	46,46,53	0.32	0	52,54,61	0.36	0
48	3PE	9	501	-	50,50,50	0.31	0	53,55,55	0.42	0
54	PNS	X	401	24	14,20,21	0.45	0	18,26,29	0.89	1 (5%)
45	SF4	9	503	7	0,12,12	-	-	-		
46	FMN	1	501	-	33,33,33	0.26	0	48,50,50	0.38	0
49	PC1	N	401	-	45,45,53	0.31	0	51,53,61	0.36	0
47	FES	2	300	2	0,4,4	-	-	-		
49	PC1	M	501	-	45,45,53	0.31	0	51,53,61	0.36	0
47	FES	3	803	3	0,4,4	-	-	-		
49	PC1	o	201	-	38,38,53	0.34	0	44,46,61	0.36	0
50	CDL	L	601	-	83,83,99	0.32	0	89,95,111	0.41	0
50	CDL	M	502	-	81,81,99	0.33	0	87,93,111	0.38	0
45	SF4	6	300	6	0,12,12	-	-	-		
52	NDP	d	401	-	51,52,52	0.42	0	71,80,80	0.51	0
53	ZMP	j	101	24	28,33,36	0.72	2 (7%)	32,40,45	1.11	1 (3%)
48	3PE	o	203	-	45,45,50	0.33	0	48,50,55	0.40	0
45	SF4	3	801	3	0,12,12	-	-	-		
50	CDL	J	300	-	78,78,99	0.33	0	84,90,111	0.38	0
45	SF4	9	502	7	0,12,12	-	-	-		
50	CDL	i	201	-	57,57,99	0.38	0	63,69,111	0.39	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
48	3PE	o	202	-	-	8/44/44/54	-
48	3PE	J	301	-	-	6/54/54/54	-
49	PC1	A	200	-	-	16/50/50/57	-
45	SF4	1	500	1	-	-	0/6/5/5
54	PNS	X	401	24	-	8/24/26/27	-
48	3PE	9	501	-	-	13/54/54/54	-
45	SF4	3	802	3	-	-	0/6/5/5
45	SF4	9	503	7	-	-	0/6/5/5
46	FMN	1	501	-	-	7/18/18/18	0/3/3/3
49	PC1	N	401	-	-	11/49/49/57	-
47	FES	2	300	2	-	-	0/1/1/1
49	PC1	M	501	-	-	13/49/49/57	-
47	FES	3	803	3	-	-	0/1/1/1
49	PC1	o	201	-	-	10/42/42/57	-
50	CDL	L	601	-	-	24/94/94/110	-
50	CDL	M	502	-	-	22/92/92/110	-
45	SF4	6	300	6	-	-	0/6/5/5
52	NDP	d	401	-	-	8/34/77/77	0/5/5/5
53	ZMP	j	101	24	-	10/38/40/43	-
48	3PE	o	203	-	-	10/49/49/54	-
45	SF4	3	801	3	-	-	0/6/5/5
50	CDL	J	300	-	-	19/89/89/110	-
45	SF4	9	502	7	-	-	0/6/5/5
50	CDL	i	201	-	-	13/68/68/110	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	j	101	ZMP	C10-S1	-2.36	1.70	1.76
53	j	101	ZMP	C9-C10	2.09	1.53	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	j	101	ZMP	O1-C10-C9	-2.83	120.71	123.98
54	X	401	PNS	C37-C38-C39	-2.24	108.66	112.39

There are no chirality outliers.

5 of 198 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	1	501	FMN	C5'-O5'-P-O1P
46	1	501	FMN	C5'-O5'-P-O2P
48	9	501	3PE	C11-O13-P-O11
48	9	501	3PE	C11-O13-P-O14
48	9	501	3PE	O13-C11-C12-N

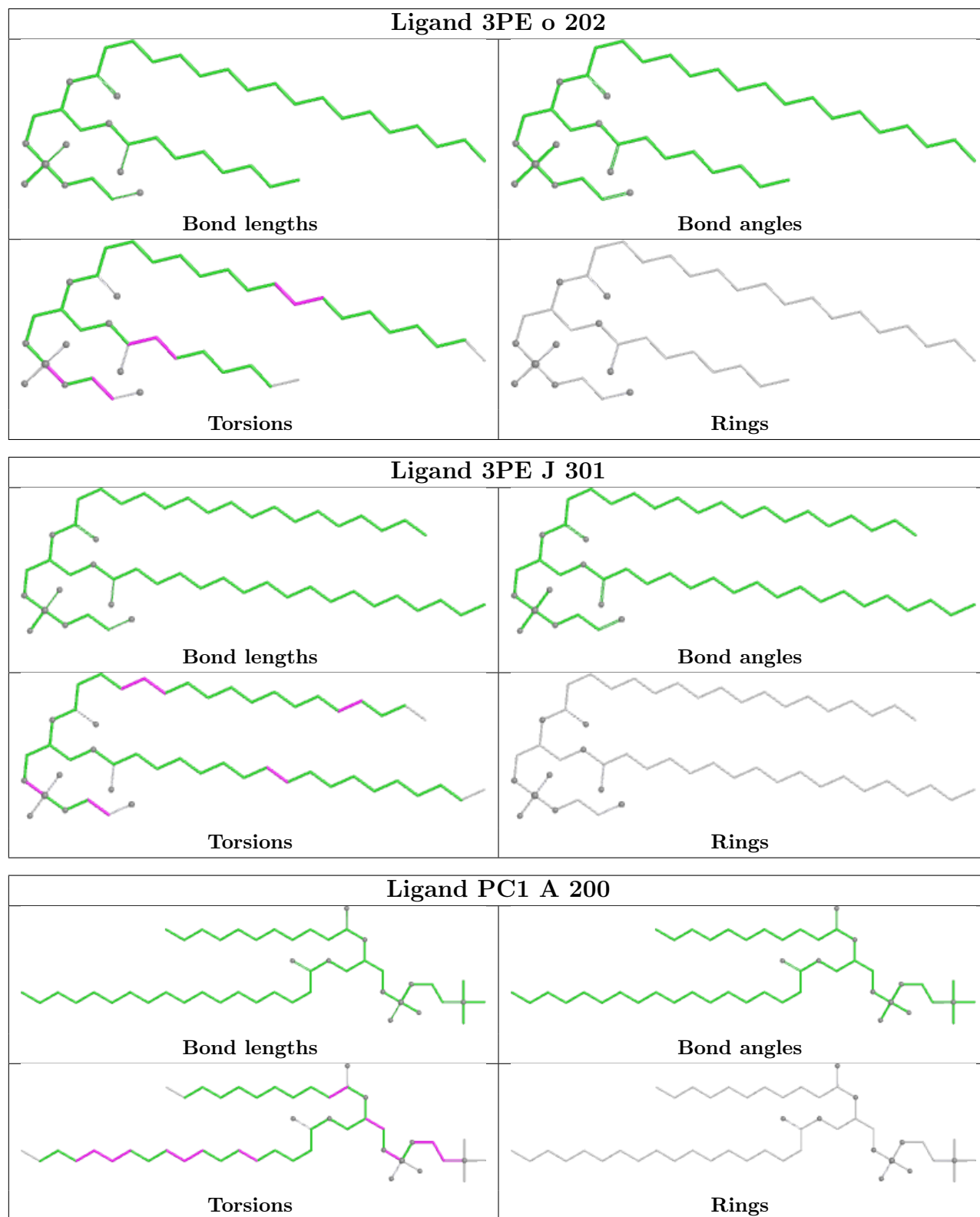
There are no ring outliers.

