



wwPDB EM Validation Summary Report ⓘ

Sep 9, 2026 – 02:49 am BST

PDB ID : 7AR8 / pdb_00007ar8
EMDB ID : EMD-11876
Title : Cryo-EM structure of Arabidopsis thaliana complex-I (closed conformation)
Authors : Klusch, N.; Kuelbrandt, W.; Yildiz, O.
Deposited on : 2020-10-23
Resolution : 3.53 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 ⓘ 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:

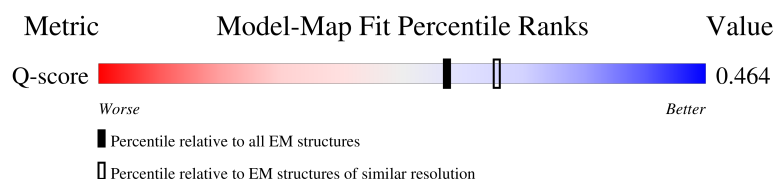
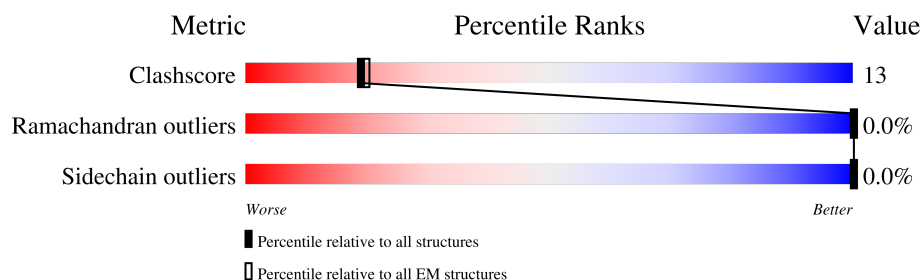
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 3.53 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	12947 (3.03 - 4.02)

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	A	119	 8% 60% 18% 23%
2	B	218	 49% 23% 28%
3	C	190	 71% 27%
4	D	394	 71% 27%

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Mol	Chain	Length	Quality of chain
5	E	255	
6	F	486	
7	G	748	
8	H	325	
9	I	222	
10	J	205	
11	K	100	
12	L	669	
13	M	495	
14	N	499	
15	O	159	
16	P	402	
17	Q	154	
18	R	110	
19	S	97	
20	T	122	
21	U	126	
22	V	169	
23	W	133	
24	X	106	
25	Z	143	
26	a	65	
27	b	65	
28	c	88	
29	d	81	

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Mol	Chain	Length	Quality of chain
30	e	83	
31	f	106	
32	g	114	
33	i	98	
34	j	69	
35	k	72	
36	l	125	
37	m	71	
38	n	117	
39	o	103	
40	p	106	
41	q	159	
42	r	131	
43	u	30	
44	v	113	
45	x	256	
46	y	278	
47	z	275	

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
48	SF4	F	501	-	-	X	-
49	FES	E	500	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 61461 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
1	A	92	Total	C	N	O	S	0	0
			785	556	108	117	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	157	Total	C	N	O	S	0	0
			1244	797	218	215	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	185	Total	C	N	O	S	0	0
			1581	1021	271	283	6		

- Molecule 4 is a protein called NADH dehydrogenase subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	385	Total	C	N	O	S	0	0
			3077	1954	542	557	24		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	363	SER	LEU	variant	UNP A0A2P2CLH2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	192	Total	C	N	O	S	0	0
			1500	954	248	287	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	434	Total	C	N	O	S	0	0
			3368	2125	600	618	25		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	688	Total	C	N	O	S	0	0
			5252	3291	921	1001	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	324	Total	C	N	O	S	0	0
			2536	1719	386	416	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	169	Total	C	N	O	S	0	0
			1381	869	234	268	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	138	Total	C	N	O	S	0	0
			1093	742	168	175	8		

- Molecule 11 is a protein called NADH dehydrogenase subunit 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	90	Total	C	N	O	S	0	0
			707	476	109	115	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	615	Total	C	N	O	S	0	0
			4807	3191	748	832	36		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	91	PHE	SER	conflict	UNP B5TM94

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	487	Total	C	N	O	S	0	0
			3887	2627	601	636	23		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	326	LEU	PRO	conflict	UNP B5TM93

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	488	Total	C	N	O	S	0	0
			3820	2573	577	642	28		

- Molecule 15 is a protein called AT3G07480.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	122	Total	C	N	O	S	0	0
			956	598	169	185	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	332	Total	C	N	O	S	0	0
			2560	1643	439	463	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	119	Total	C	N	O	S	0	0
			939	600	163	175	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	62	Total	C	N	O	S	0	0
			482	304	84	89	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	93	Total	C	N	O	S	0	0
			727	459	129	133	6		

- Molecule 20 is a protein called Acyl carrier protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	84	Total	C	N	O	S	0	0
			667	421	105	138	3		

- Molecule 21 is a protein called Acyl carrier protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	79	Total	C	N	O	S	0	0
			616	387	98	130	1		

- Molecule 22 is a protein called Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	140	Total	C	N	O	S	0	0
			1123	712	187	219	5		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	110	Total	C	N	O	S	0	0
			893	571	159	160	3		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	97	Total	C	N	O	S	0	0
			767	480	132	143	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	124	Total	C	N	O	S	0	0
			990	635	174	176	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	58	Total	C	N	O	S	0	0
			469	302	84	78	5		

- Molecule 27 is a protein called At2g46540/F11C10.23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	39	Total	C	N	O	S	0	0
			288	190	47	48	3		

- Molecule 28 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	73	Total	C	N	O	S	0	0
			595	384	110	95	6		

- Molecule 29 is a protein called Excitatory amino acid transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	73	Total	C	N	O	S	0	0
			574	368	104	97	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	64	Total	C	N	O	S	0	0
			546	338	102	99	7		

- Molecule 31 is a protein called At4g16450.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	98	Total	C	N	O	S	0	0
			734	473	118	138	5		

- Molecule 32 is a protein called ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	75	Total	C	N	O	S	0	0
			615	396	107	109	3		

- Molecule 33 is a protein called P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	i	83	Total	C	N	O	S	0	0
			721	458	132	126	5		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	j	51	Total	C	N	O	S	0	0
			415	275	73	64	3		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	k	47	Total	C	N	O	S	0	0
			374	238	71	62	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
36	l	50	Total	C	N	O	0	0
			384	255	61	68		

- Molecule 37 is a protein called B15 – 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	m	69	Total	C	N	O	S	0	0
			569	364	106	97	2		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	n	109	Total	C	N	O	S	0	0
			911	580	170	160	1		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	o	77	Total	C	N	O	S	0	0
			631	398	109	114	10		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	p	93	Total	C	N	O	S	0	0
			778	493	144	137	4		

- Molecule 41 is a protein called Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	q	65	Total	C	N	O	0	0
			536	342	95	99		

- Molecule 42 is a protein called Furry.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	r	10	Total	C	N	O	0	0
			88	57	17	14		

- Molecule 43 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	u	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 44 is a protein called Uncharacterized protein At2g27730, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	v	30	Total	C	N	O	0	0
			226	147	39	40		

- Molecule 45 is a protein called Gamma carbonic anhydrase-like 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	x	211	Total	C	N	O	S	0	0
			1637	1049	281	302	5		

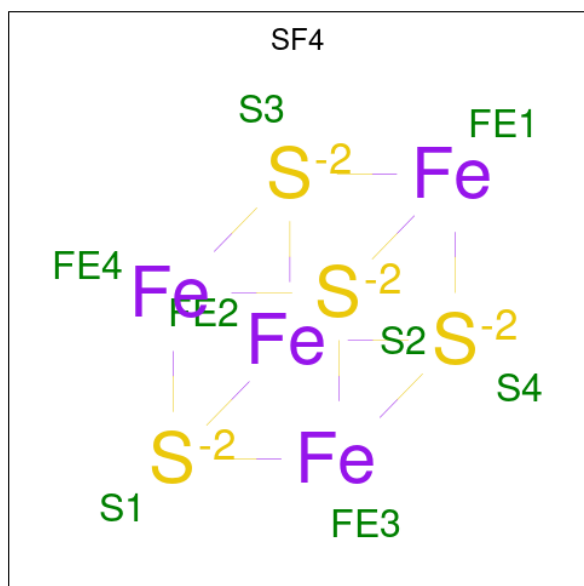
- Molecule 46 is a protein called Gamma carbonic anhydrase 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	y	263	Total	C	N	O	S	0	0
			2001	1251	357	386	7		

- Molecule 47 is a protein called Gamma carbonic anhydrase 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	z	232	Total	C	N	O	S	0	0
			1763	1105	323	329	6		

- Molecule 48 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



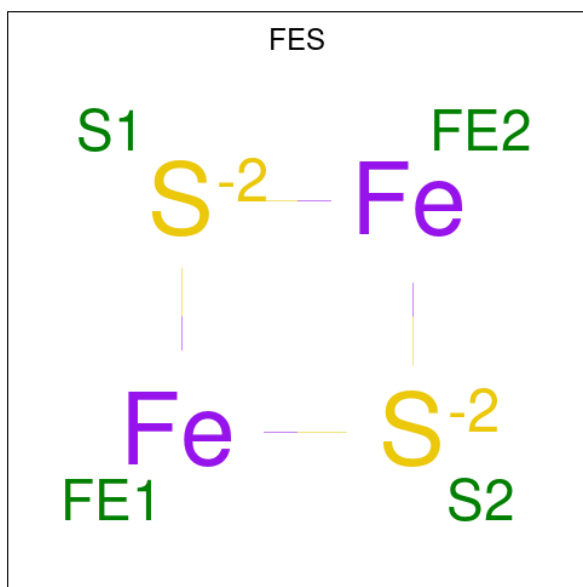
Mol	Chain	Residues	Atoms			AltConf
48	B	1	Total	Fe	S	0
			8	4	4	
48	F	1	Total	Fe	S	0
			8	4	4	
48	G	1	Total	Fe	S	0
			8	4	4	
48	G	1	Total	Fe	S	0
			8	4	4	

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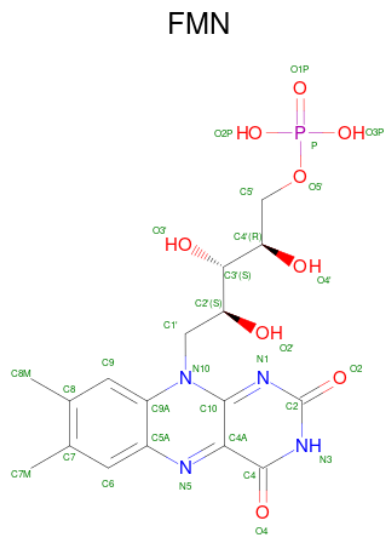
Mol	Chain	Residues	Atoms			AltConf
48	I	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	

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



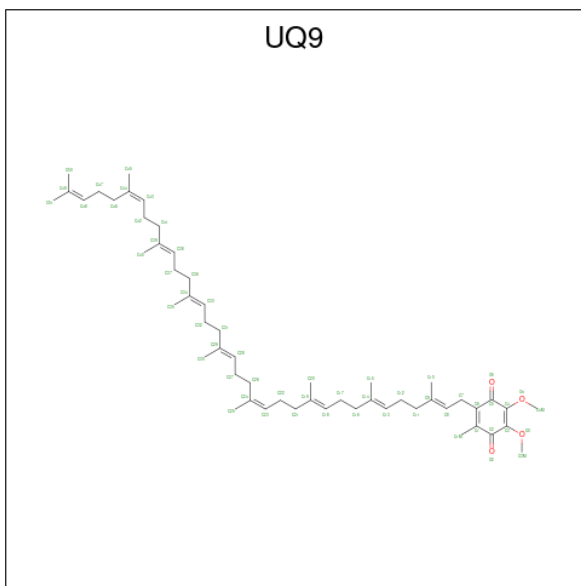
Mol	Chain	Residues	Atoms			AltConf
49	E	1	Total	Fe	S	0
			4	2	2	
49	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 50 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).



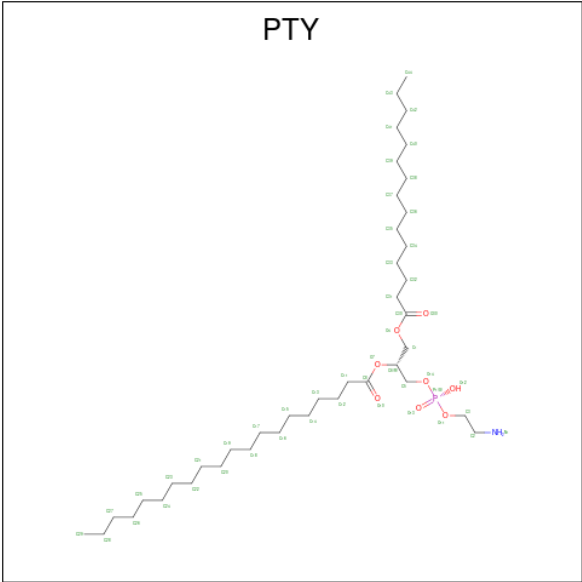
Mol	Chain	Residues	Atoms					AltConf
50	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 51 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$).



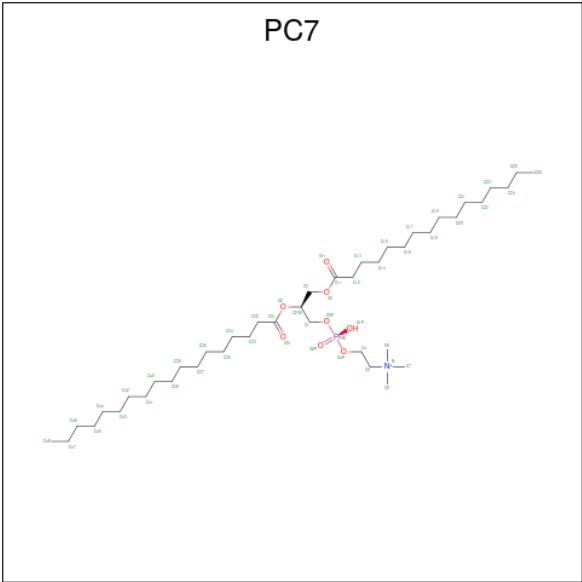
Mol	Chain	Residues	Atoms			AltConf
51	H	1	Total	C	O	0
			35	31	4	

- Molecule 52 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



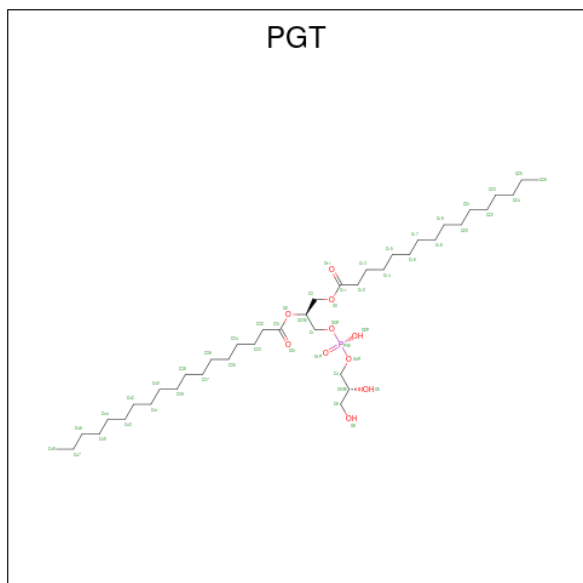
Mol	Chain	Residues	Atoms					AltConf
52	H	1	Total	C	N	O	P	0
			50	40	1	8	1	
52	M	1	Total	C	N	O	P	0
			50	40	1	8	1	
52	N	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 53 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY) METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: PC7) (formula: C₄₂H₈₅NO₈P).



Mol	Chain	Residues	Atoms					AltConf
53	M	1	Total	C	N	O	P	0
			52	42	1	8	1	
53	v	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 54 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
54	N	1	Total	C	O	P	0
			41	30	10	1	

- Molecule 55 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
55	O	1	Total	Fe	0
			1	1	

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

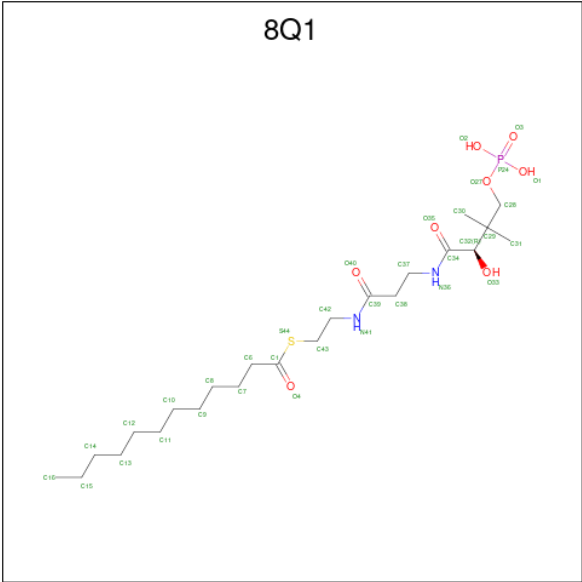


Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

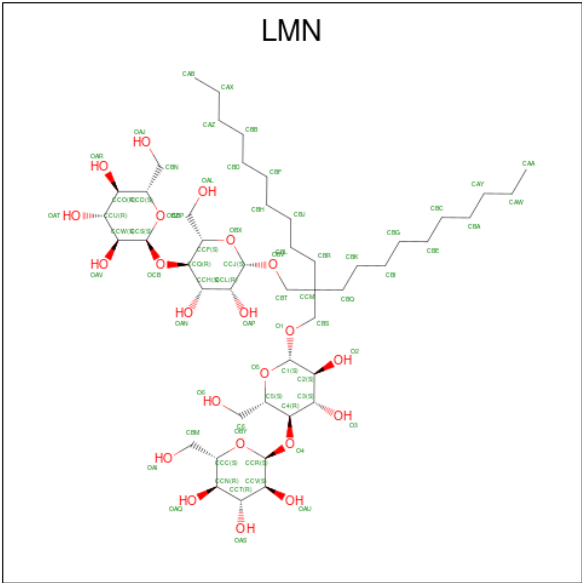
Mol	Chain	Residues	Atoms		AltConf
57	R	1	Total 1	Zn 1	0
57	y	1	Total 1	Zn 1	0

- Molecule 58 is S-[2-($\{N-[(2R)-2\text{-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl}]\text{-beta-alanyl}\}$ amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).



Mol	Chain	Residues	Atoms						AltConf
58	W	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
58	n	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

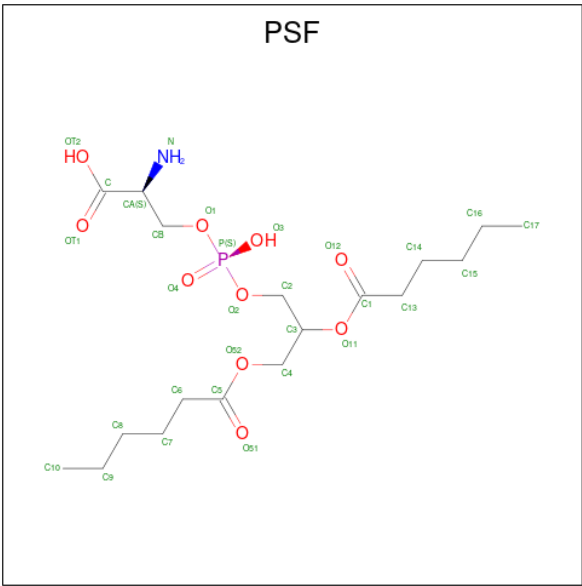
- Molecule 59 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: C₄₇H₈₈O₂₂).



Mol	Chain	Residues	Atoms			AltConf
59	d	1	Total	C	O	0
			69	47	22	

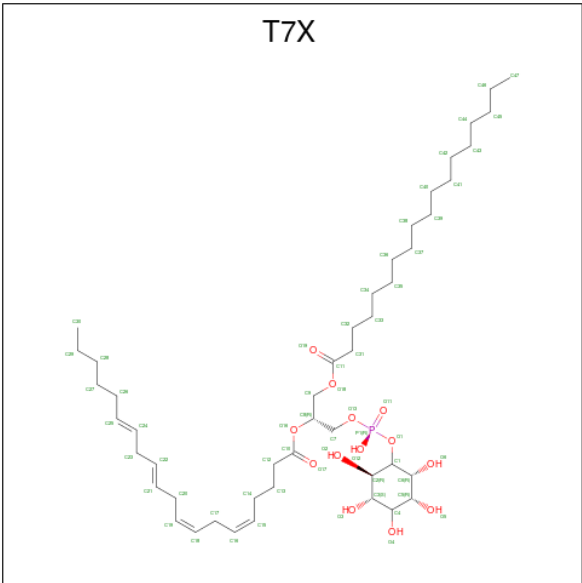
- Molecule 60 is 1,2-DICAPROYL-SN-PHOSPHATIDYL-L-SERINE (CCD ID: PSF)

(formula: C₁₈H₃₄NO₁₀P).