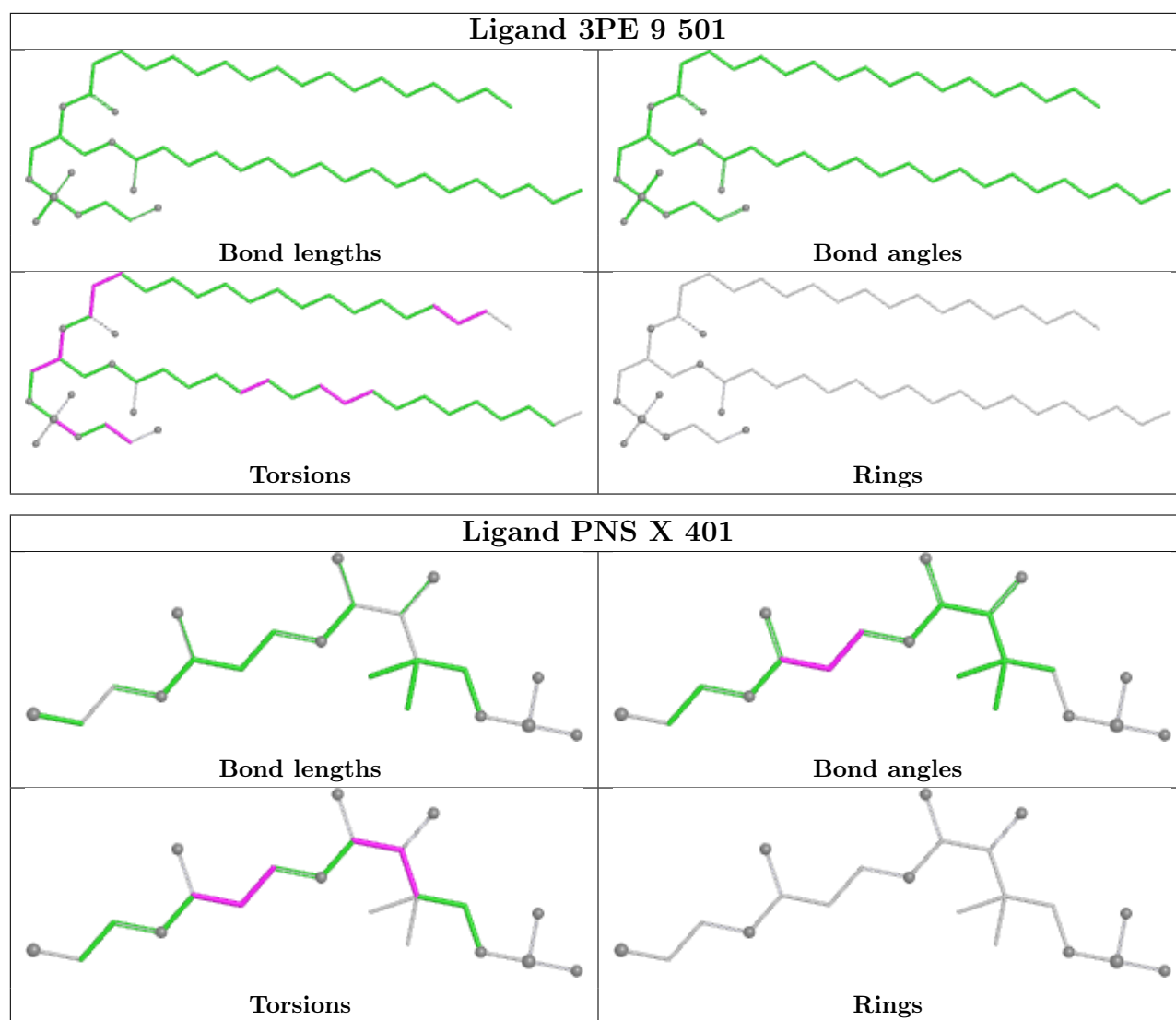
22 monomers are involved in 91 short contacts:

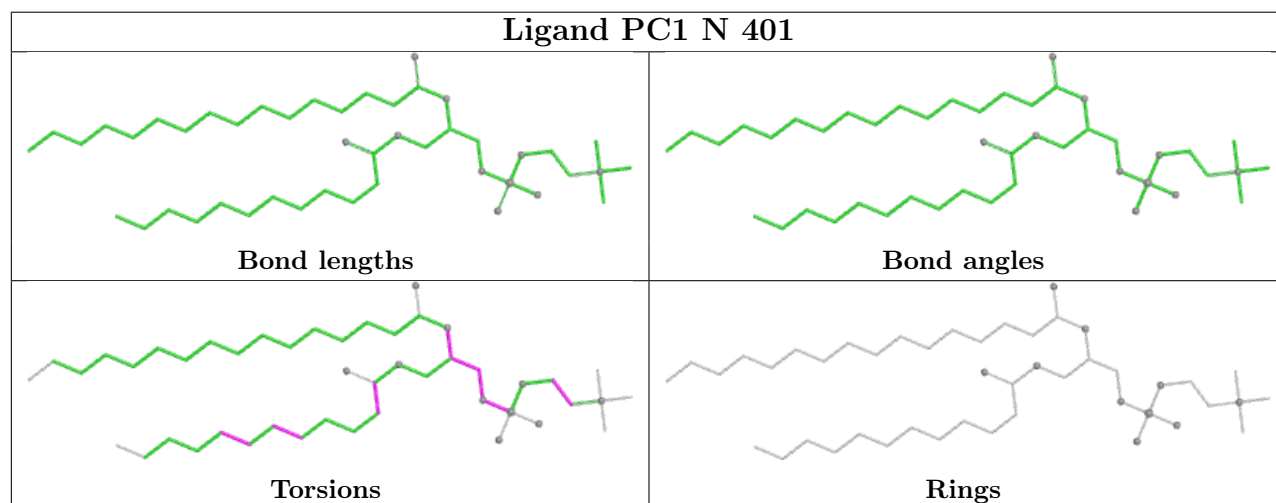
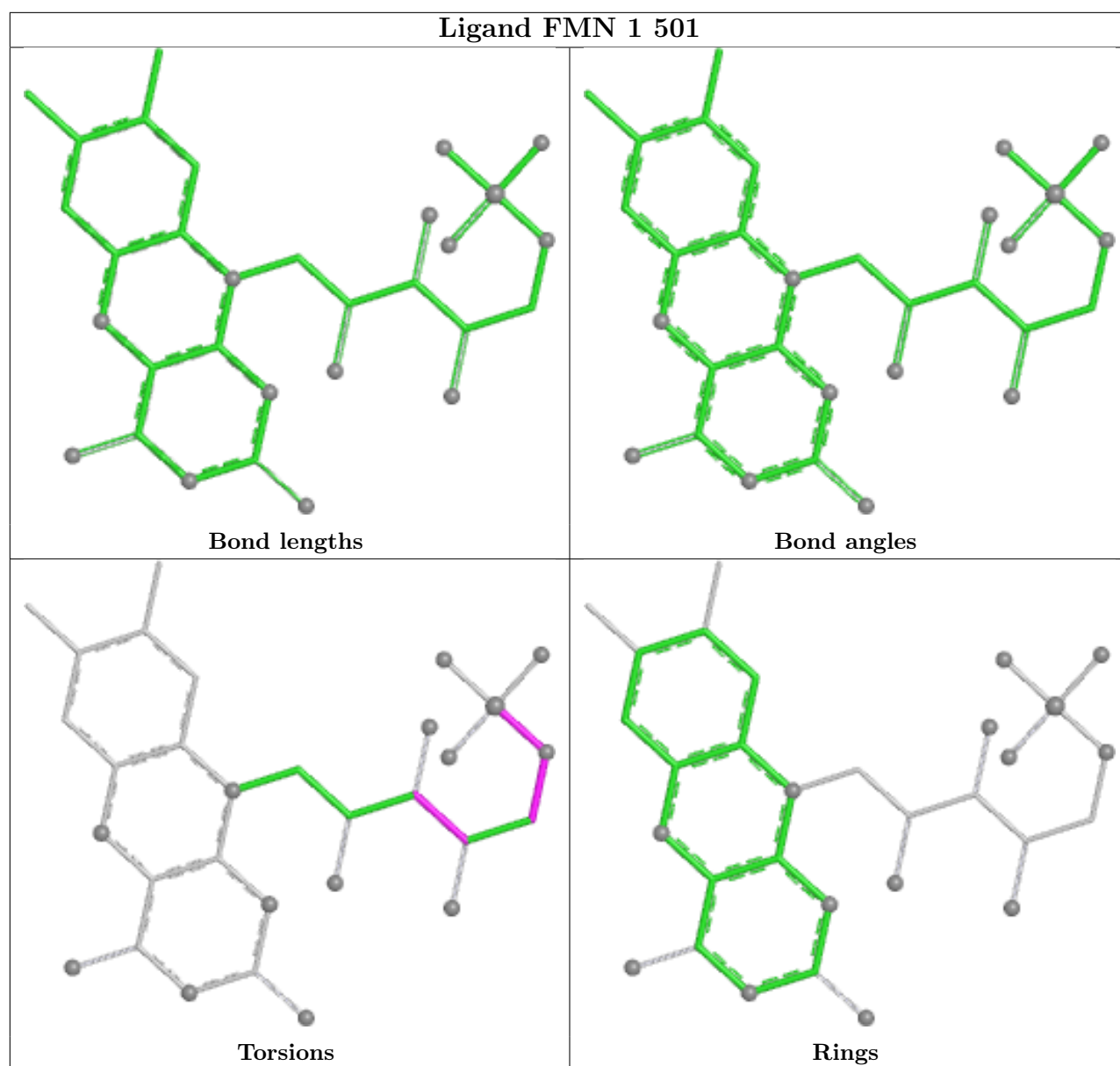
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	o	202	3PE	4	0
45	1	500	SF4	2	0
48	J	301	3PE	6	0
45	3	802	SF4	1	0
49	A	200	PC1	5	0
48	9	501	3PE	10	0
54	X	401	PNS	8	0
45	9	503	SF4	1	0
46	1	501	FMN	8	0
49	N	401	PC1	3	0
49	M	501	PC1	2	0
49	o	201	PC1	3	0
50	L	601	CDL	13	0
50	M	502	CDL	3	0
45	6	300	SF4	2	0
52	d	401	NDP	8	0
53	j	101	ZMP	3	0
48	o	203	3PE	4	0
45	3	801	SF4	1	0
50	J	300	CDL	1	0
45	9	502	SF4	3	0
50	i	201	CDL	1	0

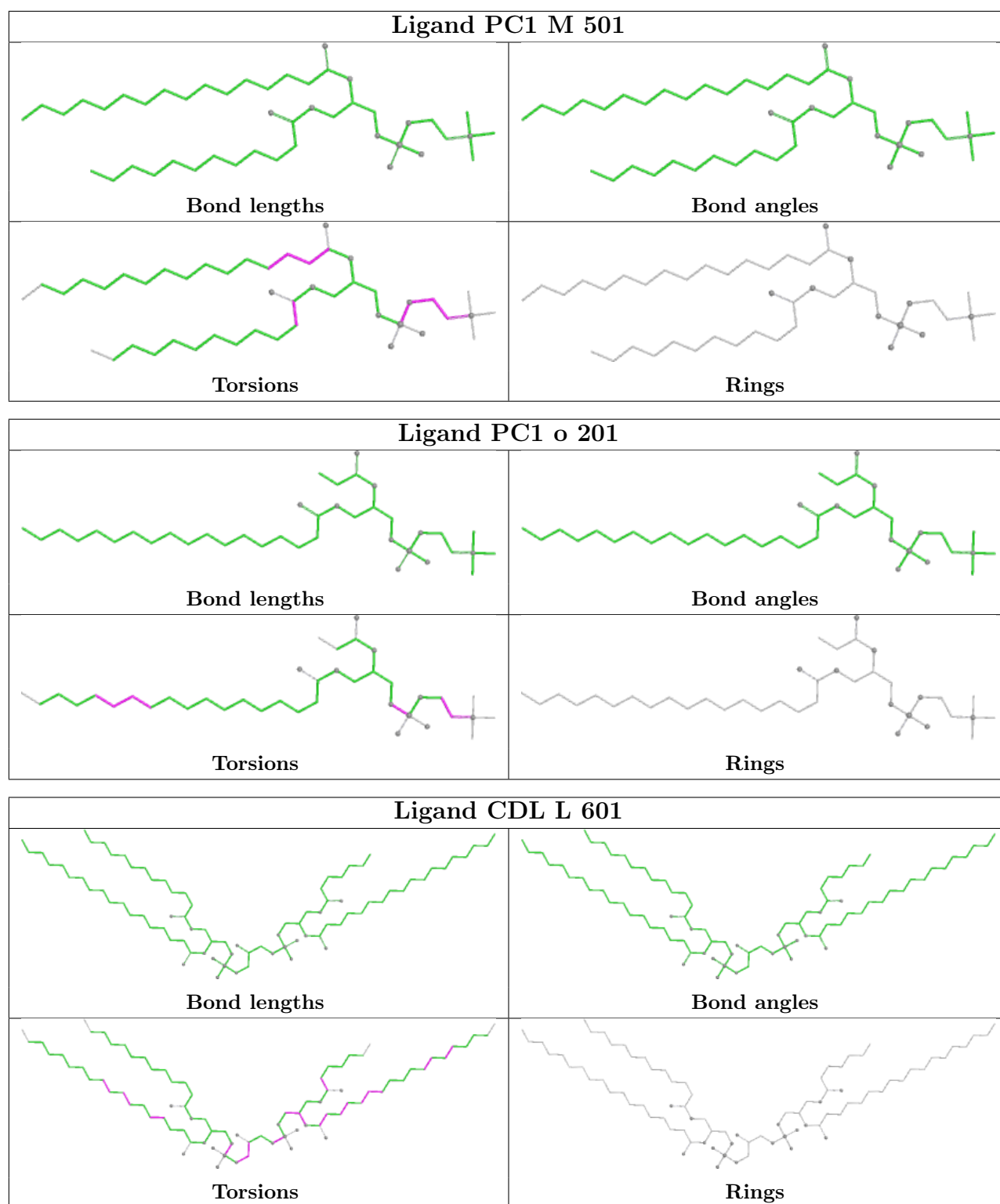
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