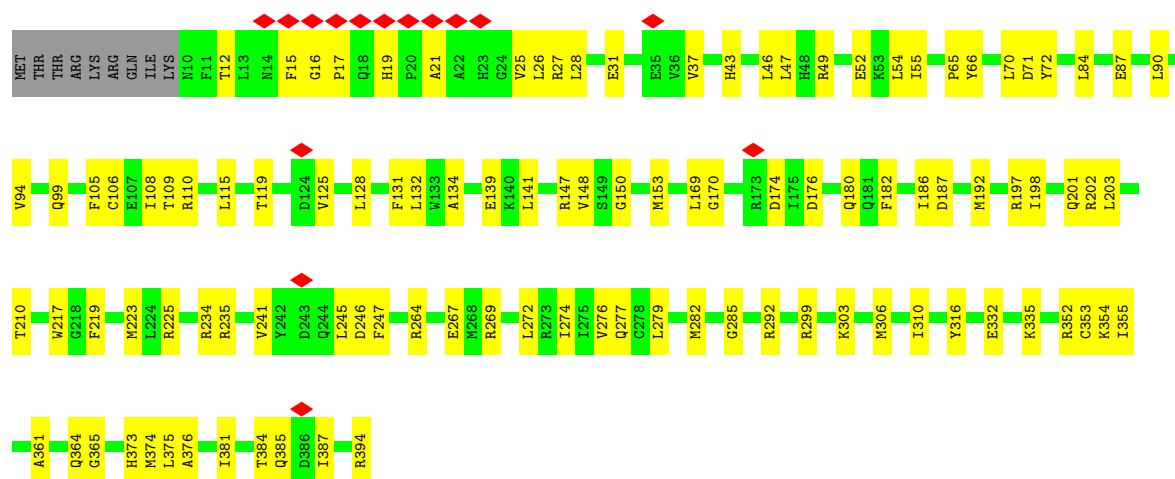
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	z	1	30	18	1	10	1	0

- Molecule 61 is Phosphatidylinositol (CCD ID: T7X) (formula: C₄₇H₈₃O₁₃P).



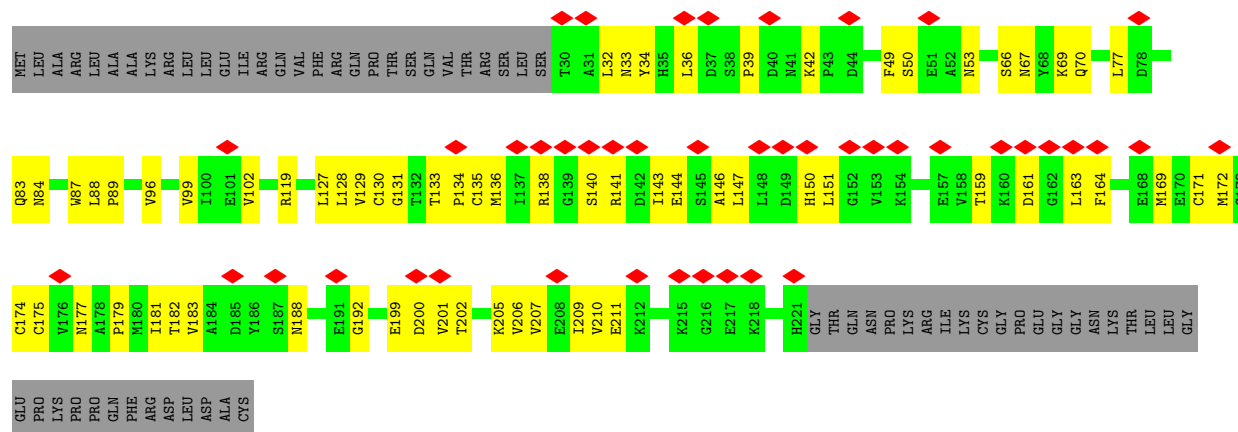
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
61	z	1	61	47	13	1	0

Chain D: 



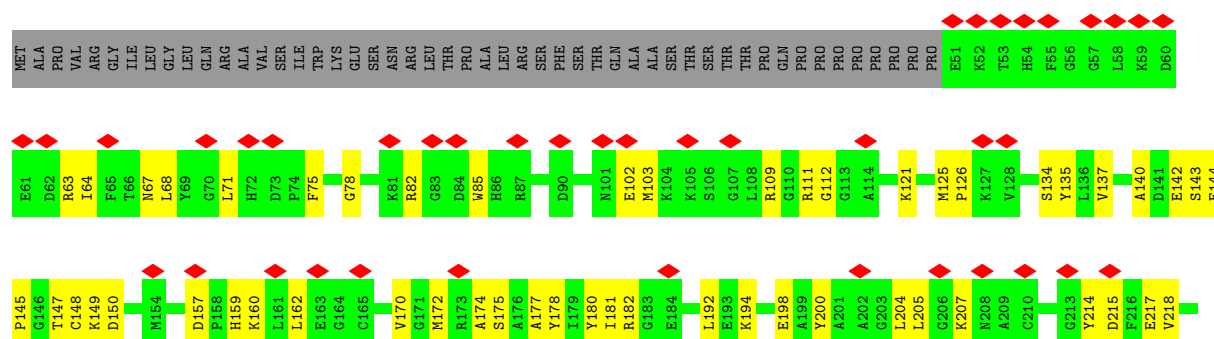
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

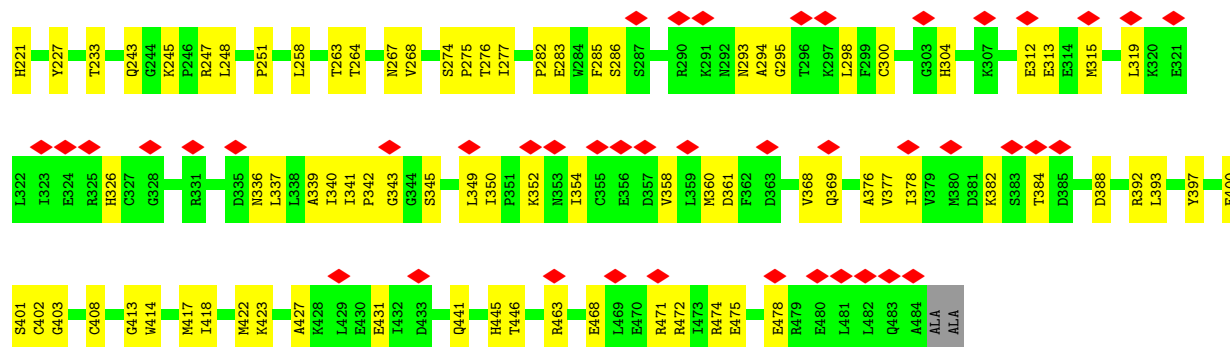
Chain E: 



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

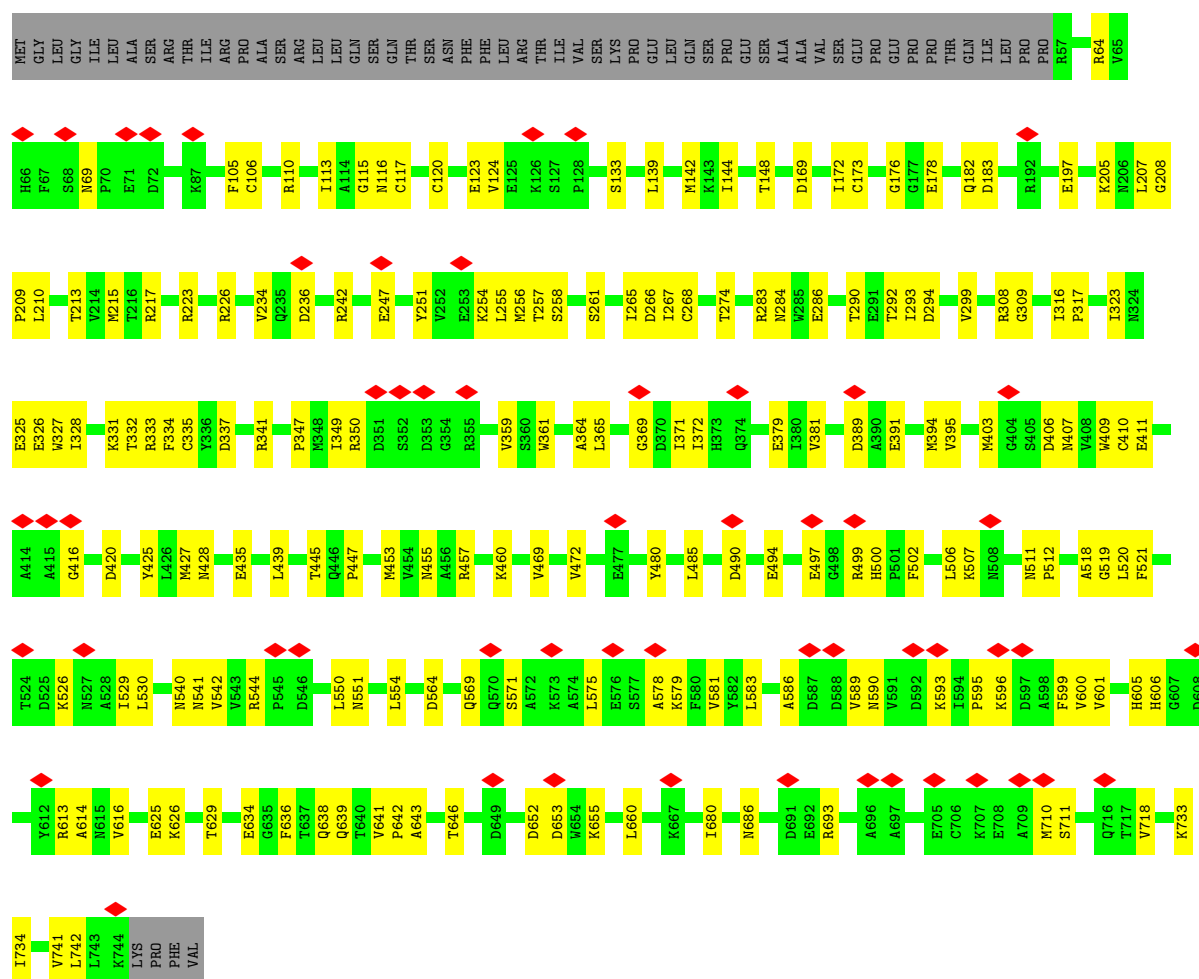
Chain F: 





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

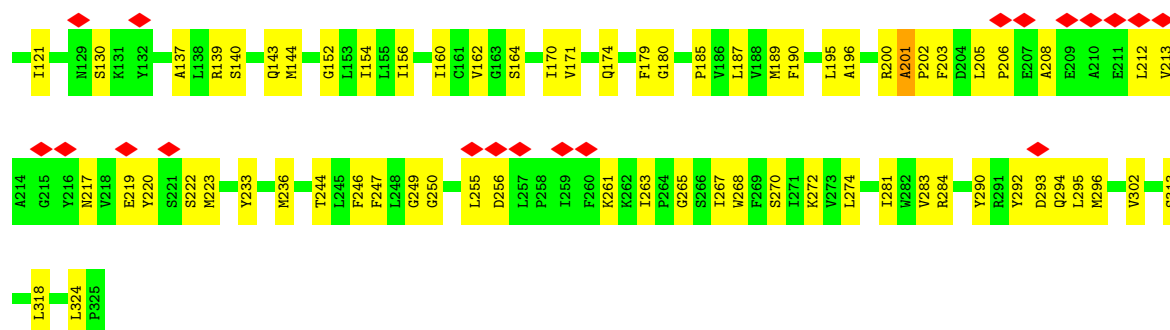
Chain G: 7% 67% 25% 8%



- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

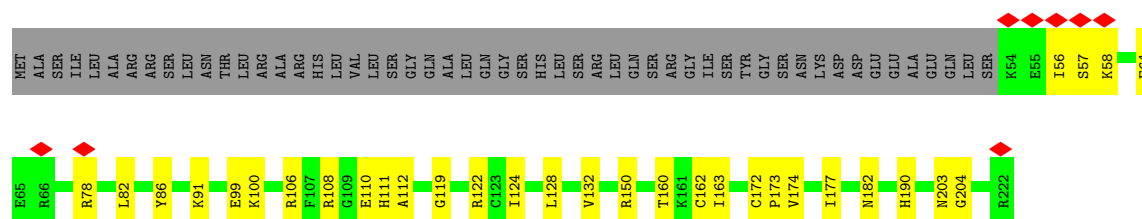
Chain H: 10% 70% 29%





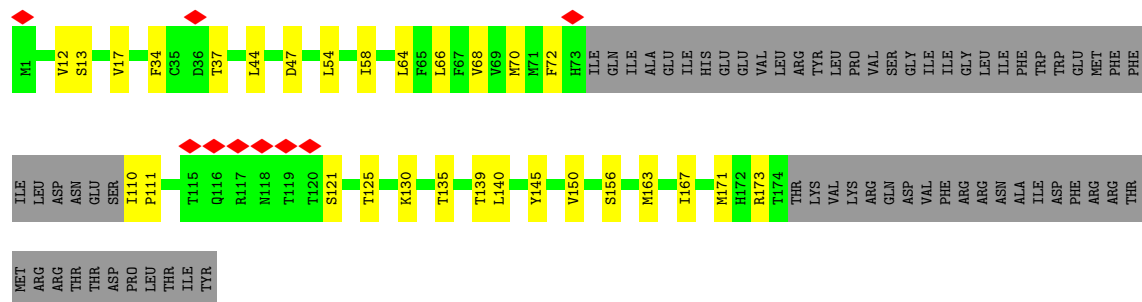
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8-A, mitochondrial

Chain I: 62% 14% 24%



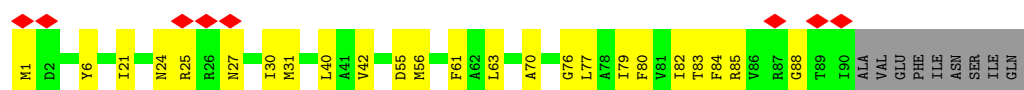
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J: 53% 14% 33%



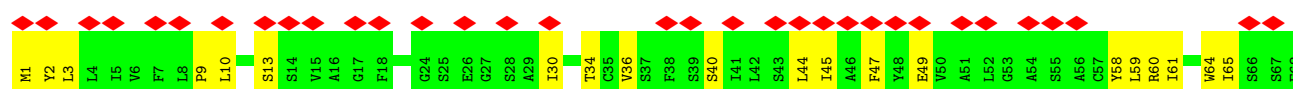
- Molecule 11: NADH dehydrogenase subunit 4L

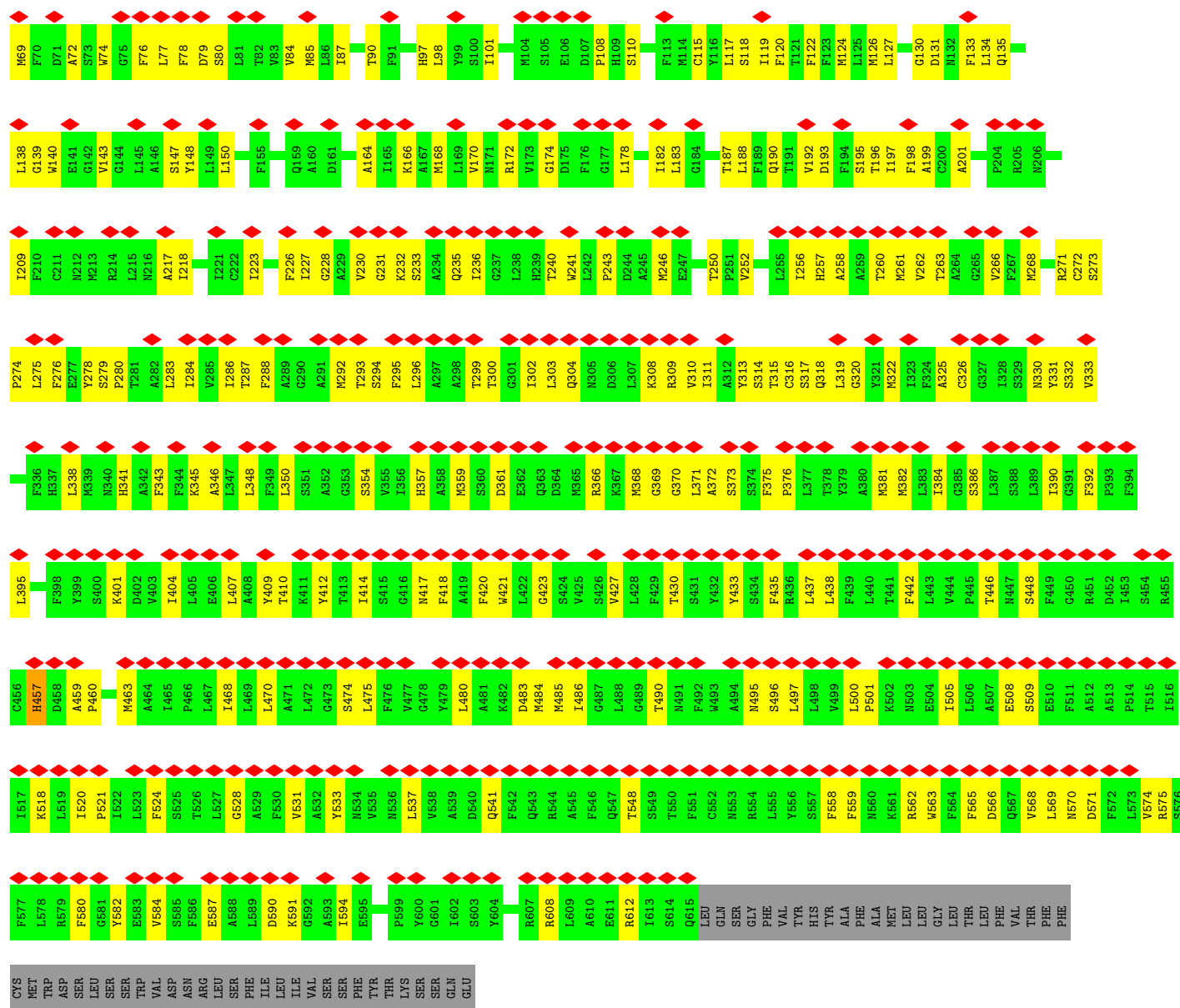
Chain K: 8% 66% 24% 10%



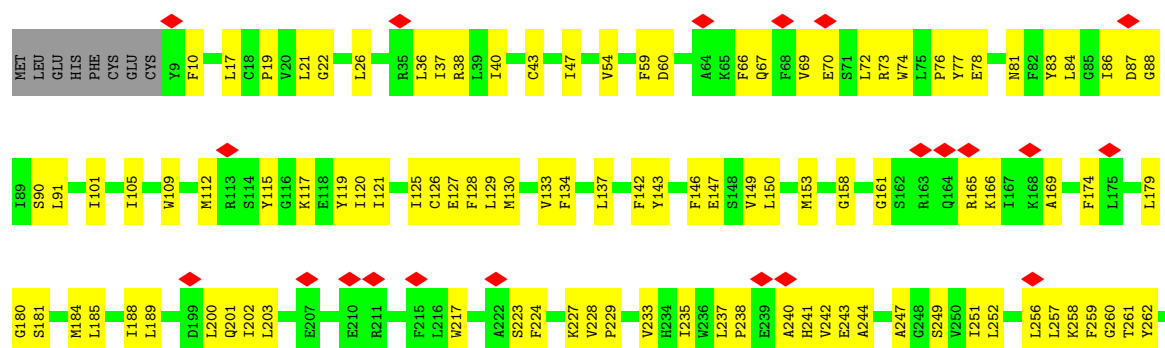
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

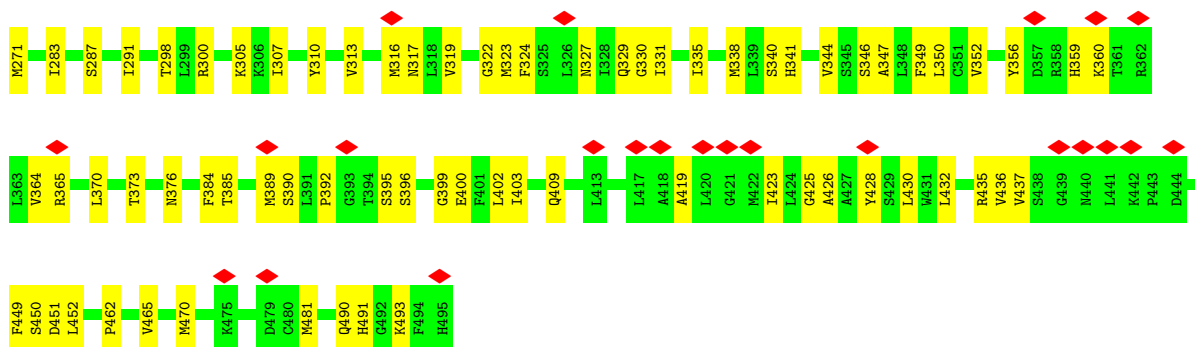
Chain L: 57% 55% 37% 8%





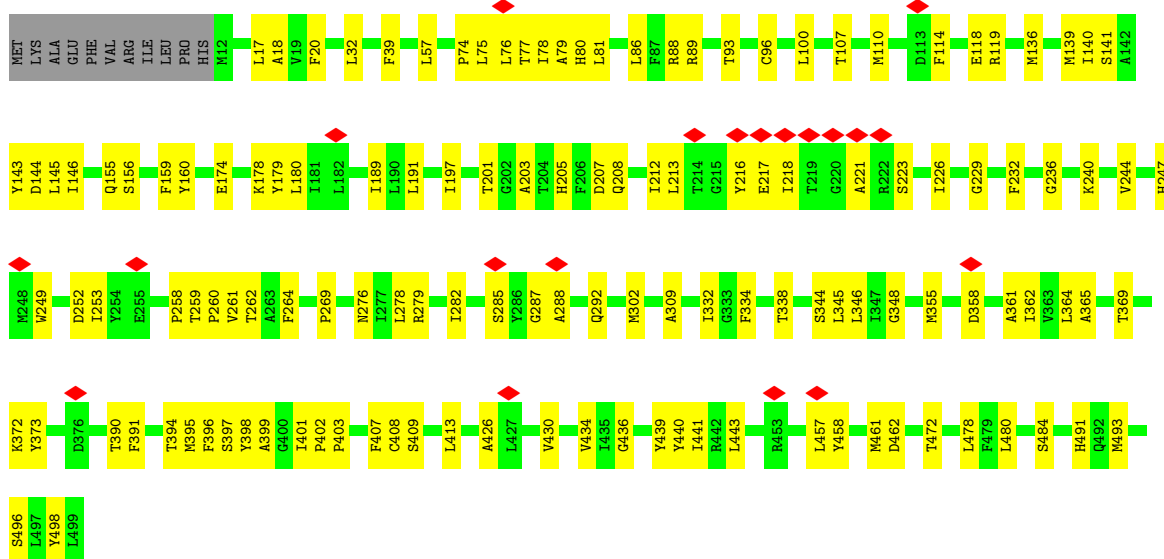
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4





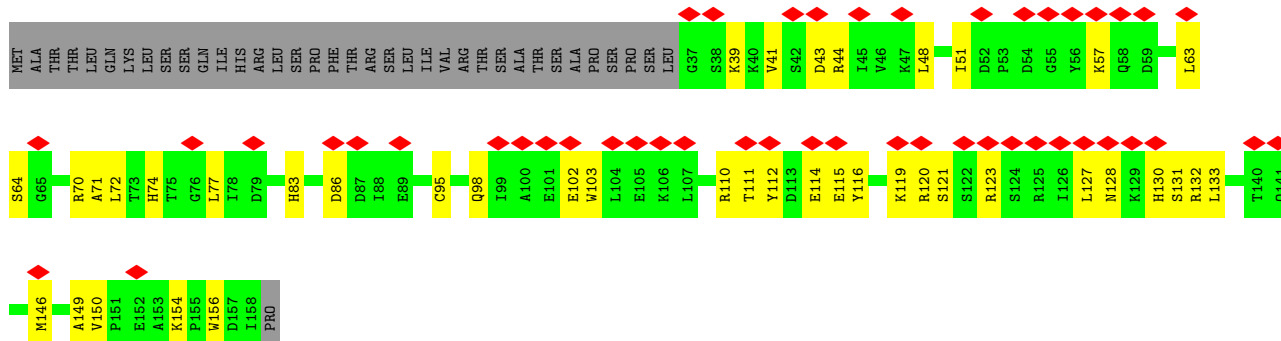
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N: 71% 27% .

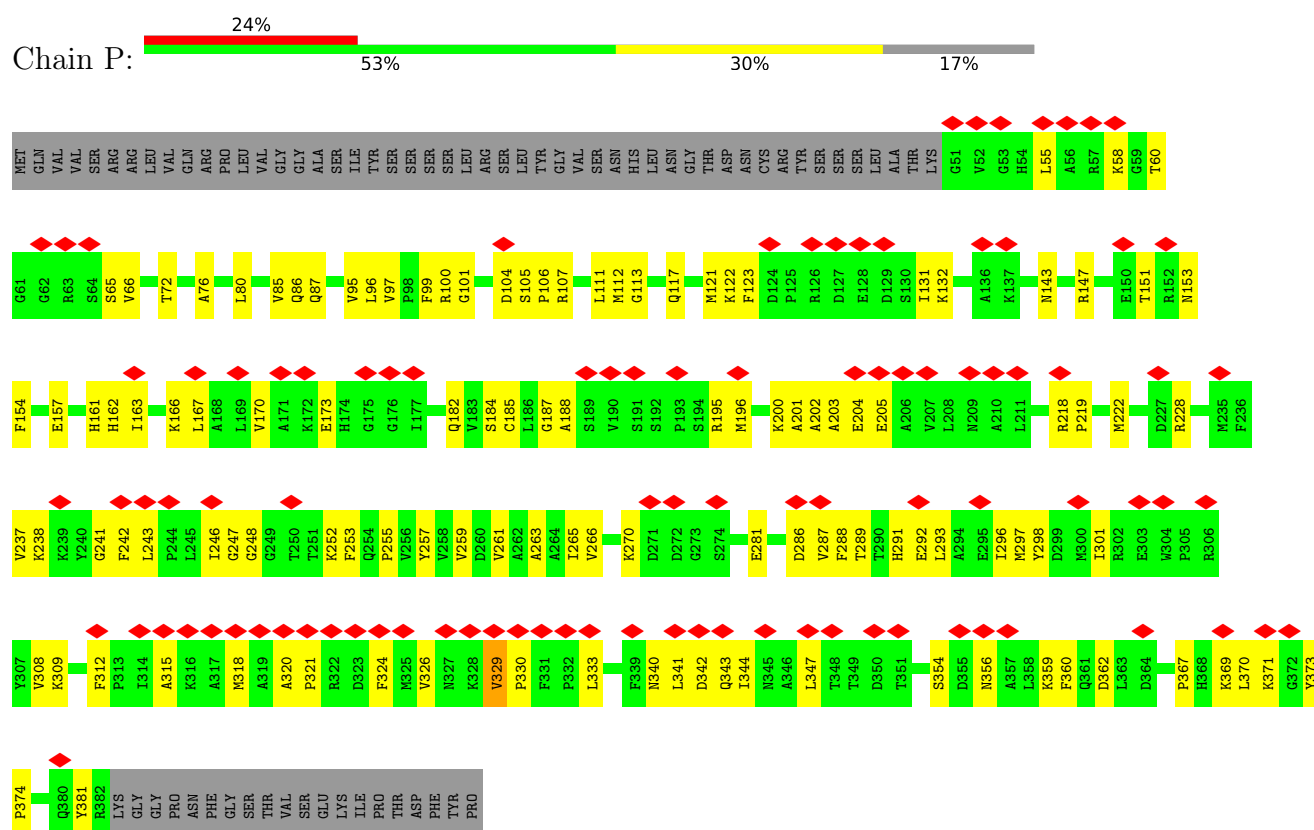


• Molecule 15: AT3G07480.1

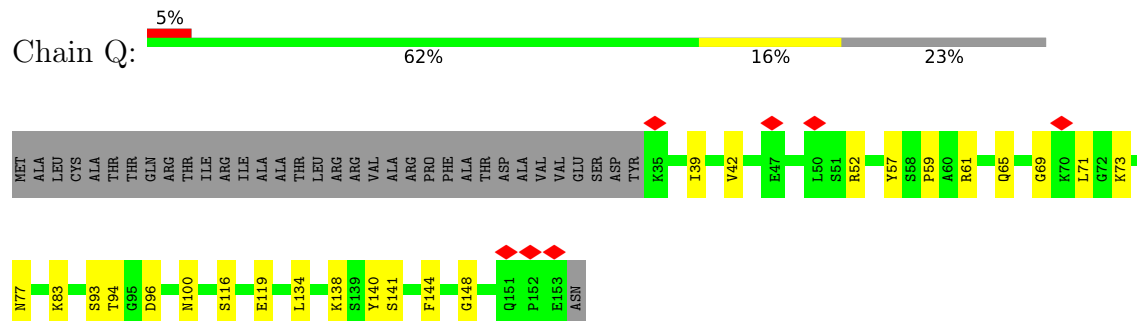
Chain O: 30% 51% 26% 23%



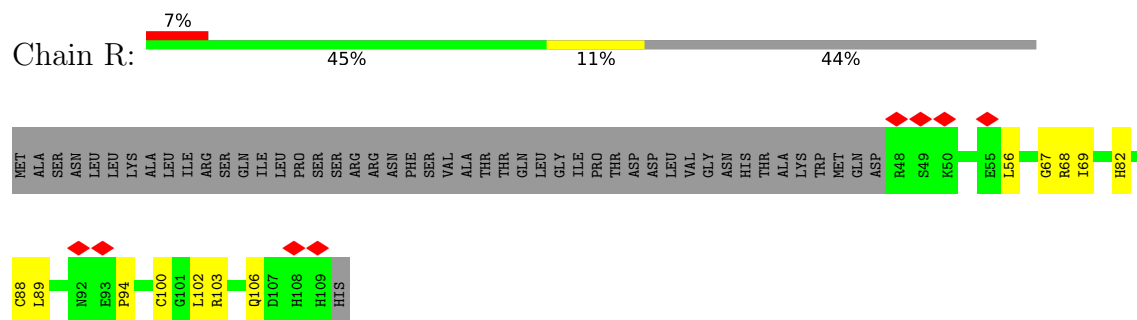
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



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

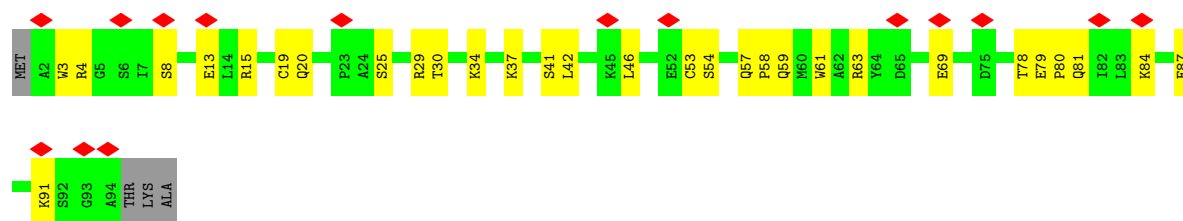


- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

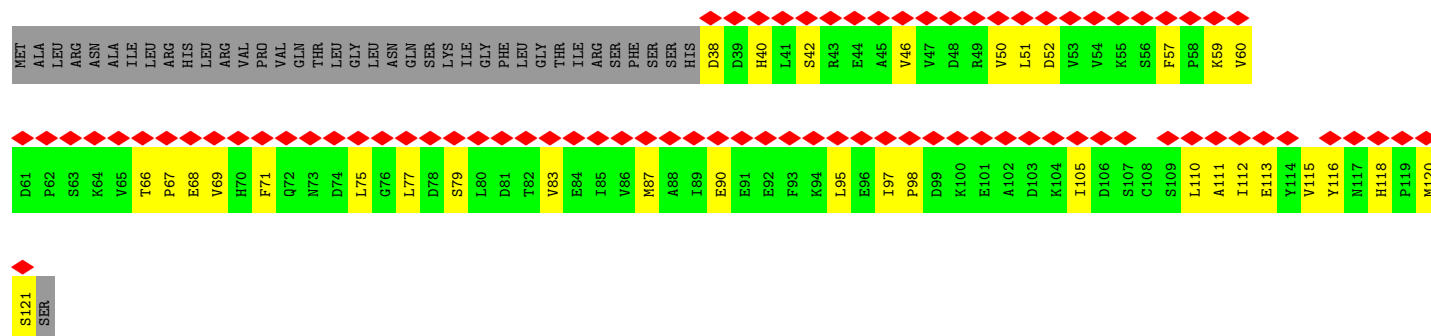


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

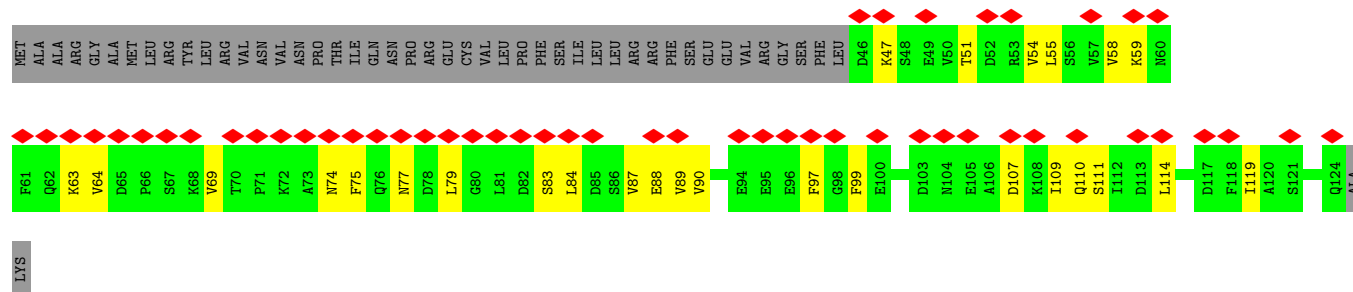




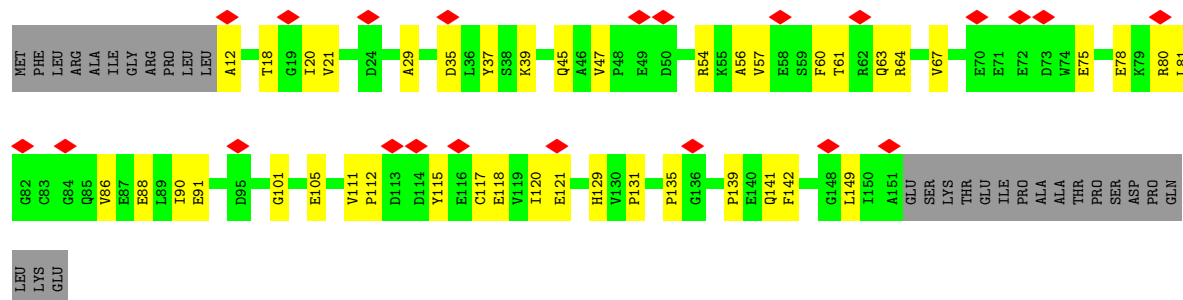
- Molecule 20: Acyl carrier protein 1, mitochondrial



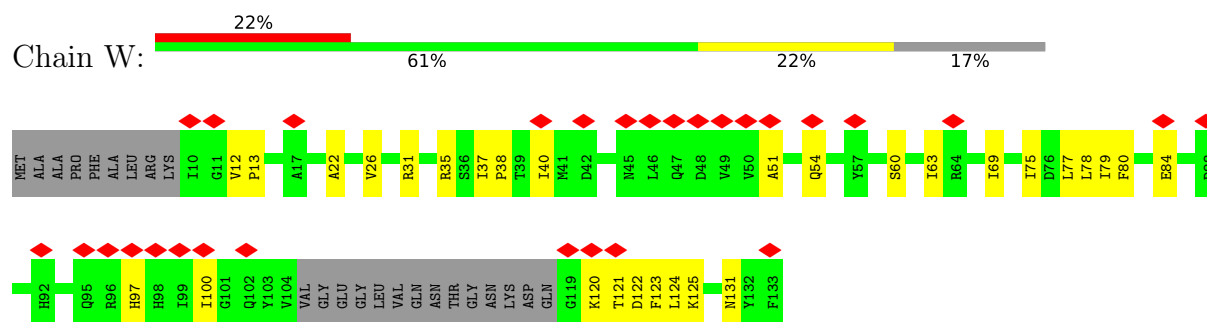
- Molecule 21: Acyl carrier protein 2, mitochondrial



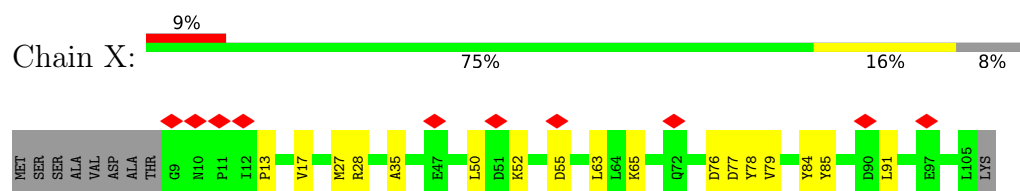
- Molecule 22: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial



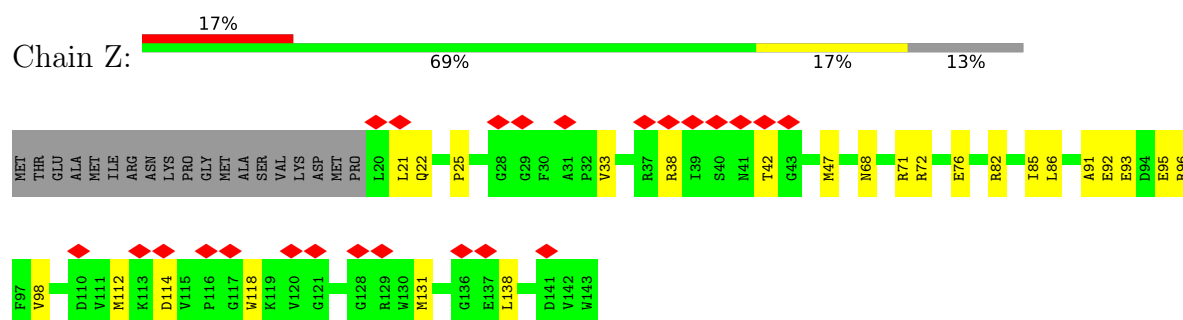
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



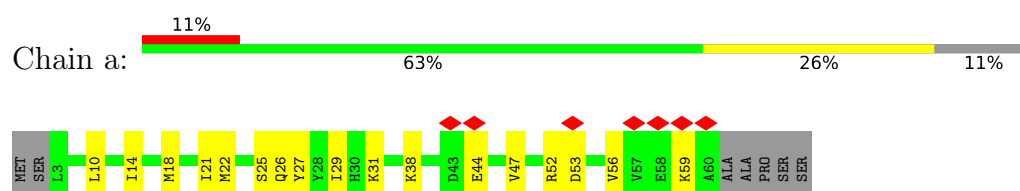
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B



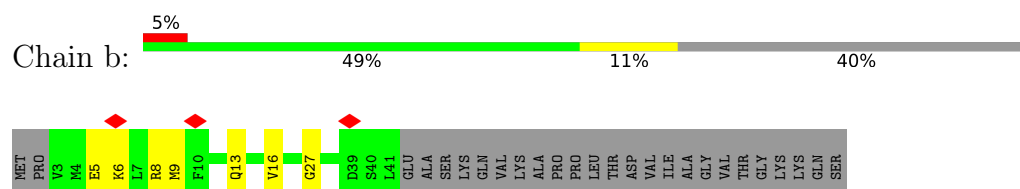
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A



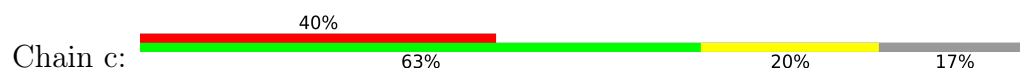
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

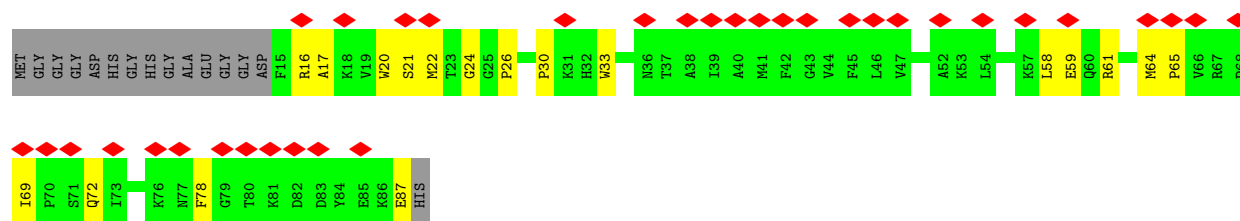


- Molecule 27: At2g46540/F11C10.23



- Molecule 28: Transmembrane protein





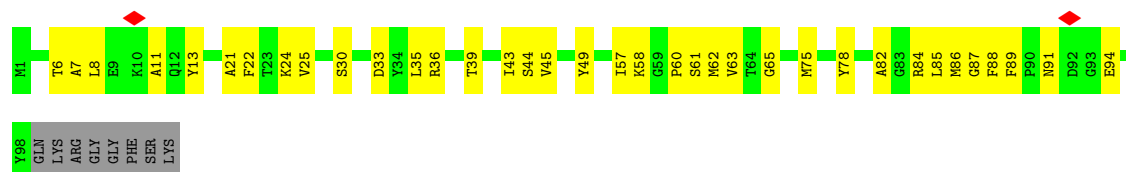
- Molecule 29: Excitatory amino acid transporter