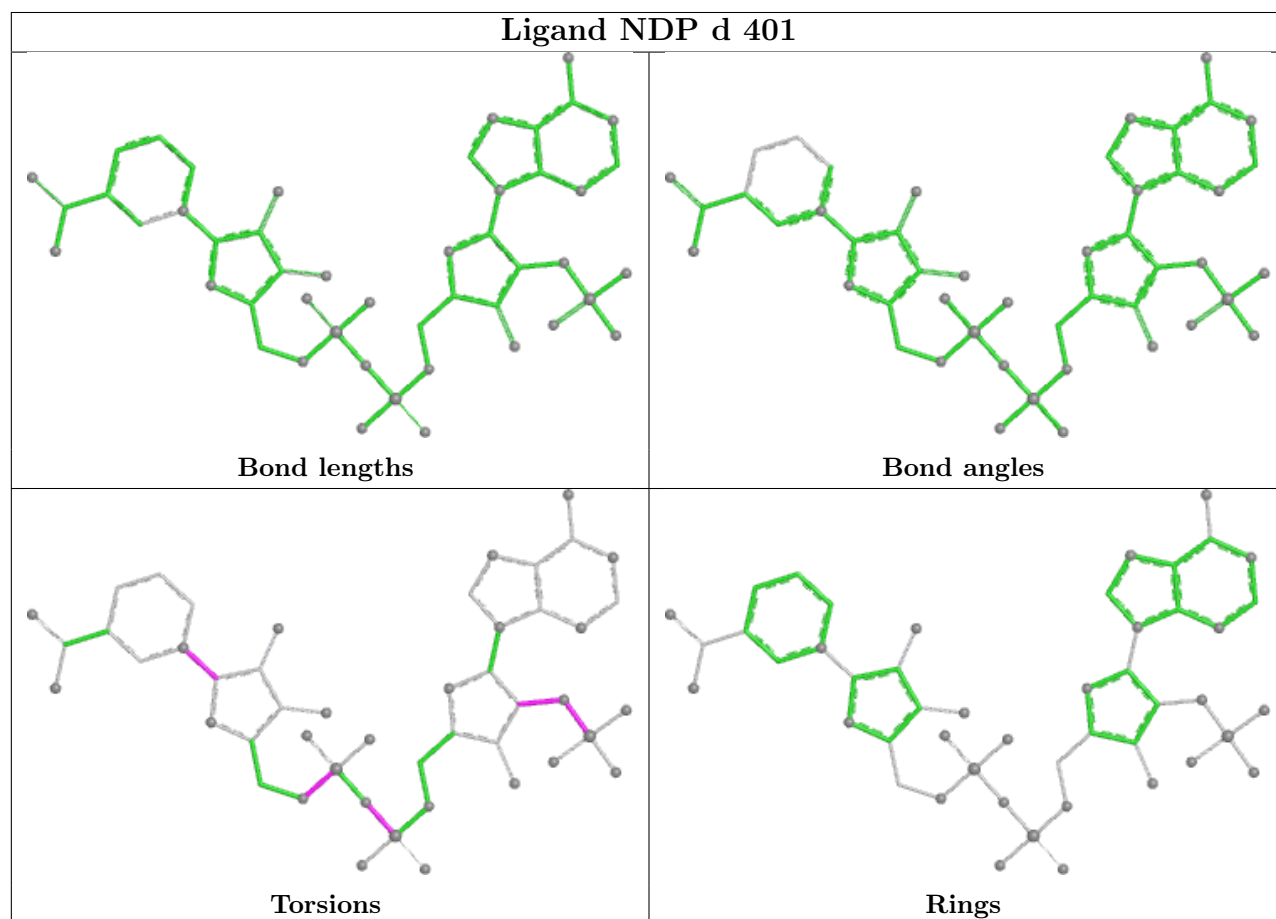
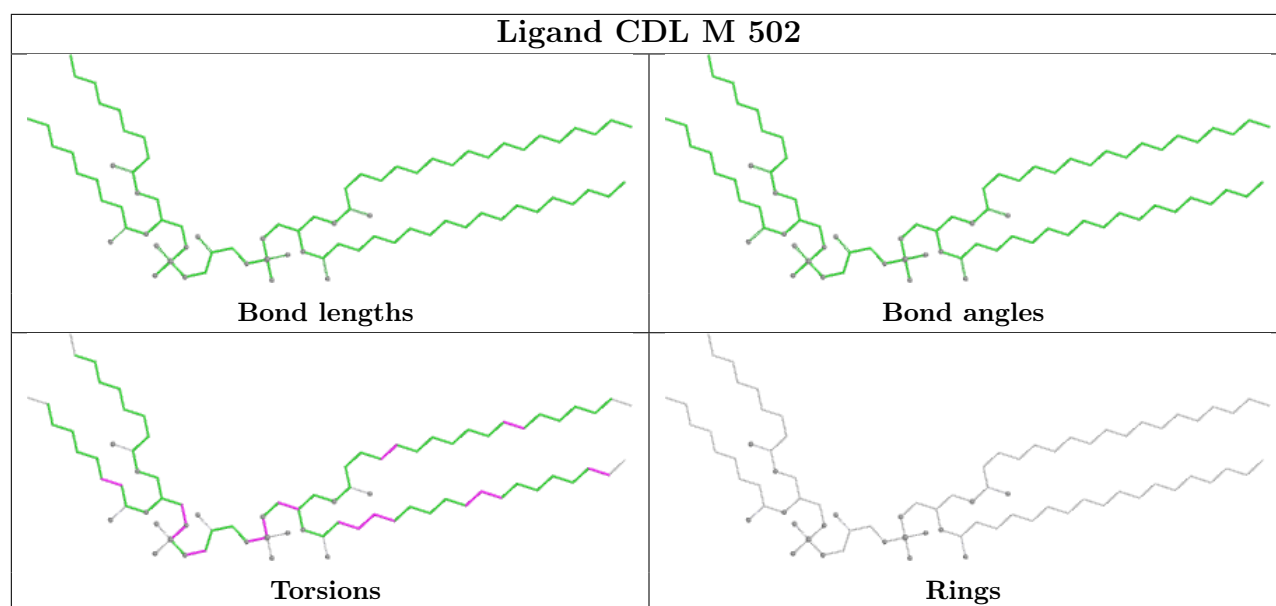
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

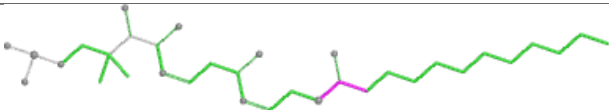
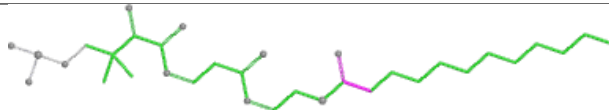
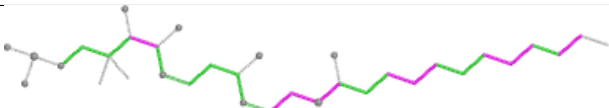
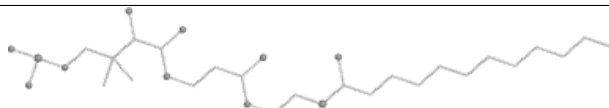


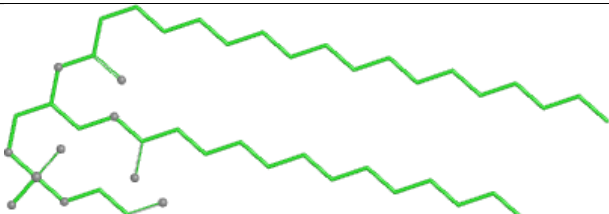
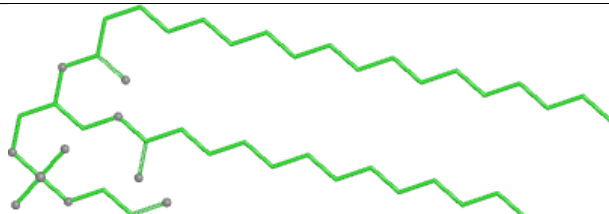
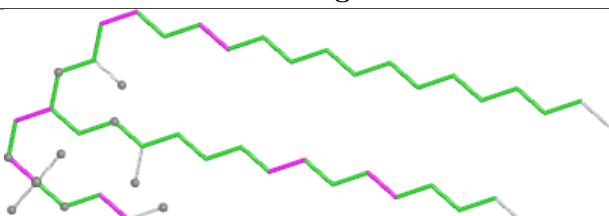
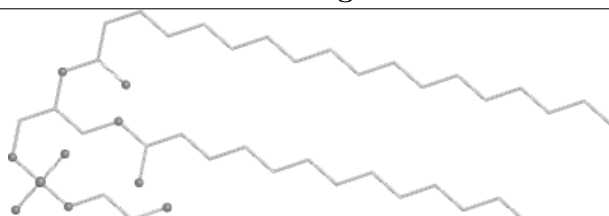