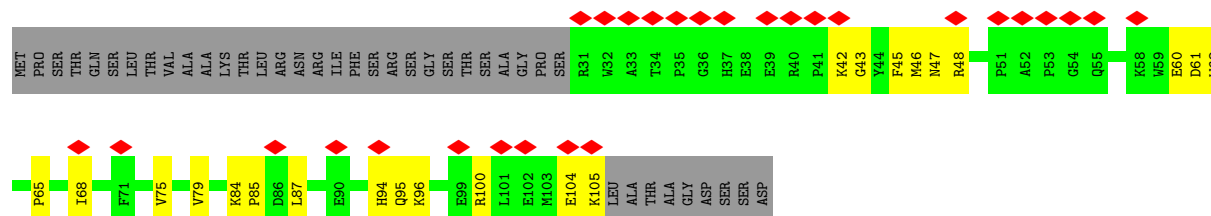
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-B



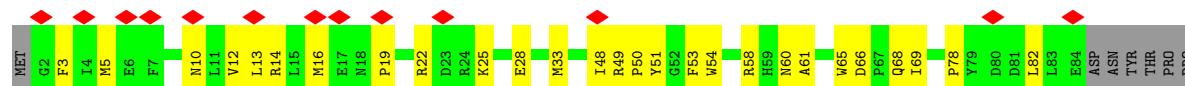
- Molecule 31: At4g16450



- Molecule 32: ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein



- Molecule 33: P1



SER
SER
SER
SER
SER
SER
SER
SER
ASP

- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2



GLY MET
GLY I10
GLY T11
GLY Y12
GLY K13
GLY G14
GLY V15
GLY T16
GLY V17
GLY H18
GLY T19
GLY P20
GLY K21
GLY T22
GLY W23
GLY H24
GLY T25
GLY V26
GLY T27
GLY G28
GLY K29
GLY G30
GLY L31
GLY C32
GLY A33
GLY V34
GLY M35
GLY W36
GLY F37
GLY W38
GLY I39
GLY L40
GLY Y41
GLY R42
GLY A43
GLY K44
GLY Q45
GLY D46
GLY G47
GLY P48
GLY V49
GLY V50
GLY M51
GLY G52
GLY W53
GLY R54
GLY H55
GLY P56
GLY W57
GLY D58
GLY G59
GLY HIS

GLY
ASP
HIS
GLY
HIS
GLY
ASP
HIS
HIS

- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3-A



GLN MET
SER ALA
SER LYS
HIS P4
HIS L5
LYS G6
GLN T7
GLN T8
PRO G9
PRO E10
HIS F11
HIS F12
HIS R13
HIS R14
HIS R15
HIS D16
HIS E17
HIS W18
HIS R19
HIS K20
HIS H21
HIS P22
HIS M23
HIS L24
HIS S25
HIS N26
HIS Q27
HIS M28
HIS R29
HIS H30
HIS A31
HIS L32
HIS P33
HIS G34
HIS I35
HIS G36
HIS I37
HIS G38
HIS V39
HIS G40
HIS A41
HIS F42
HIS C43
HIS V44
HIS Y45
HIS L46
HIS V47
HIS G48
HIS E49
HIS Q50
HIS ILE
HIS TYR
HIS SER
HIS LYS
HIS LEU
HIS MET
HIS PRO
HIS ALA
HIS SER

GLN
SER
SER
HIS
GLN
LYS
GLN
PRO
PRO
SER
HIS

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

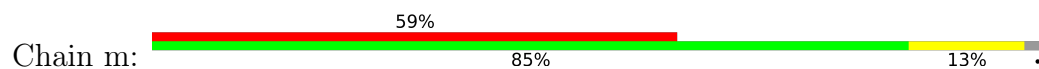


GLN MET
SER ALA
SER GLY
HIS ARG
HIS LEU
LYS SER
GLN GLY
PRO VAL
PRO ALA
SER ARG
SER ARG
SER ILE
SER MET
SER GLY
SER GLY
SER ASN
SER GLY
SER VAL
SER VAL
SER ALA
SER ARG
SER VAL
SER VAL
SER GLY
SER SER
SER SER
SER LEU
SER ARG
SER GLN
SER ARG
SER ALA
SER GLY
SER MET
SER GLY
SER VAL
SER HIS
SER ILE
SER VAL
SER PRO
SER ASP
SER LYS
SER LEU
SER LEU
SER MET
SER TRP
SER ASP
SER ASN
SER GLY
SER THR
SER ALA

PHE
PRO
GLU
PRO
CYS
ILE
ASP
ARG
ARG
ILE
ASP
ASP
THR
VAL
VAL
GLY
LYS
V76
E77
A78
L79
A80
W81
L82
S83
G84
G85
L86
G87
F88
F89
Y90
G91
L92
G93
L94
L95
A96
Y97
L98
N99
D100
K101
A102
S103
K104
V105
P106
F107
T108
P109
R110
V111
Y112
P113
Y114
D115
N116
L117
R118
V119
E120

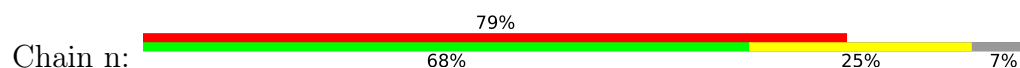
L121
G122
G123
E124
P125

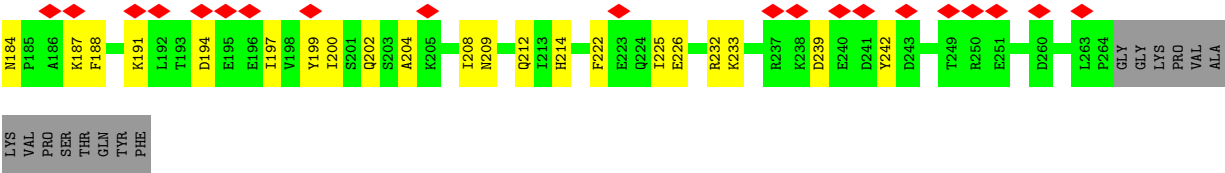
- Molecule 37: B15 – 1 beta subcomplex subunit 4



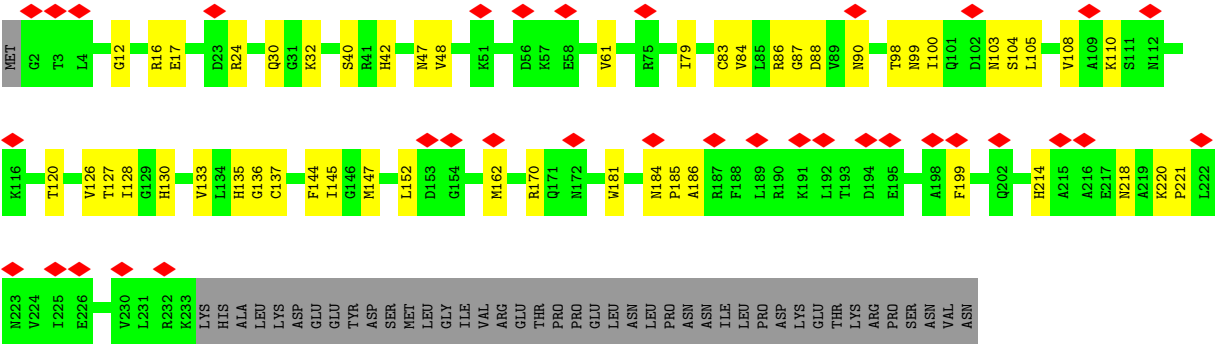
GLY MET
G2
G3
G4
H8
K9
N10
K11
F12
I13
E14
D15
W16
G17
S18
A19
R20
E21
W22
L23
E24
H25
W26
F27
R28
W29
T30
R31
R32
N33
F34
A35
L36
I37
G38
I39
F40
G41
I42
M58
Q59
D60
E61
D62
A63
G64
R65
P66
H67
R68
K69
F70
LEU

- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9





● Molecule 47: Gamma carbonic anhydrase 1, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42096	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 ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.119	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	502.2, 502.2, 502.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	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: FMN, 8Q1, NDP, PSF, PTY, ZN, LMN, UQ9, FE, FES, T7X, SF4, PGT, PC7

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	0.17	0/813	0.35	0/1103
2	B	0.18	0/1279	0.35	0/1734
3	C	0.17	0/1629	0.36	0/2207
4	D	0.17	0/3147	0.35	0/4256
5	E	0.14	0/1535	0.39	0/2084
6	F	0.13	0/3441	0.32	0/4641
7	G	0.14	0/5347	0.31	0/7242
8	H	0.18	0/2609	0.39	0/3553
9	I	0.17	0/1410	0.29	0/1904
10	J	0.16	0/1118	0.32	0/1523
11	K	0.16	0/717	0.33	0/969
12	L	0.14	0/4938	0.38	0/6706
13	M	0.15	0/3996	0.33	0/5431
14	N	0.16	0/3924	0.34	0/5327
15	O	0.11	0/971	0.30	0/1314
16	P	0.13	0/2617	0.33	0/3544
17	Q	0.13	0/966	0.26	0/1305
18	R	0.12	0/493	0.26	0/668
19	S	0.11	0/739	0.30	0/996
20	T	0.10	0/679	0.28	0/922
21	U	0.11	0/625	0.29	0/847
22	V	0.13	0/1146	0.32	0/1555
23	W	0.14	0/912	0.39	0/1234
24	X	0.12	0/781	0.30	0/1049
25	Z	0.15	0/1019	0.34	0/1381
26	a	0.14	0/481	0.36	0/646
27	b	0.13	0/292	0.28	0/396
28	c	0.11	0/614	0.31	0/829
29	d	0.16	0/585	0.35	0/788
30	e	0.15	0/559	0.28	0/745
31	f	0.16	0/750	0.34	0/1015
32	g	0.14	0/635	0.38	0/863

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	i	0.14	0/741	0.36	0/997
34	j	0.11	0/433	0.29	0/592
35	k	0.11	0/384	0.32	0/515
36	l	0.11	0/395	0.32	0/538
37	m	0.10	0/584	0.25	0/782
38	n	0.12	0/938	0.32	0/1273
39	o	0.12	0/640	0.35	0/852
40	p	0.12	0/799	0.30	0/1074
41	q	0.11	0/553	0.29	0/750
42	r	1.62	1/89 (1.1%)	3.40	4/118 (3.4%)
44	v	0.12	0/230	0.30	0/311
45	x	0.15	0/1677	0.33	0/2290
46	y	0.12	0/2034	0.31	0/2757
47	z	0.13	0/1795	0.31	0/2430
All	All	0.16	1/62059 (0.0%)	0.36	4/84056 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	r	83	PRO	C-N	14.79	1.51	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	r	83	PRO	CA-C-N	-24.16	90.97	123.10
42	r	83	PRO	C-N-CA	-24.16	90.97	123.10
42	r	83	PRO	O-C-N	9.49	138.18	123.00
42	r	83	PRO	CA-N-CD	-8.92	99.51	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	785	0	807	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1244	0	1231	54	0
3	C	1581	0	1529	42	0
4	D	3077	0	3043	98	0
5	E	1500	0	1473	49	0
6	F	3368	0	3353	95	0
7	G	5252	0	5241	129	0
8	H	2536	0	2641	80	0
9	I	1381	0	1328	30	0
10	J	1093	0	1171	31	0
11	K	707	0	771	28	0
12	L	4807	0	4847	193	0
13	M	3887	0	4037	135	0
14	N	3820	0	3926	113	0
15	O	956	0	969	30	0
16	P	2560	0	2601	87	0
17	Q	939	0	928	20	0
18	R	482	0	478	7	0
19	S	727	0	759	20	0
20	T	667	0	648	28	0
21	U	616	0	597	17	0
22	V	1123	0	1112	35	0
23	W	893	0	889	24	0
24	X	767	0	764	13	0
25	Z	990	0	971	23	0
26	a	469	0	472	15	0
27	b	288	0	314	7	0
28	c	595	0	605	14	0
29	d	574	0	593	21	0
30	e	546	0	514	10	0
31	f	734	0	733	30	0
32	g	615	0	604	19	0
33	i	721	0	695	25	0
34	j	415	0	406	9	0
35	k	374	0	369	15	0
36	l	384	0	383	21	0
37	m	569	0	553	11	0
38	n	911	0	879	28	0
39	o	631	0	646	18	0
40	p	778	0	768	28	0
41	q	536	0	495	8	0
42	r	88	0	97	6	0
43	u	150	0	33	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	v	226	0	235	6	0
45	x	1637	0	1647	52	0
46	y	2001	0	2009	61	0
47	z	1763	0	1754	38	0
48	B	8	0	0	0	0
48	F	8	0	0	2	0
48	G	16	0	0	1	0
48	I	16	0	0	0	0
49	E	4	0	0	2	0
49	G	4	0	0	0	0
50	F	31	0	19	3	0
51	H	35	0	40	2	0
52	H	50	0	79	3	0
52	M	50	0	79	0	0
52	N	50	0	79	1	0
53	M	52	0	84	6	0
53	v	52	0	84	4	0
54	N	41	0	52	1	0
55	O	1	0	0	0	0
56	P	48	0	22	4	0
57	R	1	0	0	0	0
57	y	1	0	0	0	0
58	W	35	0	0	2	0
58	n	35	0	0	0	0
59	d	69	0	88	7	0
60	z	30	0	32	0	0
61	z	61	0	0	0	0
All	All	61461	0	61576	1574	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 13.

The worst 5 of 1574 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)
22:V:67:VAL:HG11	22:V:81:LEU:HD21	1.56	0.87
18:R:82:HIS:CD2	18:R:100:CYS:SG	2.67	0.87
3:C:9:TYR:HH	3:C:48:HIS:HE2	1.26	0.84
15:O:110:ARG:HD3	15:O:115:GLU:HB3	1.58	0.83
36:l:107:PHE:HB2	39:o:69:ARG:HG2	1.63	0.81

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	88/119 (74%)	86 (98%)	2 (2%)	0	100	100
2	B	155/218 (71%)	136 (88%)	19 (12%)	0	100	100
3	C	183/190 (96%)	164 (90%)	19 (10%)	0	100	100
4	D	383/394 (97%)	354 (92%)	29 (8%)	0	100	100
5	E	190/255 (74%)	172 (90%)	18 (10%)	0	100	100
6	F	432/486 (89%)	399 (92%)	33 (8%)	0	100	100
7	G	686/748 (92%)	618 (90%)	68 (10%)	0	100	100
8	H	322/325 (99%)	290 (90%)	31 (10%)	1 (0%)	36	66
9	I	167/222 (75%)	164 (98%)	3 (2%)	0	100	100
10	J	134/205 (65%)	129 (96%)	5 (4%)	0	100	100
11	K	88/100 (88%)	85 (97%)	3 (3%)	0	100	100
12	L	613/669 (92%)	569 (93%)	44 (7%)	0	100	100
13	M	485/495 (98%)	466 (96%)	19 (4%)	0	100	100
14	N	486/499 (97%)	469 (96%)	17 (4%)	0	100	100
15	O	120/159 (76%)	113 (94%)	7 (6%)	0	100	100
16	P	330/402 (82%)	299 (91%)	30 (9%)	1 (0%)	36	66
17	Q	117/154 (76%)	111 (95%)	6 (5%)	0	100	100
18	R	60/110 (54%)	60 (100%)	0	0	100	100
19	S	91/97 (94%)	82 (90%)	9 (10%)	0	100	100
20	T	82/122 (67%)	78 (95%)	4 (5%)	0	100	100
21	U	77/126 (61%)	72 (94%)	5 (6%)	0	100	100
22	V	138/169 (82%)	133 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	W	106/133 (80%)	102 (96%)	4 (4%)	0	100	100
24	X	95/106 (90%)	90 (95%)	5 (5%)	0	100	100
25	Z	122/143 (85%)	113 (93%)	9 (7%)	0	100	100
26	a	56/65 (86%)	54 (96%)	2 (4%)	0	100	100
27	b	37/65 (57%)	37 (100%)	0	0	100	100
28	c	71/88 (81%)	62 (87%)	9 (13%)	0	100	100
29	d	71/81 (88%)	68 (96%)	3 (4%)	0	100	100
30	e	62/83 (75%)	58 (94%)	4 (6%)	0	100	100
31	f	96/106 (91%)	86 (90%)	10 (10%)	0	100	100
32	g	73/114 (64%)	67 (92%)	6 (8%)	0	100	100
33	i	81/98 (83%)	75 (93%)	6 (7%)	0	100	100
34	j	49/69 (71%)	40 (82%)	9 (18%)	0	100	100
35	k	45/72 (62%)	38 (84%)	7 (16%)	0	100	100
36	l	48/125 (38%)	47 (98%)	1 (2%)	0	100	100
37	m	67/71 (94%)	63 (94%)	4 (6%)	0	100	100
38	n	107/117 (92%)	97 (91%)	10 (9%)	0	100	100
39	o	75/103 (73%)	69 (92%)	6 (8%)	0	100	100
40	p	91/106 (86%)	81 (89%)	10 (11%)	0	100	100
41	q	63/159 (40%)	55 (87%)	8 (13%)	0	100	100
42	r	8/131 (6%)	8 (100%)	0	0	100	100
44	v	28/113 (25%)	27 (96%)	1 (4%)	0	100	100
45	x	209/256 (82%)	190 (91%)	19 (9%)	0	100	100
46	y	261/278 (94%)	239 (92%)	22 (8%)	0	100	100
47	z	230/275 (84%)	211 (92%)	19 (8%)	0	100	100
All	All	7578/9221 (82%)	7026 (93%)	550 (7%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	201	ALA
16	P	329	VAL

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	A	84/106 (79%)	84 (100%)	0	100	100
2	B	132/184 (72%)	132 (100%)	0	100	100
3	C	175/179 (98%)	175 (100%)	0	100	100
4	D	331/340 (97%)	331 (100%)	0	100	100
5	E	166/220 (76%)	166 (100%)	0	100	100
6	F	353/396 (89%)	353 (100%)	0	100	100
7	G	571/625 (91%)	571 (100%)	0	100	100
8	H	271/272 (100%)	271 (100%)	0	100	100
9	I	151/195 (77%)	151 (100%)	0	100	100
10	J	123/186 (66%)	123 (100%)	0	100	100
11	K	78/86 (91%)	78 (100%)	0	100	100
12	L	518/568 (91%)	517 (100%)	1 (0%)	87	85
13	M	426/434 (98%)	426 (100%)	0	100	100
14	N	406/416 (98%)	406 (100%)	0	100	100
15	O	107/141 (76%)	107 (100%)	0	100	100
16	P	273/334 (82%)	273 (100%)	0	100	100
17	Q	100/128 (78%)	100 (100%)	0	100	100
18	R	55/97 (57%)	55 (100%)	0	100	100
19	S	82/85 (96%)	82 (100%)	0	100	100
20	T	79/112 (70%)	79 (100%)	0	100	100
21	U	72/113 (64%)	72 (100%)	0	100	100
22	V	123/148 (83%)	123 (100%)	0	100	100
23	W	97/114 (85%)	97 (100%)	0	100	100
24	X	87/94 (93%)	87 (100%)	0	100	100
25	Z	99/115 (86%)	99 (100%)	0	100	100
26	a	48/53 (91%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	b	32/53 (60%)	32 (100%)	0	100	100
28	c	64/71 (90%)	64 (100%)	0	100	100
29	d	58/66 (88%)	58 (100%)	0	100	100
30	e	59/73 (81%)	58 (98%)	1 (2%)	53	69
31	f	78/84 (93%)	78 (100%)	0	100	100
32	g	65/96 (68%)	65 (100%)	0	100	100
33	i	75/90 (83%)	75 (100%)	0	100	100
34	j	42/51 (82%)	42 (100%)	0	100	100
35	k	38/60 (63%)	38 (100%)	0	100	100
36	l	39/97 (40%)	39 (100%)	0	100	100
37	m	57/59 (97%)	57 (100%)	0	100	100
38	n	92/99 (93%)	92 (100%)	0	100	100
39	o	67/87 (77%)	67 (100%)	0	100	100
40	p	83/93 (89%)	83 (100%)	0	100	100
41	q	54/133 (41%)	54 (100%)	0	100	100
42	r	10/118 (8%)	10 (100%)	0	100	100
44	v	23/84 (27%)	23 (100%)	0	100	100
45	x	180/216 (83%)	180 (100%)	0	100	100
46	y	220/232 (95%)	220 (100%)	0	100	100
47	z	187/228 (82%)	187 (100%)	0	100	100
All	All	6530/7831 (83%)	6528 (100%)	2 (0%)	100	100

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

Mol	Chain	Res	Type
12	L	457	HIS
30	e	52	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
18	R	109	HIS
23	W	126	ASN
46	y	125	ASN

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Mol	Chain	Res	Type
19	S	35	ASN
21	U	74	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 3 are monoatomic - leaving 22 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	SF4	I	501	9	0,12,12	-	-	-		
61	T7X	z	302	-	61,61,61	0.84	4 (6%)	71,73,73	1.07	3 (4%)
60	PSF	z	301	47	28,29,29	1.18	4 (14%)	32,36,36	1.19	2 (6%)
54	PGT	N	501	-	40,40,50	1.16	3 (7%)	43,46,56	1.10	2 (4%)
52	PTY	N	502	-	49,49,49	0.87	4 (8%)	52,54,54	1.07	2 (3%)
49	FES	E	500	5	0,4,4	-	-	-		
53	PC7	v	201	-	51,51,51	0.96	4 (7%)	57,59,59	1.05	2 (3%)
56	NDP	P	500	16	49,52,52	2.19	7 (14%)	66,80,80	1.64	14 (21%)
59	LMN	d	101	-	72,72,72	1.67	14 (19%)	96,98,98	1.13	5 (5%)
48	SF4	B	500	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	PTY	H	402	-	49,49,49	0.87	4 (8%)	52,54,54	1.11	2 (3%)
48	SF4	I	500	9	0,12,12	-	-	-	-	-
51	UQ9	H	401	8	35,35,58	2.61	13 (37%)	42,45,73	1.66	10 (23%)
58	8Q1	n	200	38	31,34,34	1.69	6 (19%)	40,43,43	1.47	4 (10%)
48	SF4	G	802	7	0,12,12	-	-	-	-	-
48	SF4	F	501	6	0,12,12	-	-	-	-	-
49	FES	G	801	7	0,4,4	-	-	-	-	-
58	8Q1	W	200	-	31,34,34	1.69	6 (19%)	40,43,43	1.49	4 (10%)
53	PC7	M	501	-	51,51,51	0.97	4 (7%)	57,59,59	1.09	2 (3%)
50	FMN	F	500	-	33,33,33	1.09	2 (6%)	48,50,50	1.21	8 (16%)
48	SF4	G	803	7	0,12,12	-	-	-	-	-
52	PTY	M	502	13	49,49,49	0.87	4 (8%)	52,54,54	1.11	2 (3%)

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	SF4	I	501	9	-	-	0/6/5/5
61	T7X	z	302	-	-	32/56/80/80	0/1/1/1
60	PSF	z	301	47	-	15/35/35/35	-
54	PGT	N	501	-	-	29/45/45/55	-
52	PTY	N	502	-	-	21/53/53/53	-
49	FES	E	500	5	-	-	0/1/1/1
53	PC7	v	201	-	-	28/55/55/55	-
56	NDP	P	500	16	-	6/34/77/77	0/5/5/5
59	LMN	d	101	-	-	28/50/130/130	0/4/4/4
48	SF4	B	500	2	-	-	0/6/5/5
52	PTY	H	402	-	-	17/53/53/53	-
48	SF4	I	500	9	-	-	0/6/5/5
51	UQ9	H	401	8	-	9/30/54/81	0/1/1/1
58	8Q1	n	200	38	-	11/41/41/41	-
48	SF4	G	802	7	-	-	0/6/5/5
48	SF4	F	501	6	-	-	0/6/5/5
49	FES	G	801	7	-	-	0/1/1/1
58	8Q1	W	200	-	-	20/41/41/41	-
53	PC7	M	501	-	-	19/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	FMN	F	500	-	-	4/18/18/18	0/3/3/3
48	SF4	G	803	7	-	-	0/6/5/5
52	PTY	M	502	13	-	24/53/53/53	-

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	500	NDP	P2B-O2B	12.23	1.82	1.59
51	H	401	UQ9	C6-C1	10.53	1.54	1.35
58	W	200	8Q1	C34-N36	5.50	1.45	1.33
58	n	200	8Q1	C34-N36	5.48	1.45	1.33
58	W	200	8Q1	C39-N41	5.39	1.45	1.33

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	P	500	NDP	PN-O3-PA	-7.00	108.80	132.83
58	n	200	8Q1	C6-C1-S44	5.39	119.73	113.46
58	W	200	8Q1	C6-C1-S44	5.30	119.63	113.46
51	H	401	UQ9	C7-C8-C9	-4.64	119.07	126.79
61	z	302	T7X	O16-C10-C12	4.28	120.72	111.50

There are no chirality outliers.

5 of 263 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	F	500	FMN	N10-C1'-C2'-O2'
50	F	500	FMN	N10-C1'-C2'-C3'
50	F	500	FMN	C5'-O5'-P-O1P
51	H	401	UQ9	C25-C24-C26-C27
51	H	401	UQ9	C23-C24-C26-C27

There are no ring outliers.

13 monomers are involved in 38 short contacts:

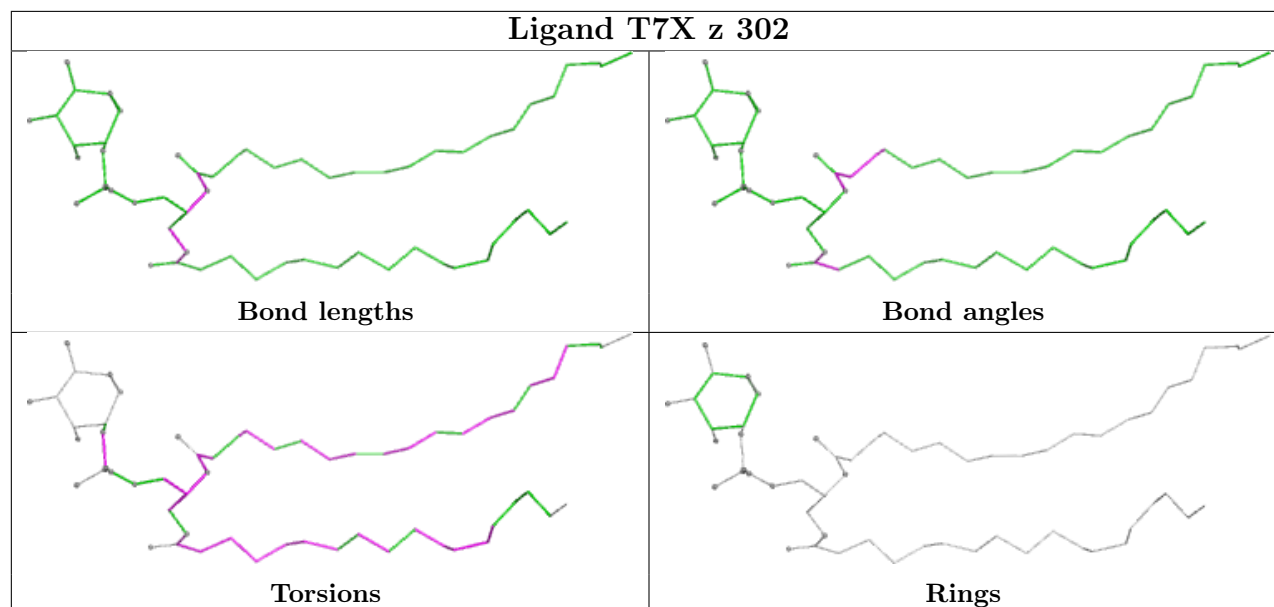
Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	N	501	PGT	1	0
52	N	502	PTY	1	0
49	E	500	FES	2	0
53	v	201	PC7	4	0

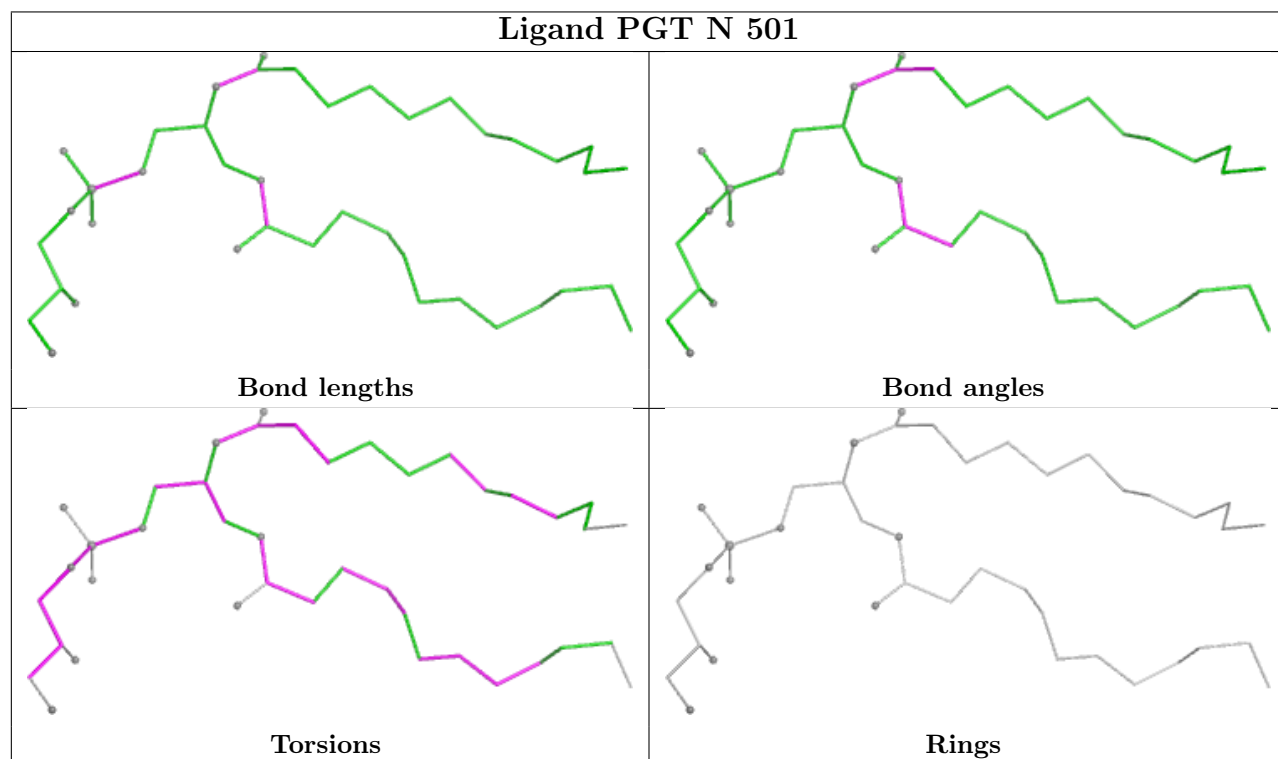
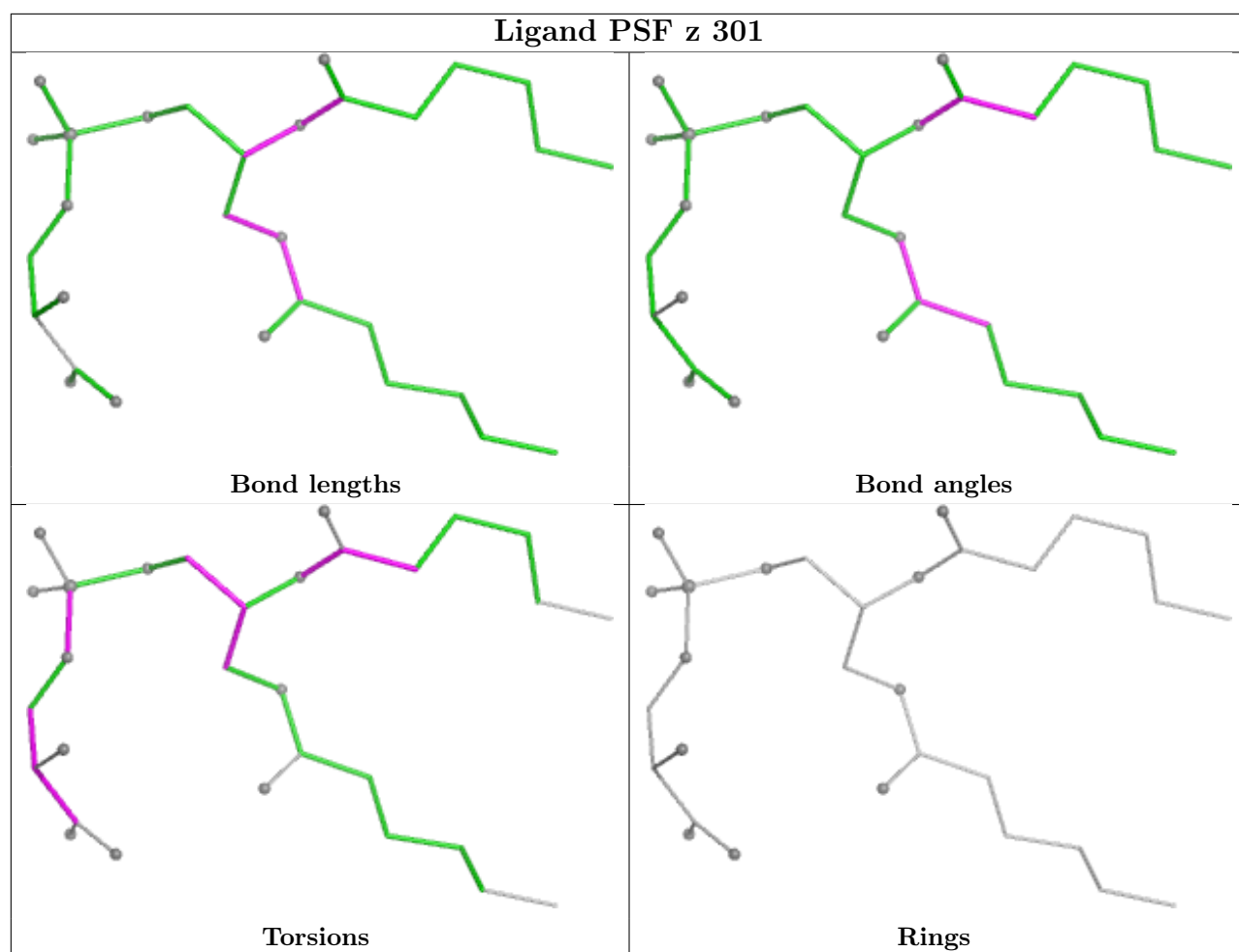
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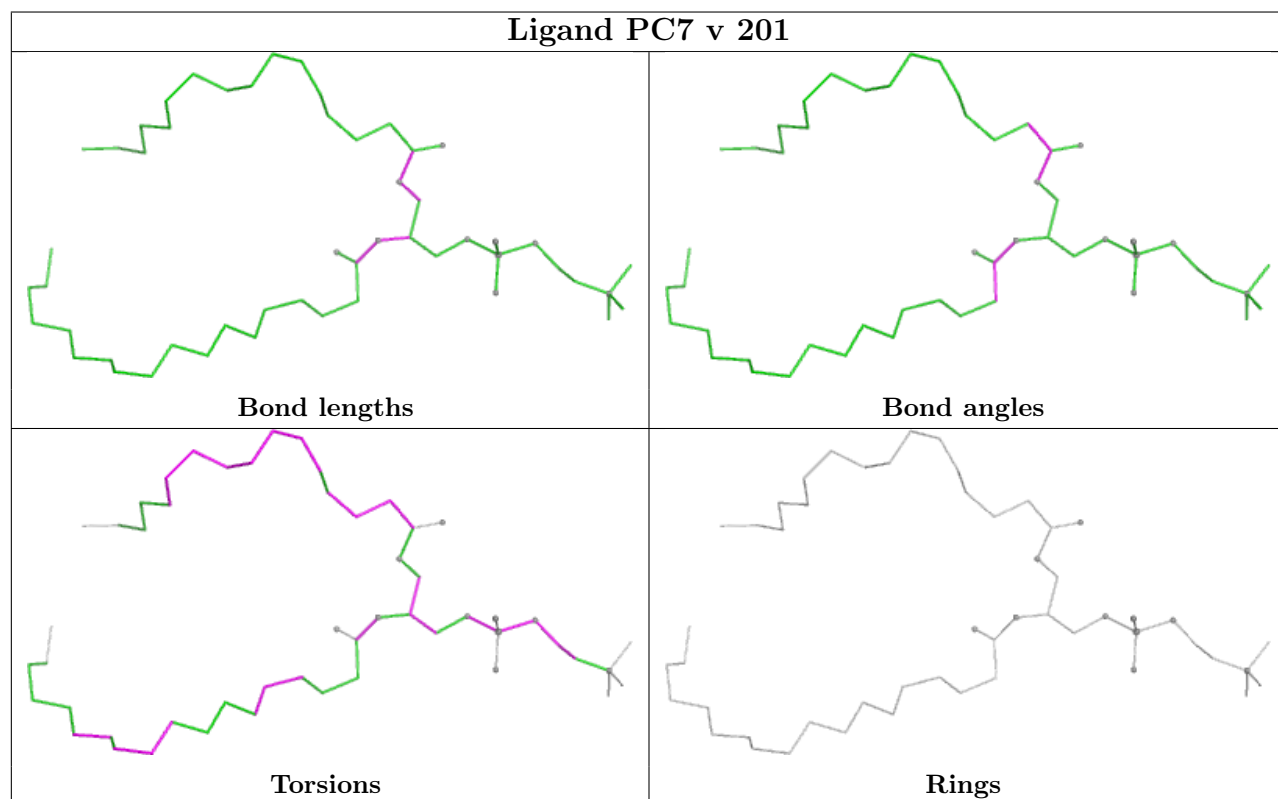
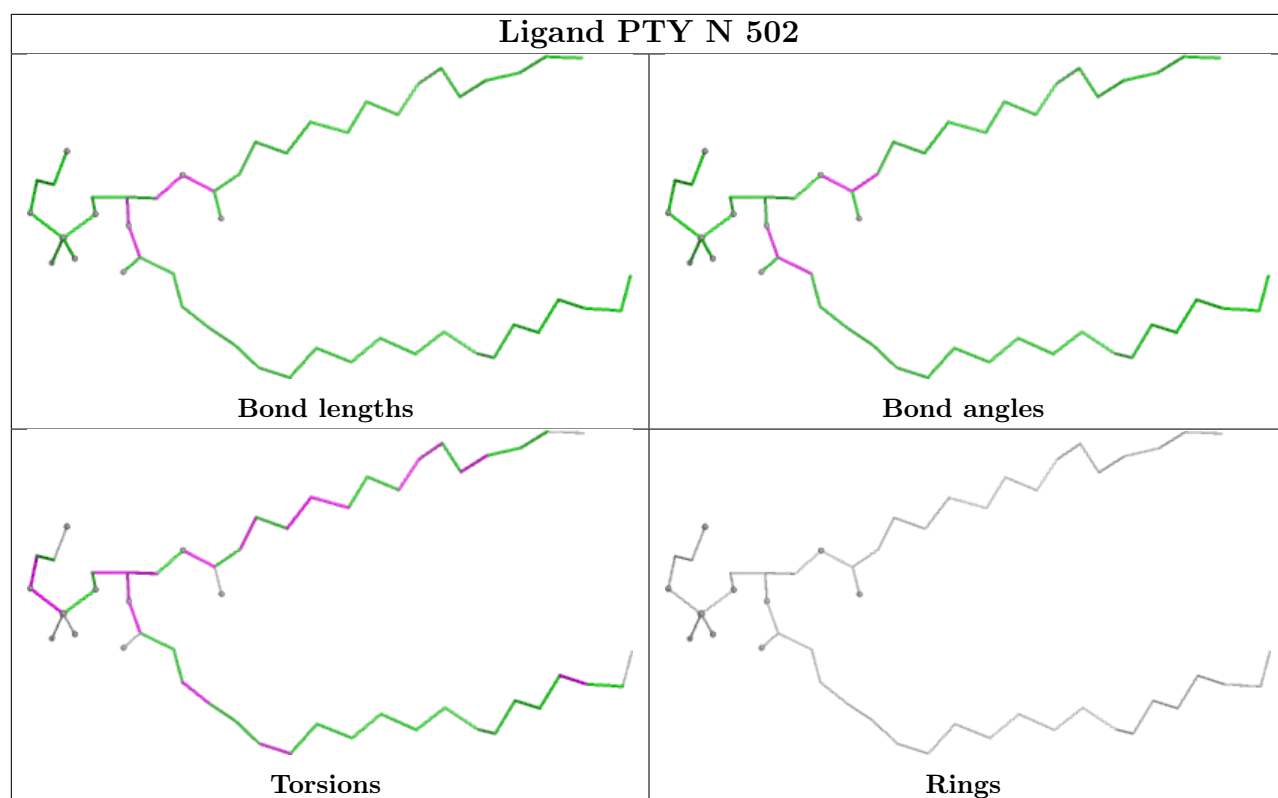
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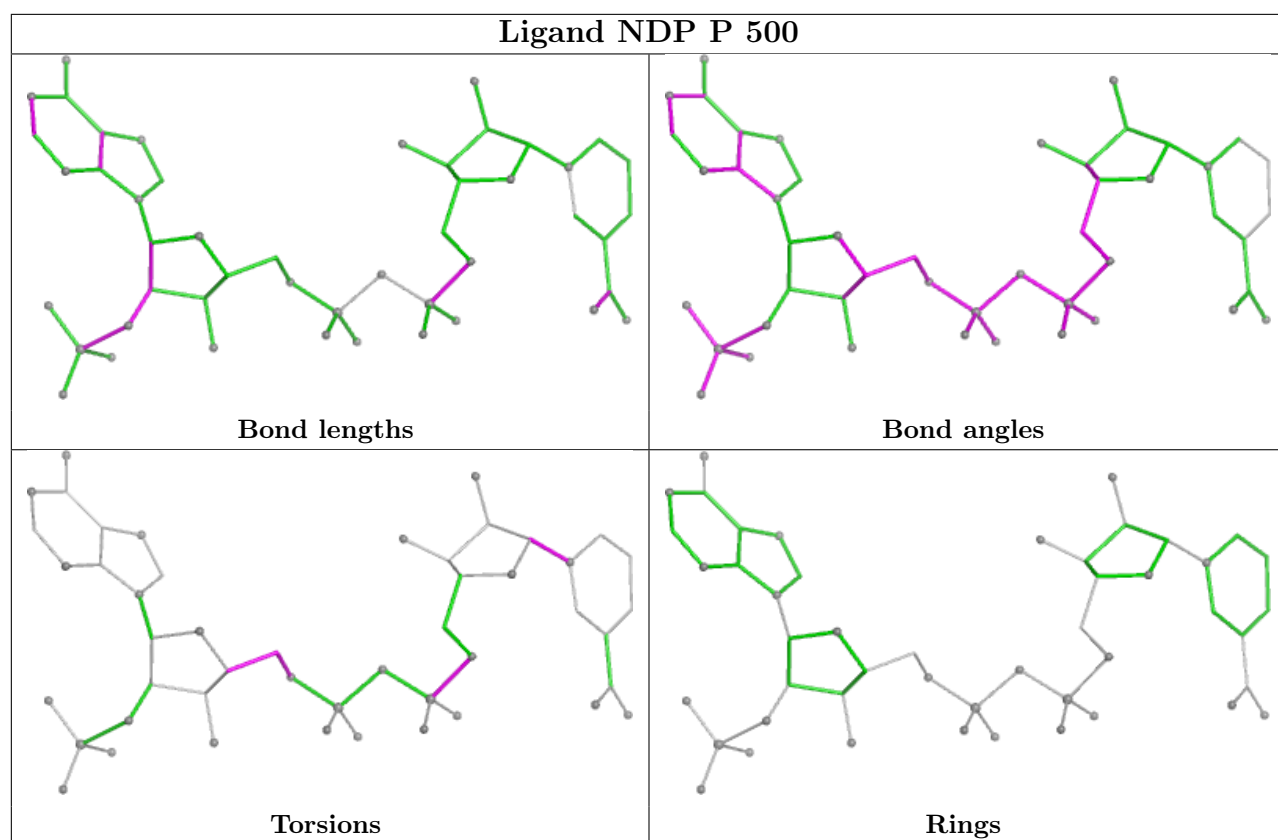
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	P	500	NDP	4	0
59	d	101	LMN	7	0
52	H	402	PTY	3	0
51	H	401	UQ9	2	0
48	G	802	SF4	1	0
48	F	501	SF4	2	0
58	W	200	8Q1	2	0
53	M	501	PC7	6	0
50	F	500	FMN	3	0