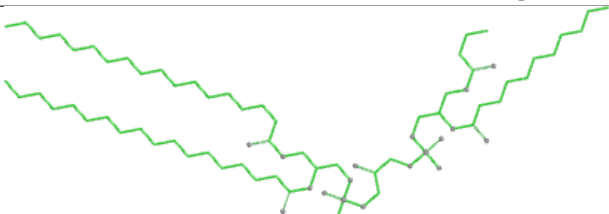
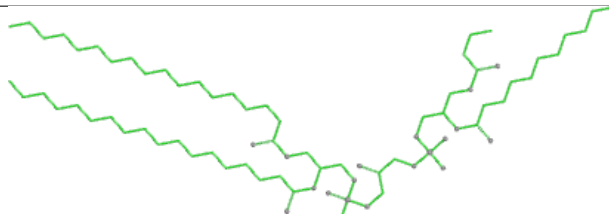
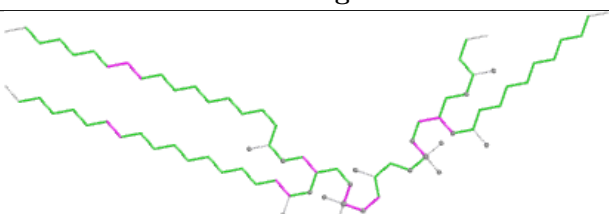
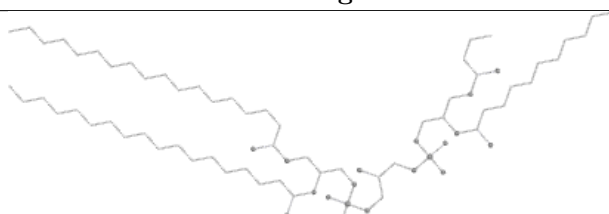


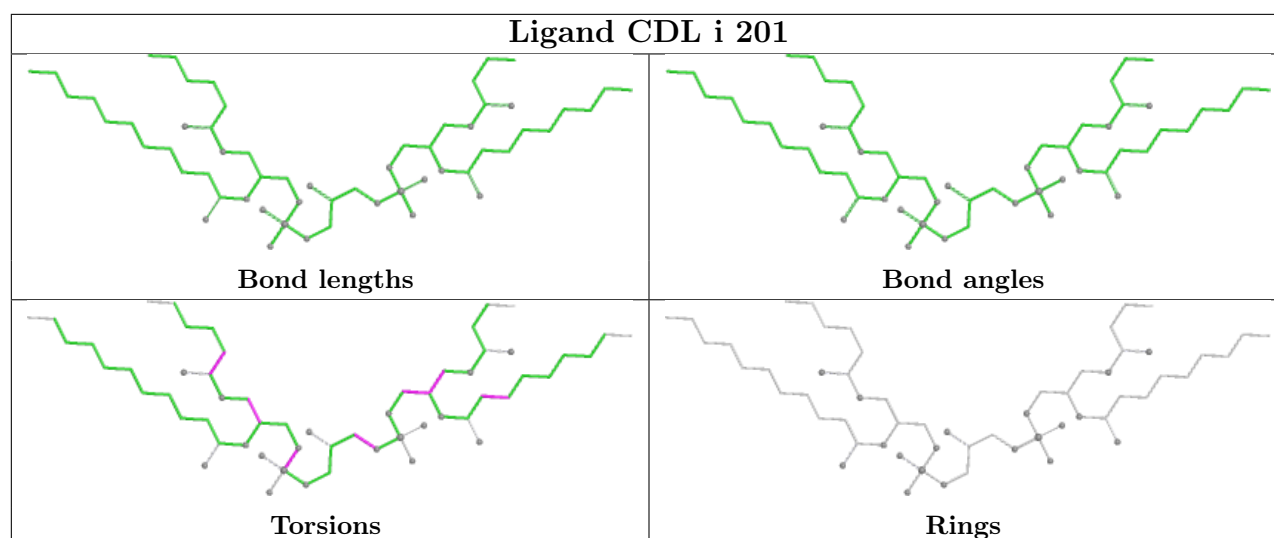




Ligand ZMP j 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 3PE o 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CDL J 300	
	
Bond lengths	Bond angles
	
Torsions	Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	k	1
9	N	1
19	e	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	k	174:VAL	C	175:PRO	N	1.18
1	N	304:MET	C	305:PHE	N	1.16
1	e	50:LEU	C	51:PRO	N	1.15

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4093. These allow visual inspection of the internal detail of the map and identification of artifacts.

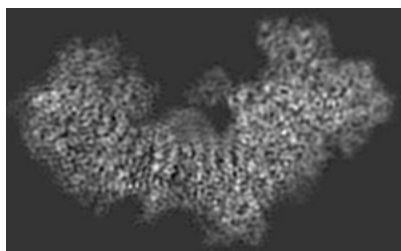
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

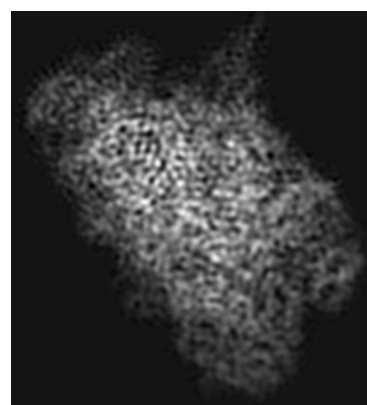
6.1.1 Primary map



X



Y

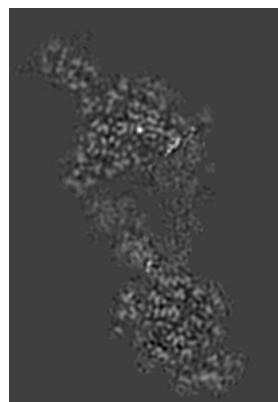


Z

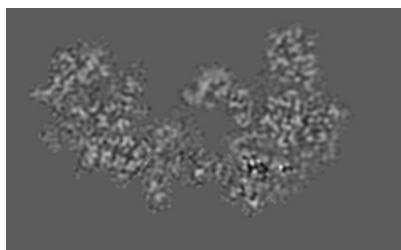
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

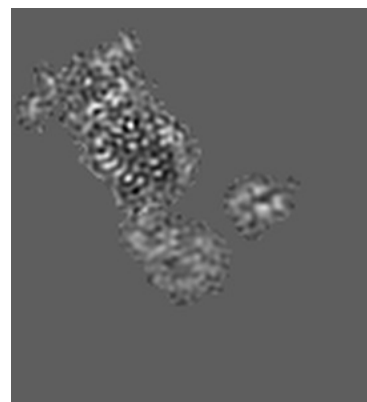
6.2.1 Primary map



X Index: 64



Y Index: 70

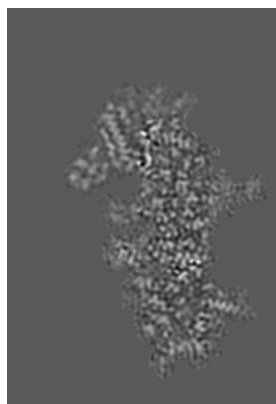


Z Index: 104

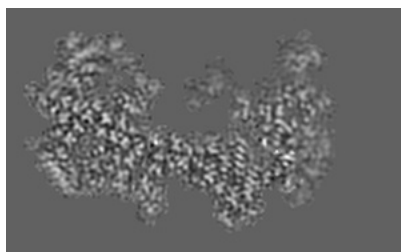
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