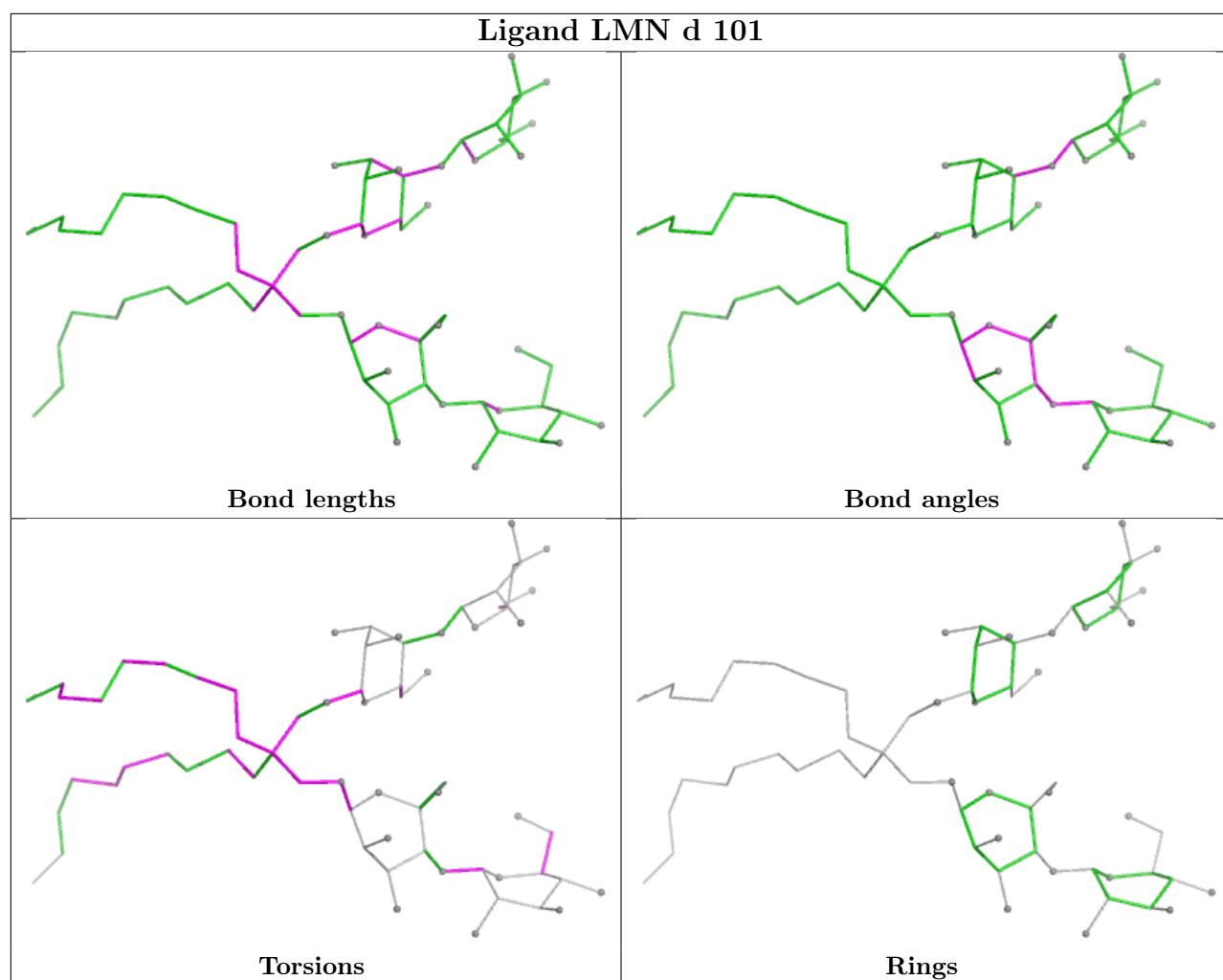
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

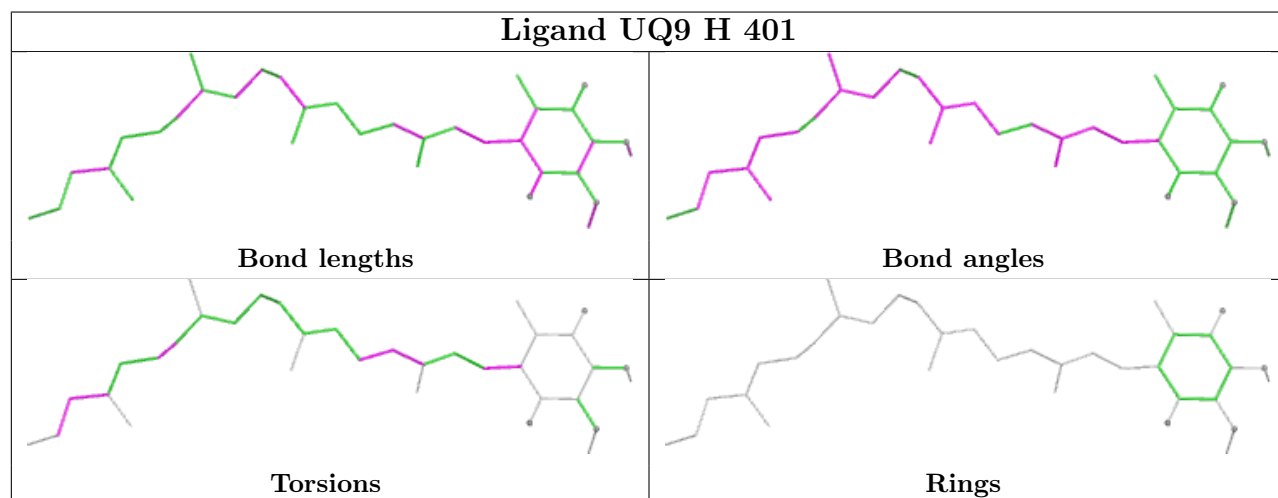
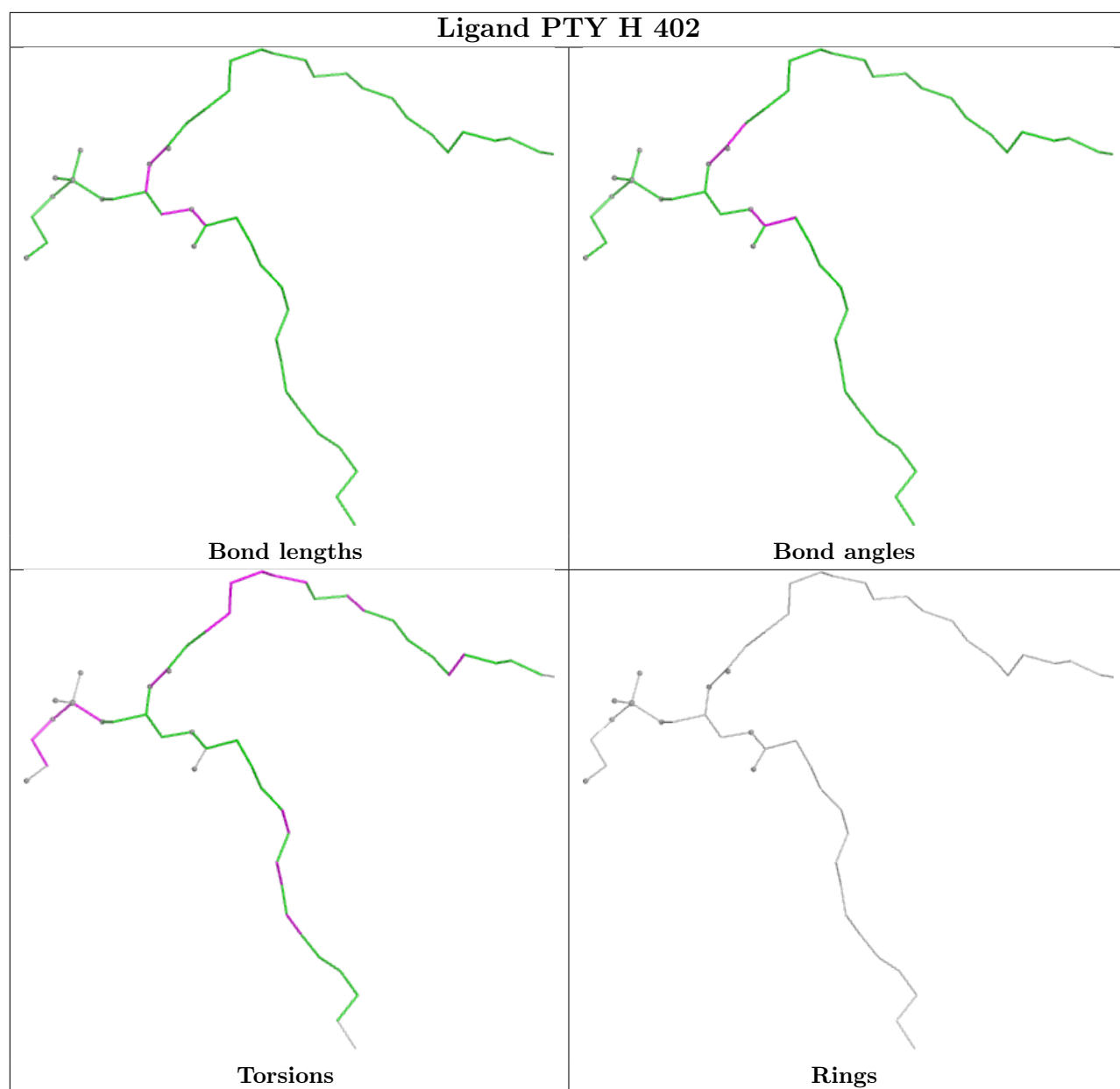


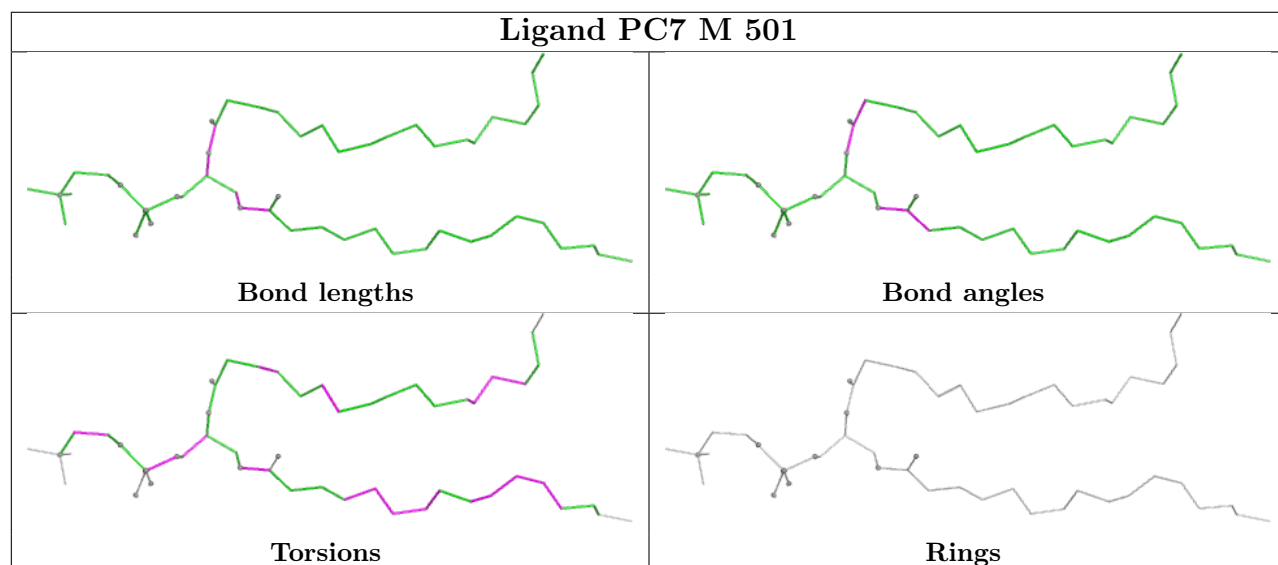
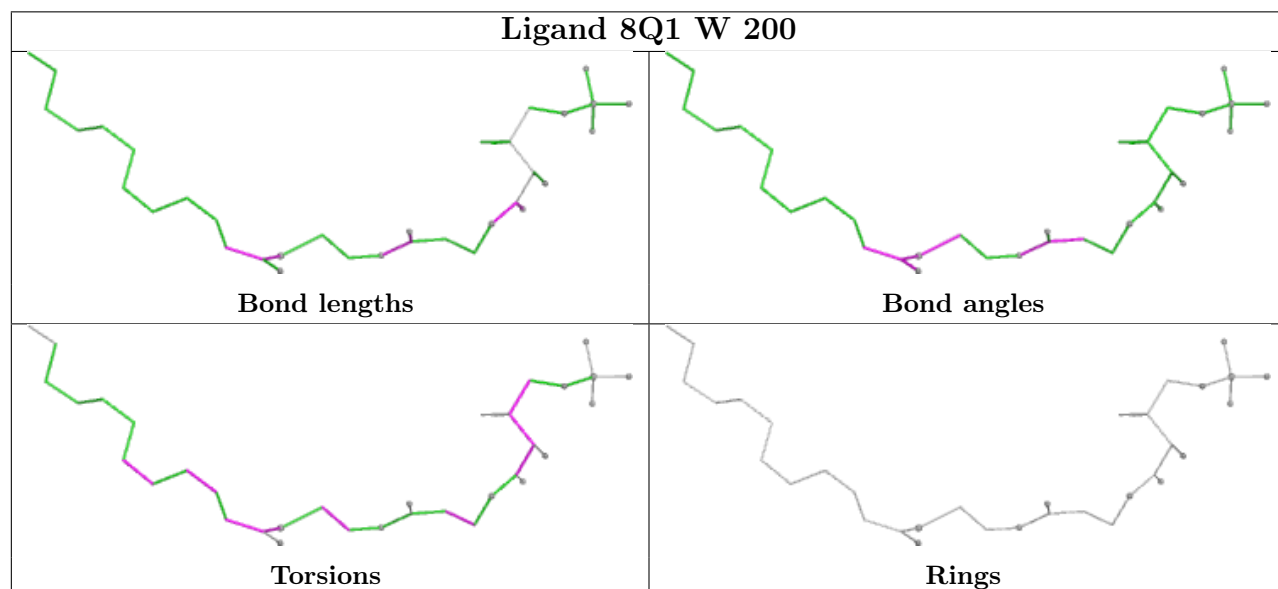
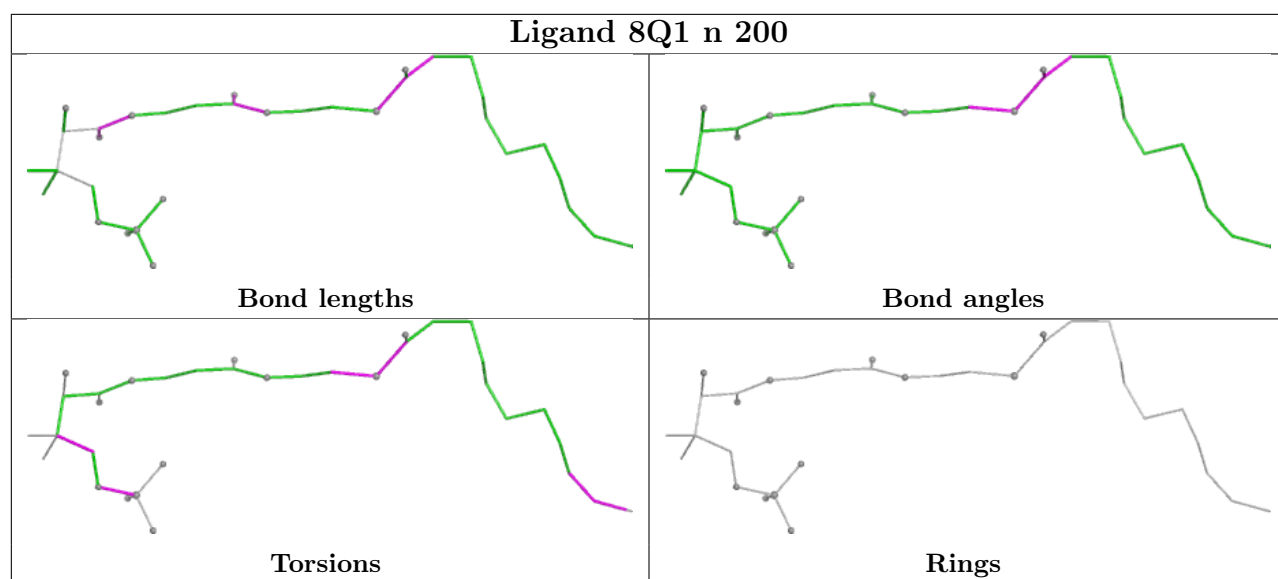