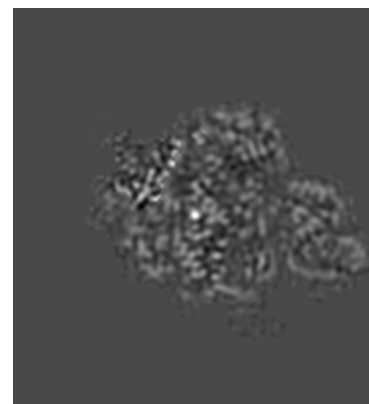
6.3.1 Primary map



X Index: 46



Y Index: 80

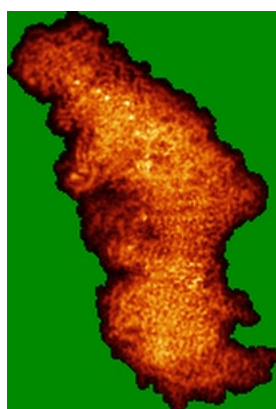


Z Index: 145

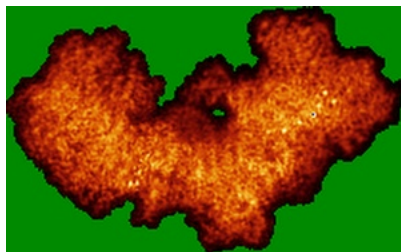
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

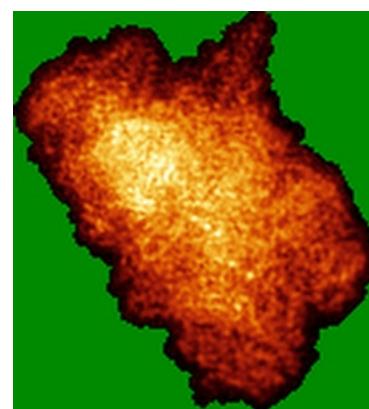
6.4.1 Primary map



X



Y

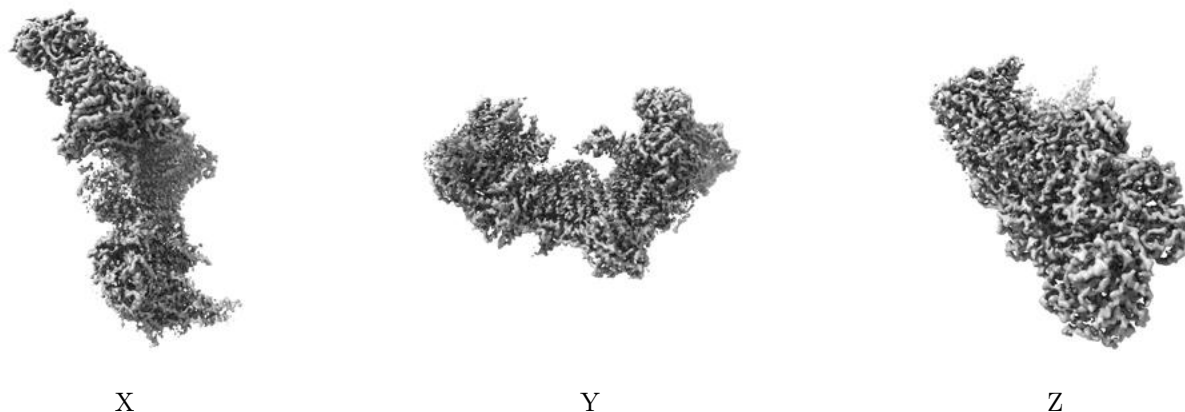


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

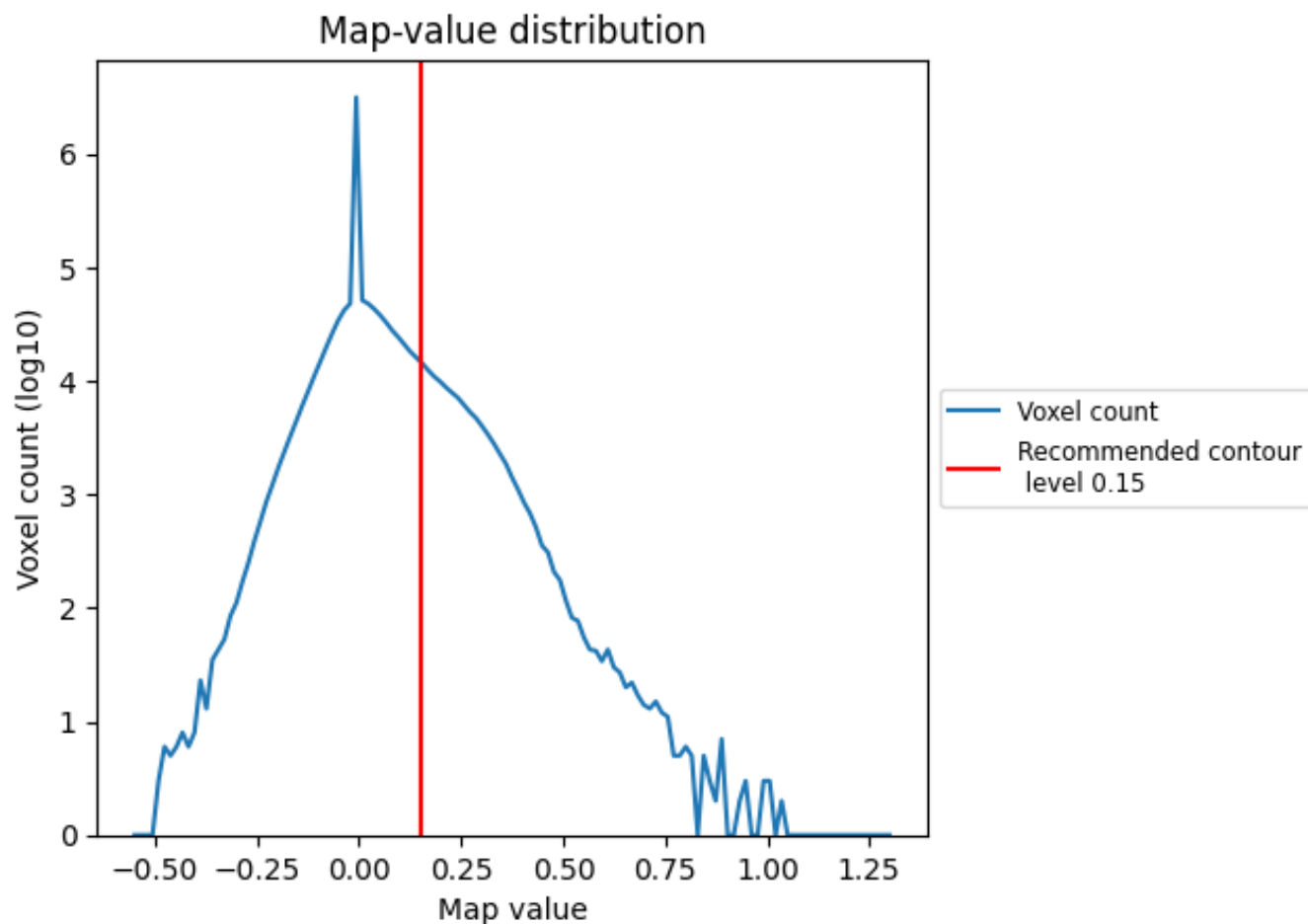
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