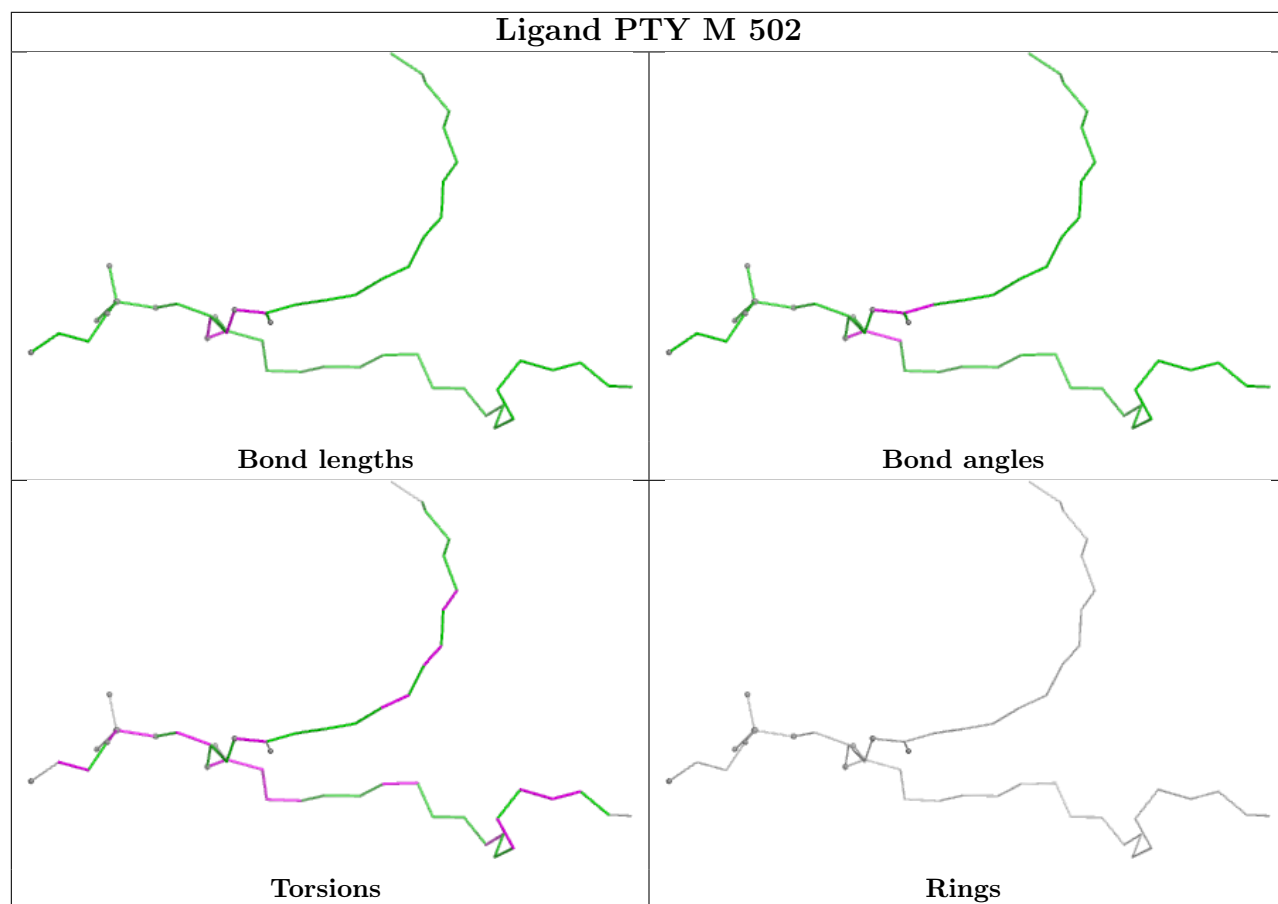
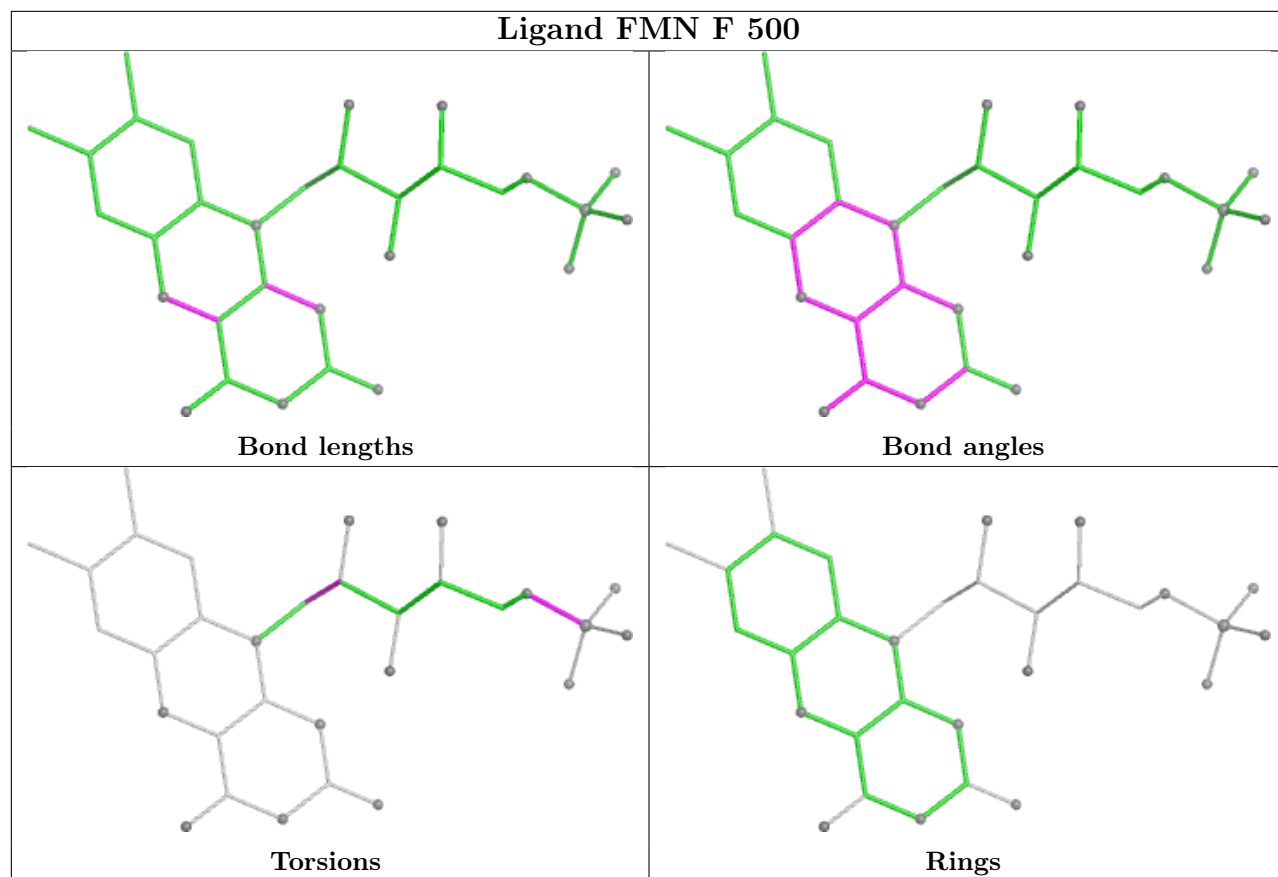












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

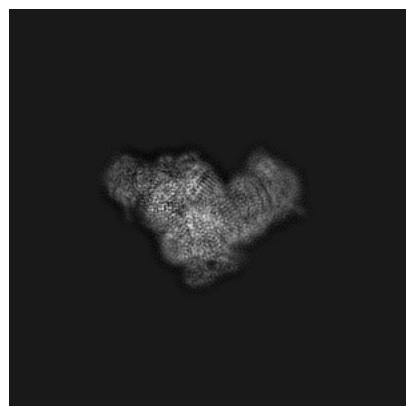
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11876. These allow visual inspection of the internal detail of the map and identification of artifacts.

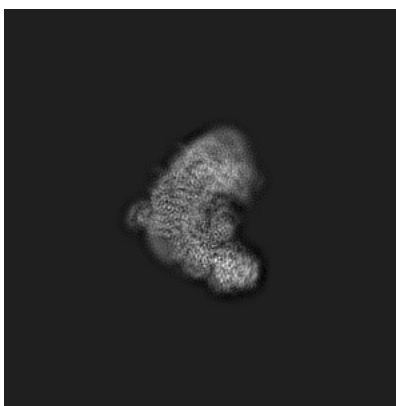
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

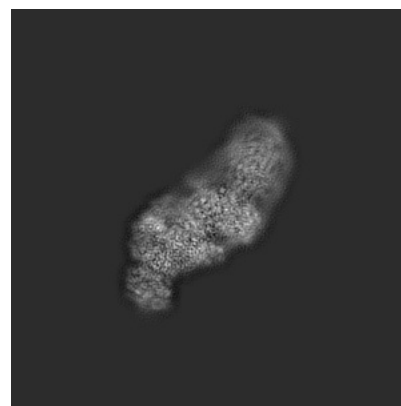
6.1.1 Primary map



X

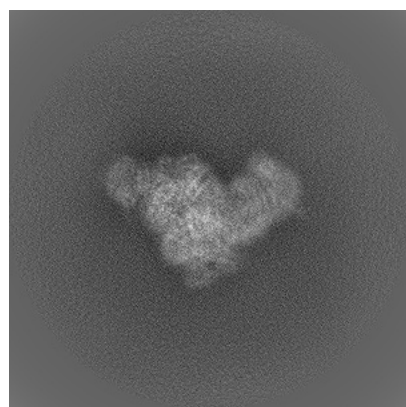


Y

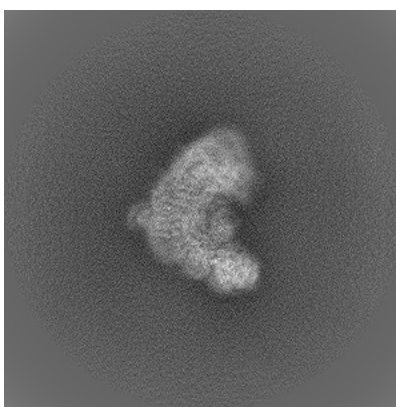


Z

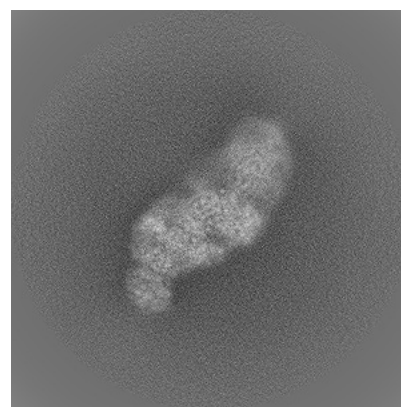
6.1.2 Raw map



X



Y

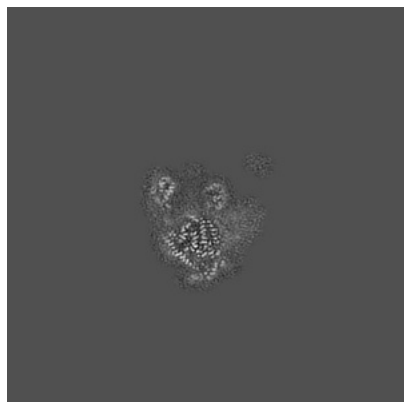


Z

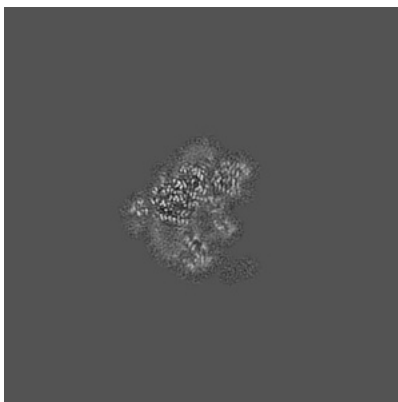
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

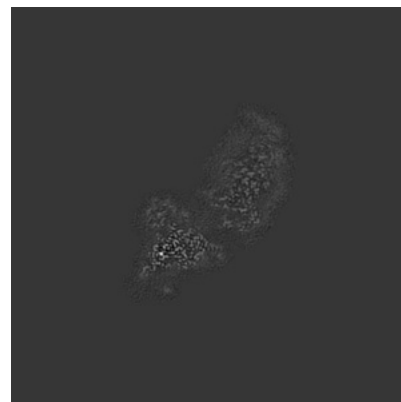
6.2.1 Primary map



X Index: 300

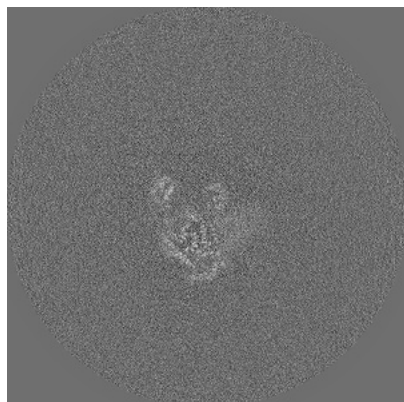


Y Index: 300

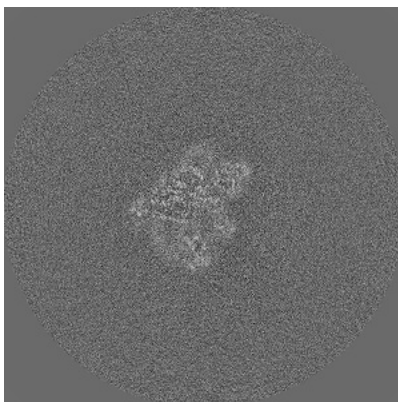


Z Index: 300

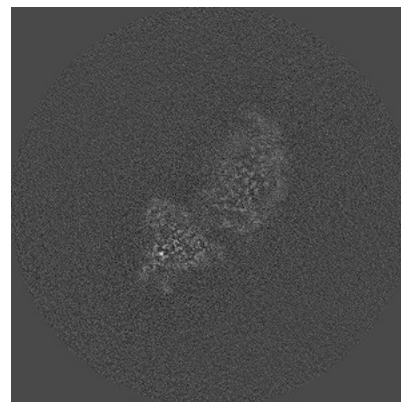
6.2.2 Raw map



X Index: 300



Y Index: 300



Z Index: 300

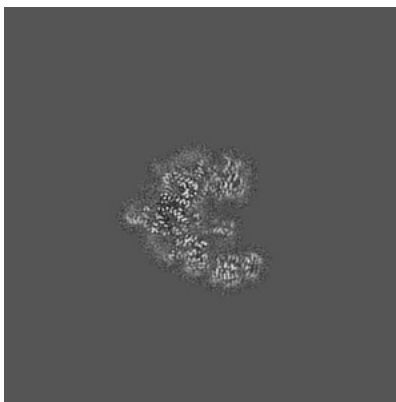
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

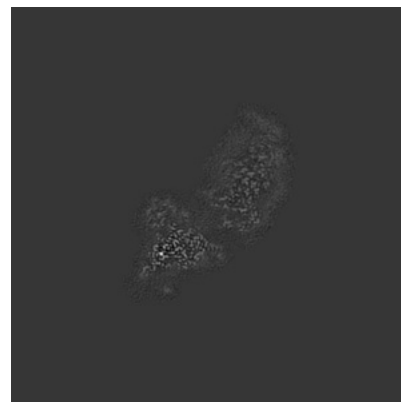
6.3.1 Primary map



X Index: 222

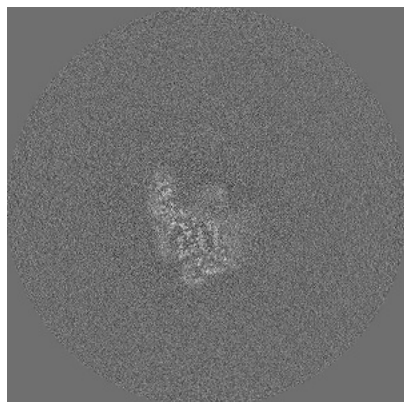


Y Index: 273

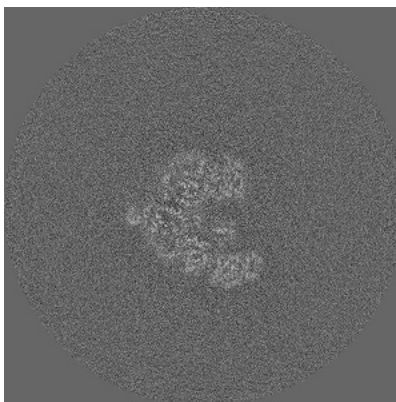


Z Index: 300

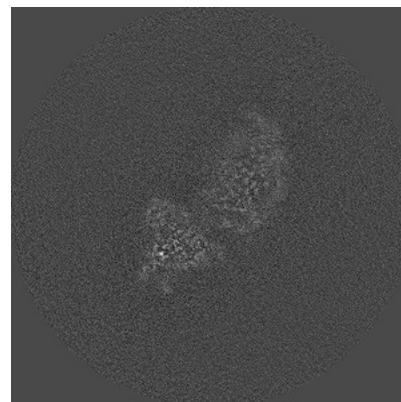
6.3.2 Raw map



X Index: 289



Y Index: 272

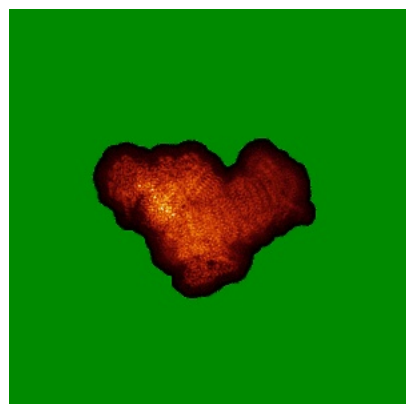


Z Index: 300

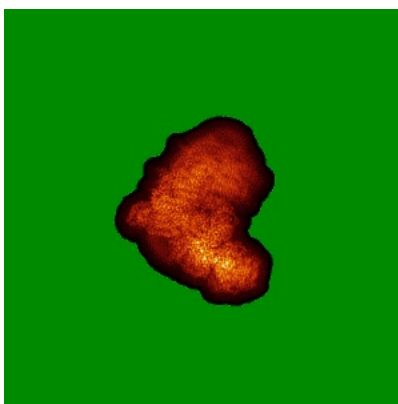
The images above show the largest variance slices of the map in three orthogonal directions.

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

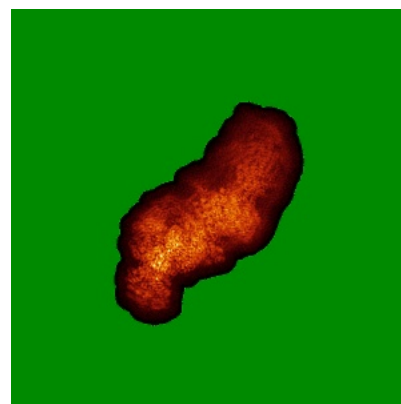
6.4.1 Primary map



X

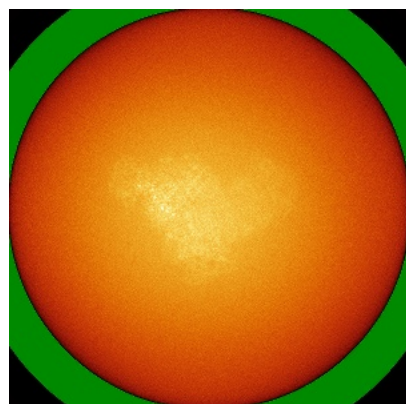


Y

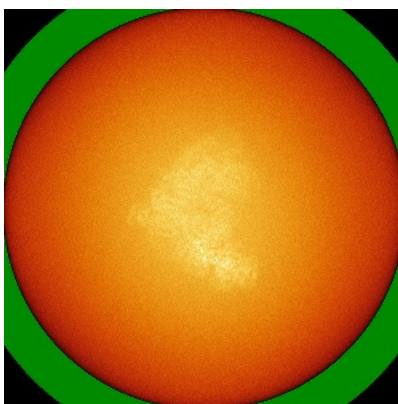


Z

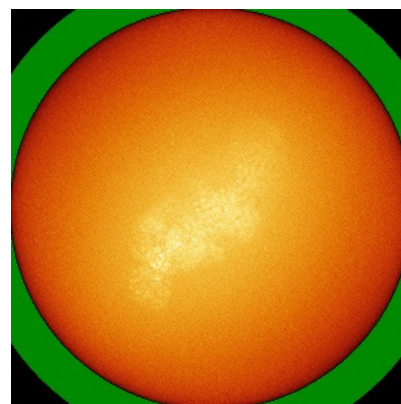
6.4.2 Raw map



X



Y

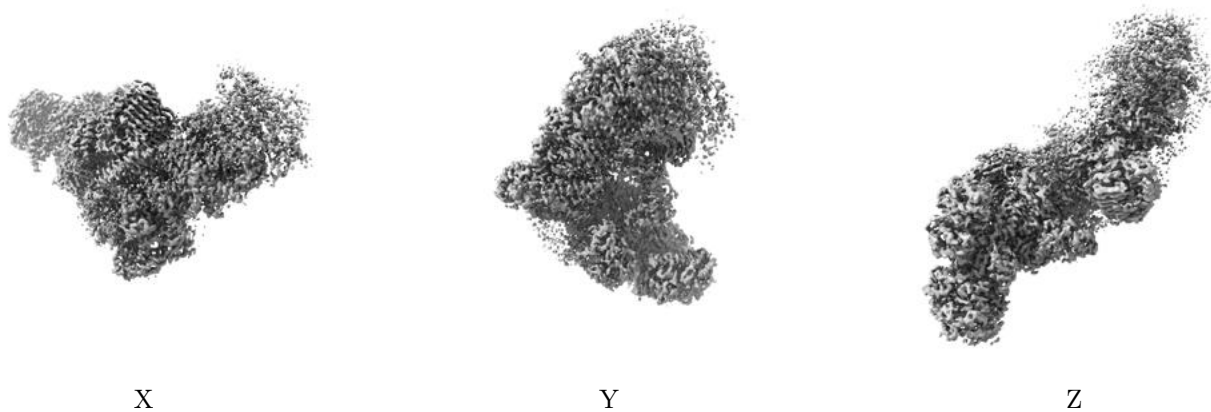


Z

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.