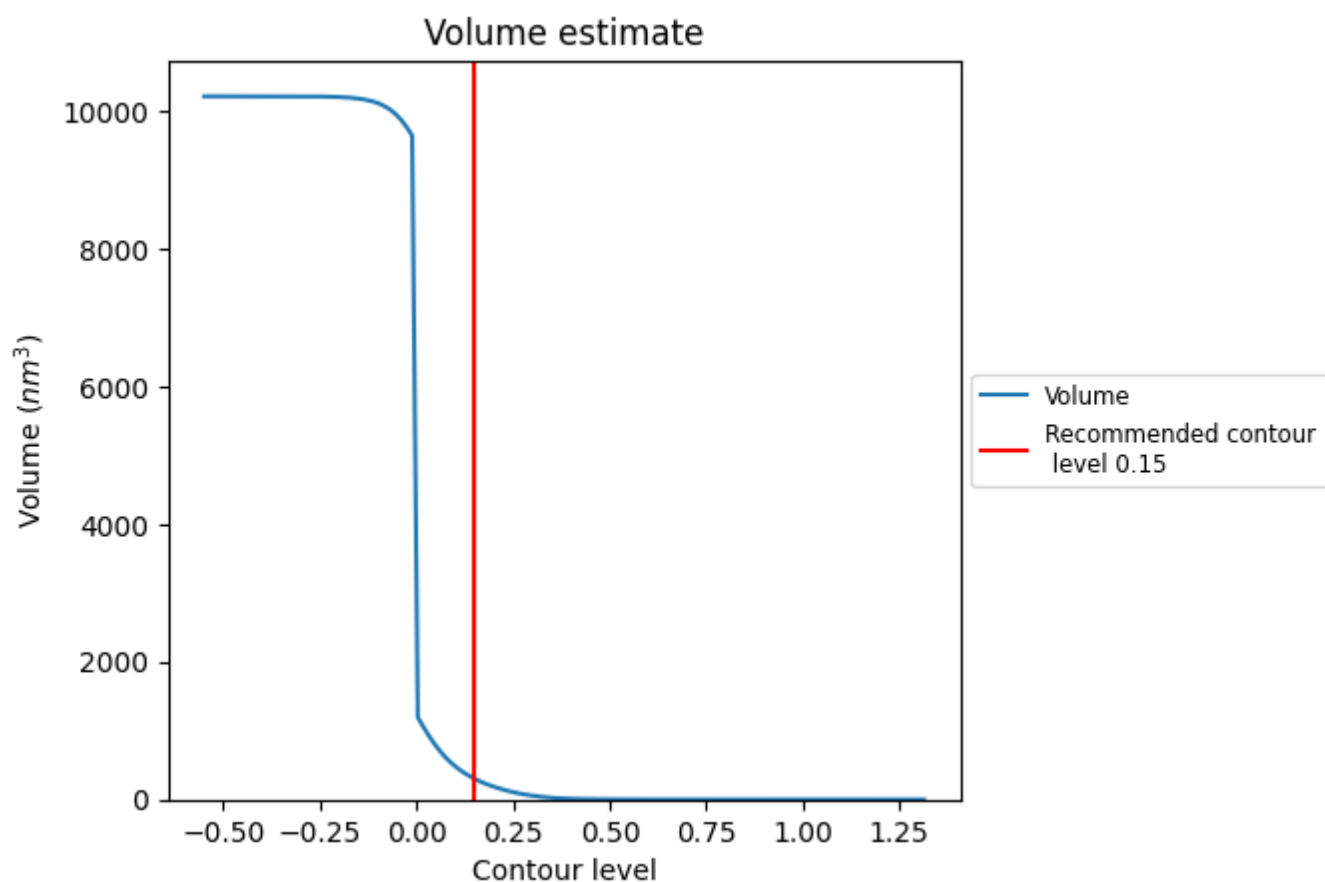
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 304 nm³; this corresponds to an approximate mass of 275 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

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

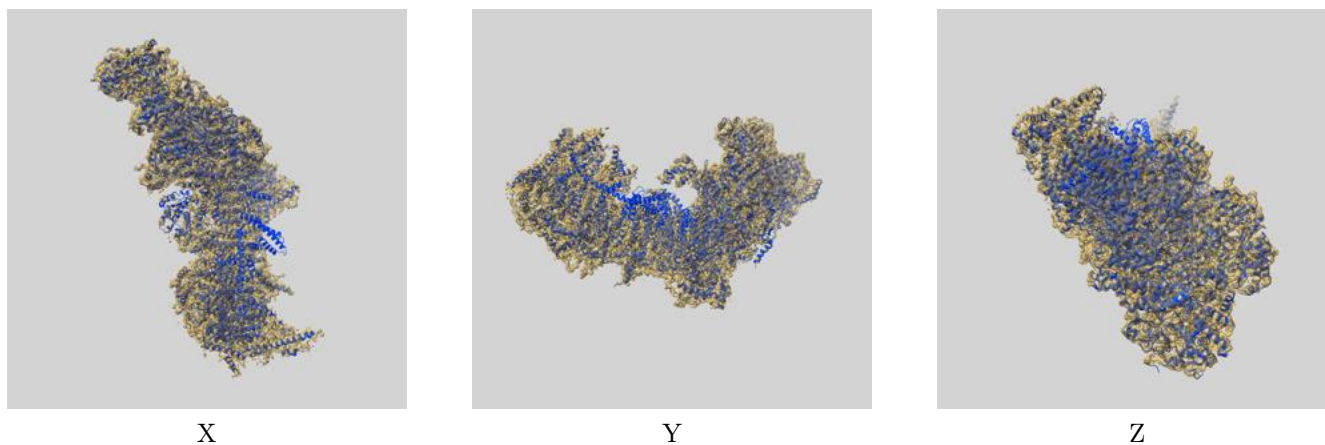
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

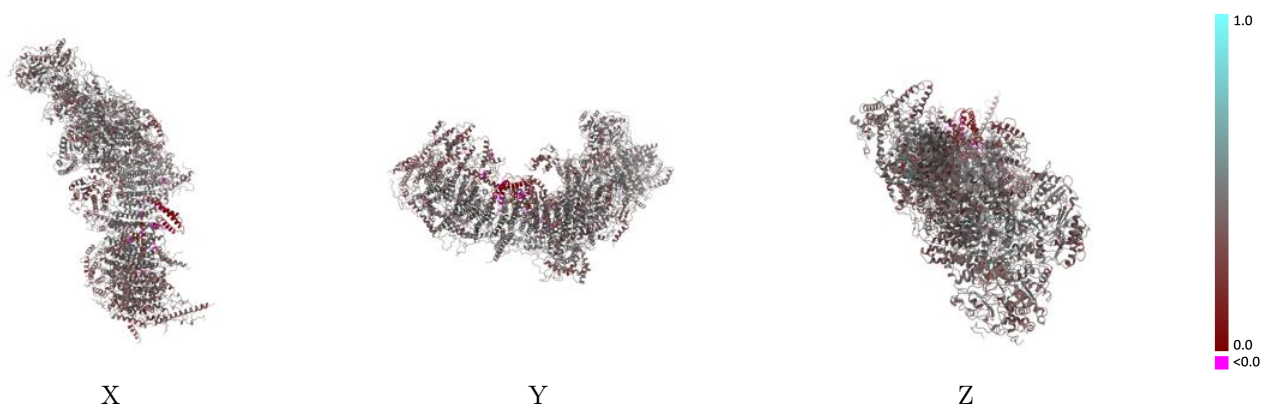
This section contains information regarding the fit between EMDB map EMD-4093 and PDB model 5LNK. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



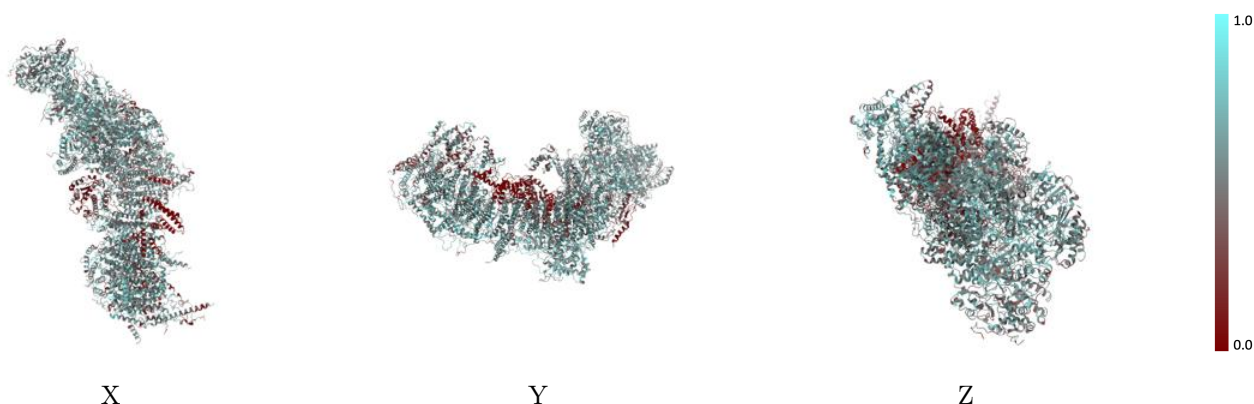
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



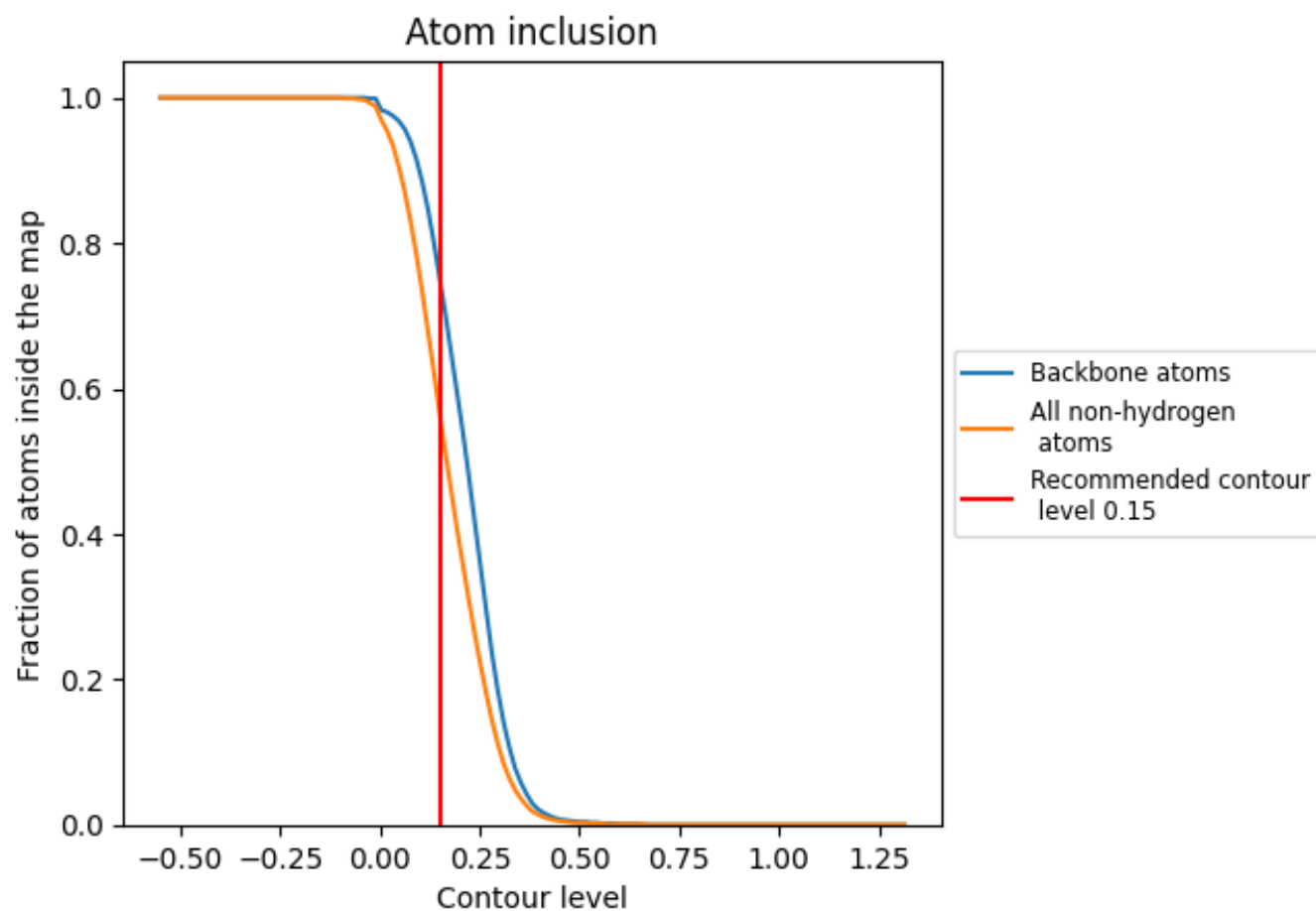
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5640	 0.4080
1	 0.5680	 0.4170
2	 0.5520	 0.4100
3	 0.5970	 0.4350
4	 0.5970	 0.4320
5	 0.6410	 0.4560
6	 0.6280	 0.4200
9	 0.6450	 0.4310
A	 0.5470	 0.4270
H	 0.6250	 0.4320
J	 0.4000	 0.4110
K	 0.5820	 0.4330
L	 0.5520	 0.3890
M	 0.6440	 0.4460
N	 0.6540	 0.4480
V	 0.0120	 0.0190
W	 0.6680	 0.4390
X	 0.5330	 0.3640
Y	 0.6240	 0.4060
Z	 0.6260	 0.4120
a	 0.5210	 0.4050
b	 0.5780	 0.4570
c	 0.5970	 0.4570
d	 0.5280	 0.3940
e	 0.5790	 0.3900
f	 0.5920	 0.3920
g	 0.5780	 0.4250
h	 0.4940	 0.4070
i	 0.3370	 0.3900
j	 0.4760	 0.3610
k	 0.3010	 0.3100
l	 0.6180	 0.4400
m	 0.6010	 0.4360
n	 0.5550	 0.3680
o	 0.5800	 0.4420



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Chain	Atom inclusion	Q-score
p	 0.4730	 0.3660
q	 0.5880	 0.4050
r	 0.5360	 0.3660
s	 0.5210	 0.3630
t	 0.6030	 0.3700
u	 0.5420	 0.3750
v	 0.4940	 0.3360
w	 0.6350	 0.4340
x	 0.5860	 0.3870
y	 0.5110	 0.3860
z	 0.6550	 0.4260