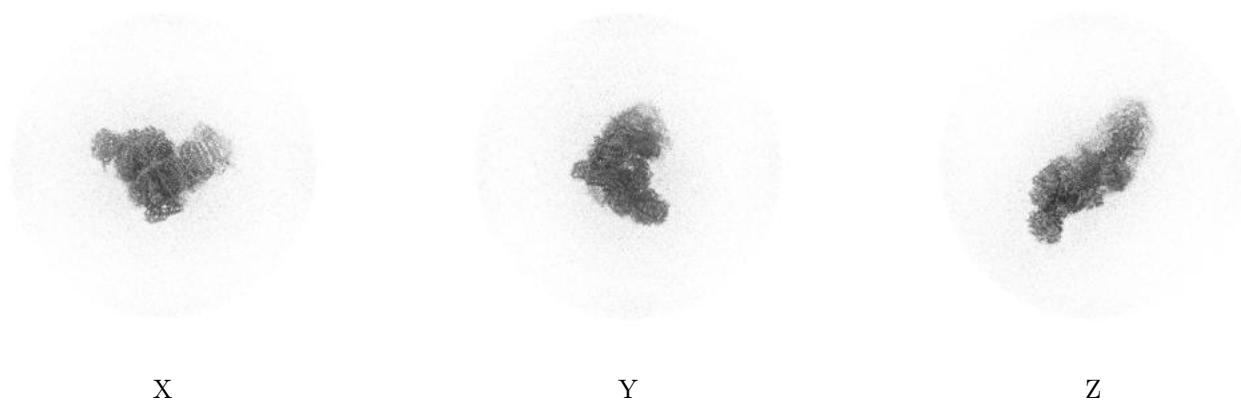
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.011. 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



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.

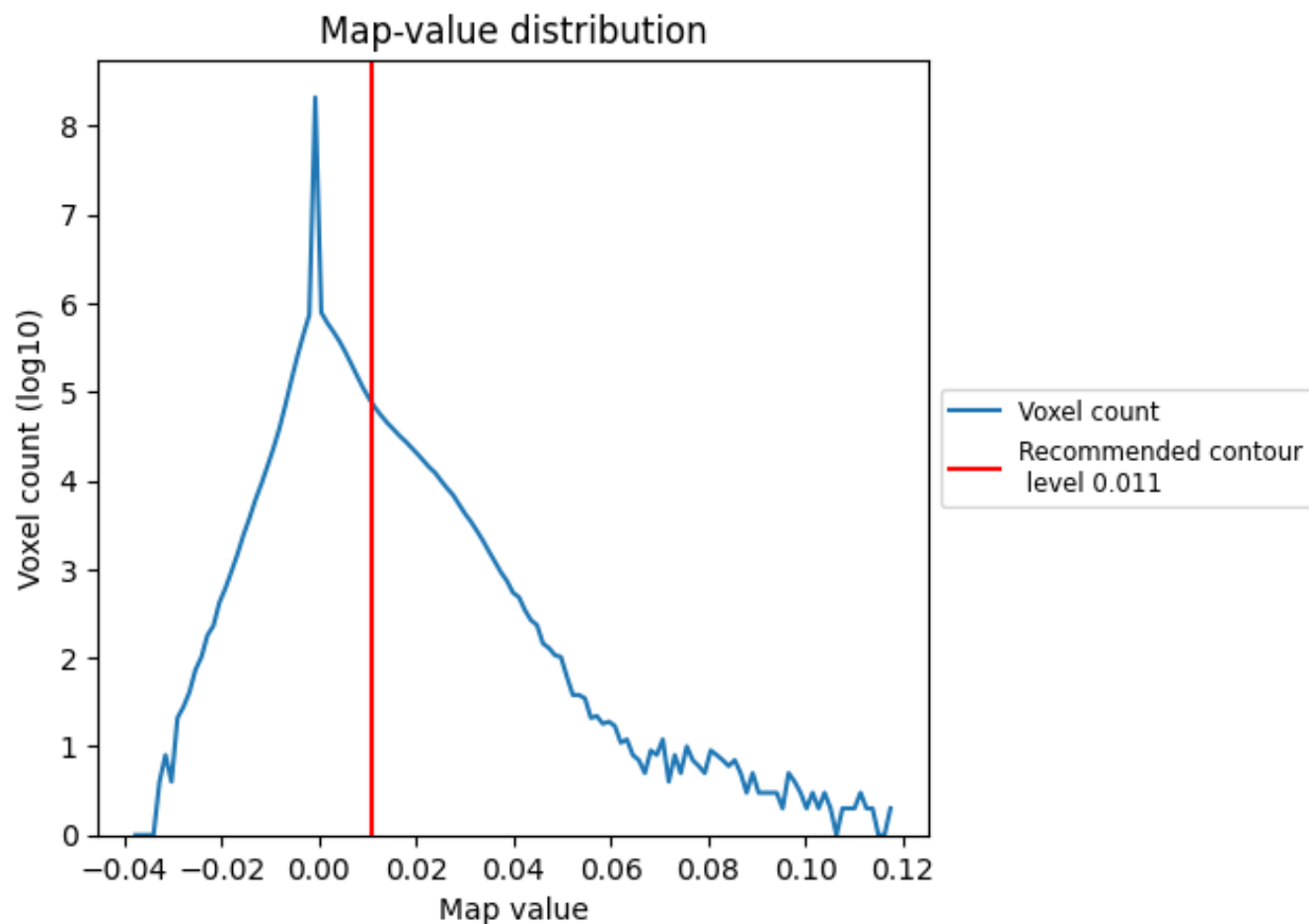
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

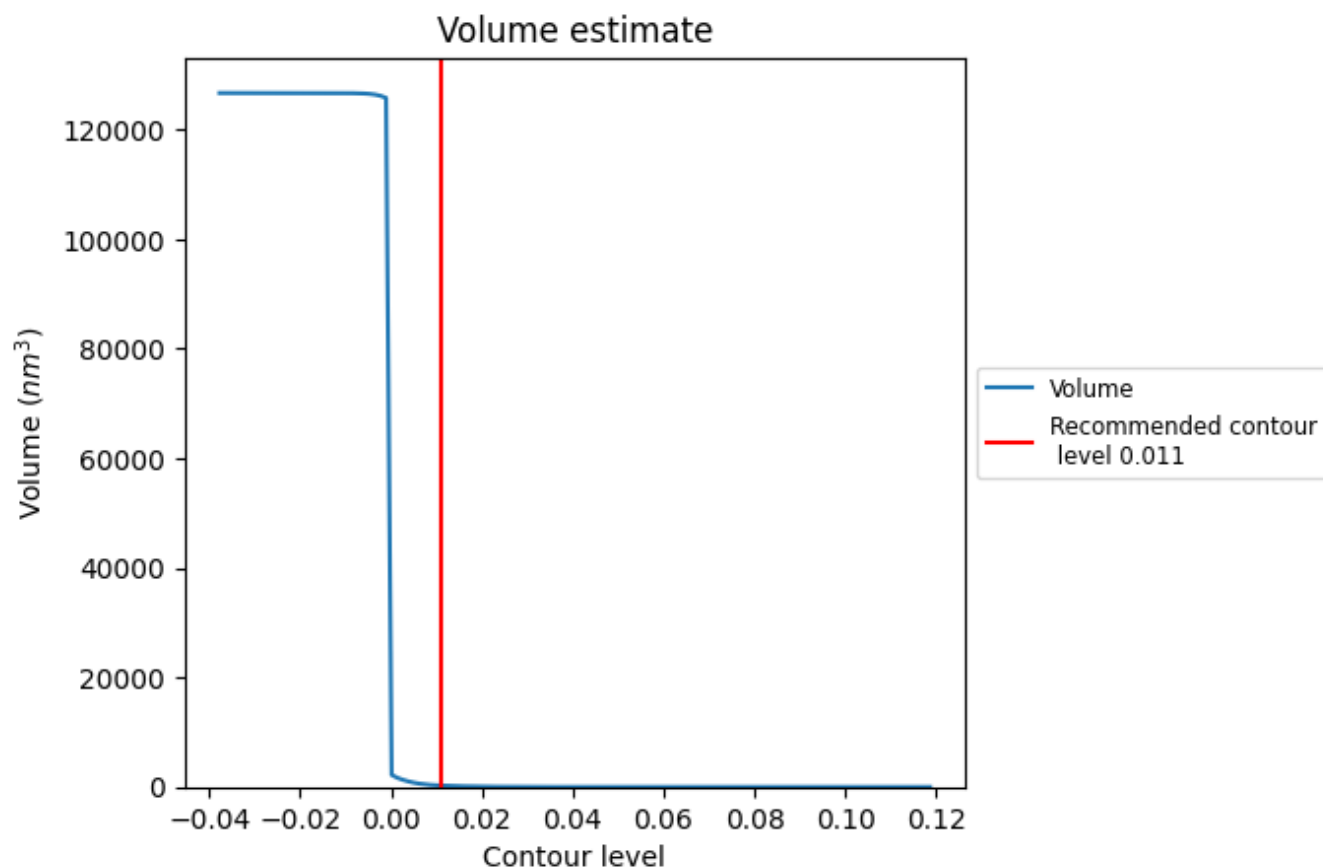
This section contains the results of statistical analysis of the map.

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.

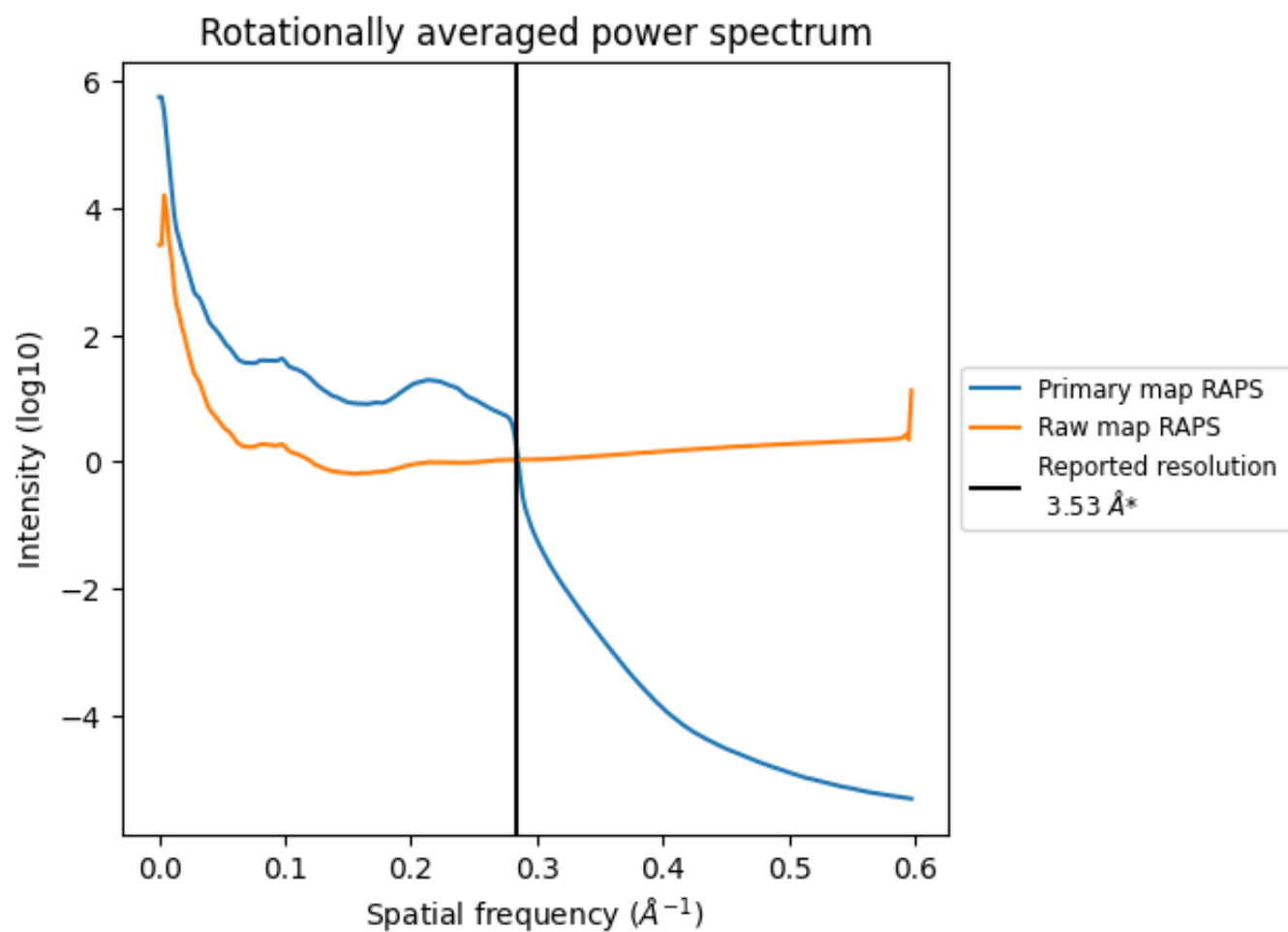
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 255 nm³; this corresponds to an approximate mass of 230 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 ⓘ

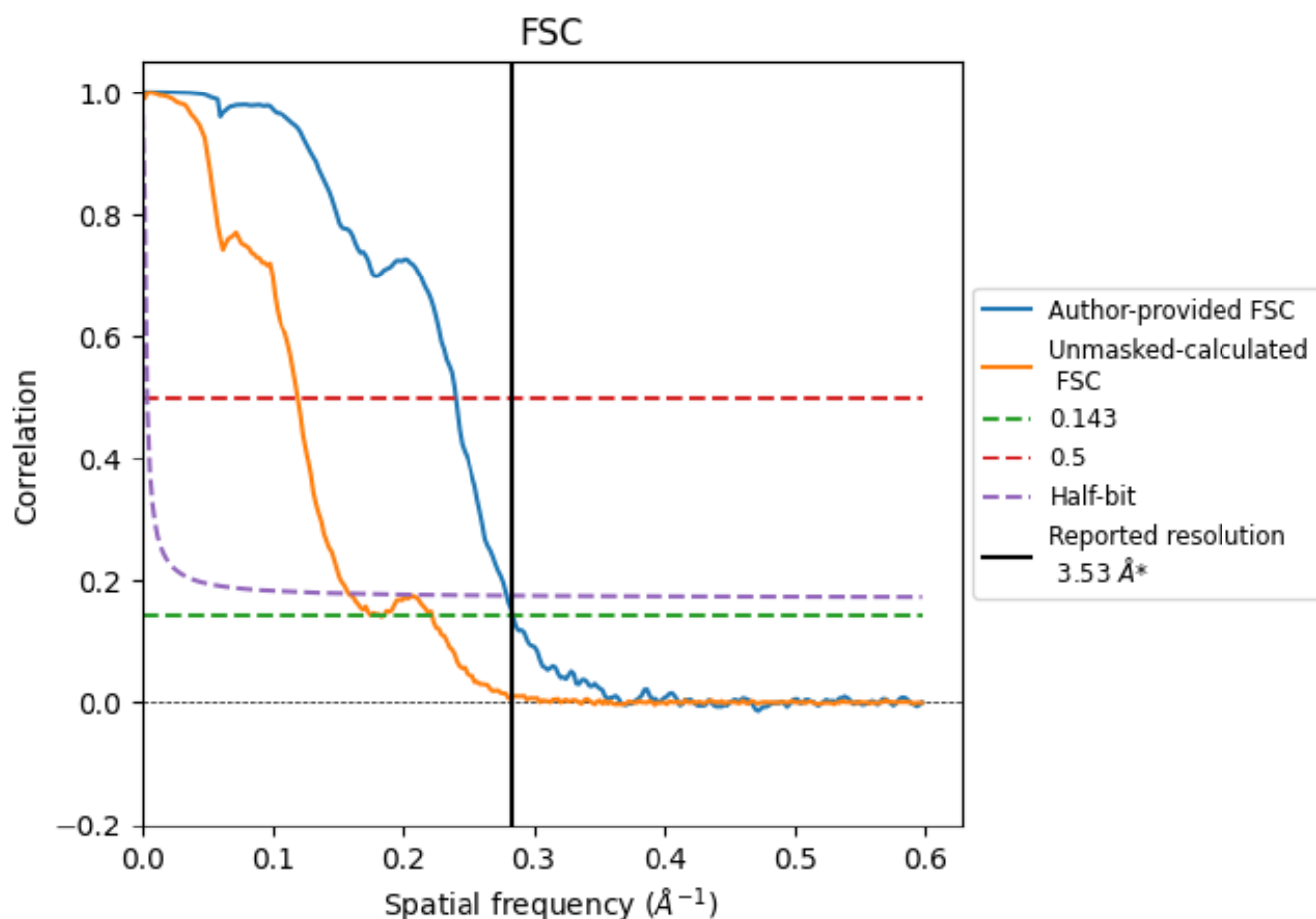


*Reported resolution corresponds to spatial frequency of $0.283 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.283 Å⁻¹

8.2 Resolution estimates [i](#)

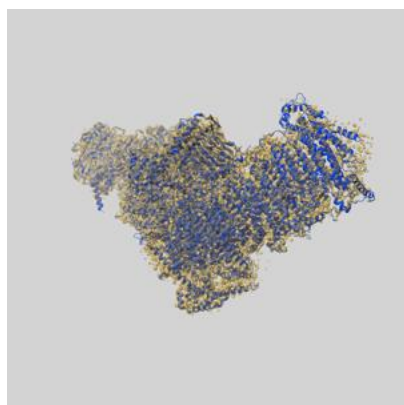
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.53	-	-
Author-provided FSC curve	3.52	4.17	3.58
Unmasked-calculated*	5.48	8.38	6.31

*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 5.48 differs from the reported value 3.53 by more than 10 %

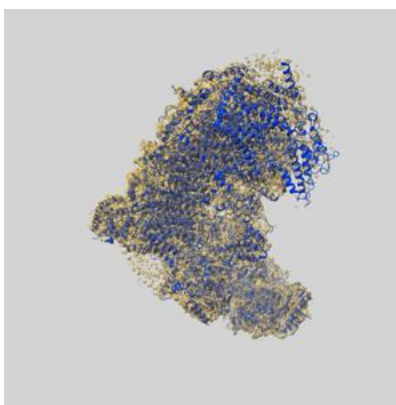
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11876 and PDB model 7AR8. Per-residue inclusion information can be found in section [3](#) on page [20](#).

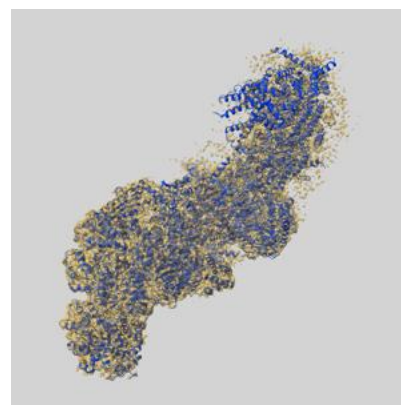
9.1 Map-model overlay [i](#)



X



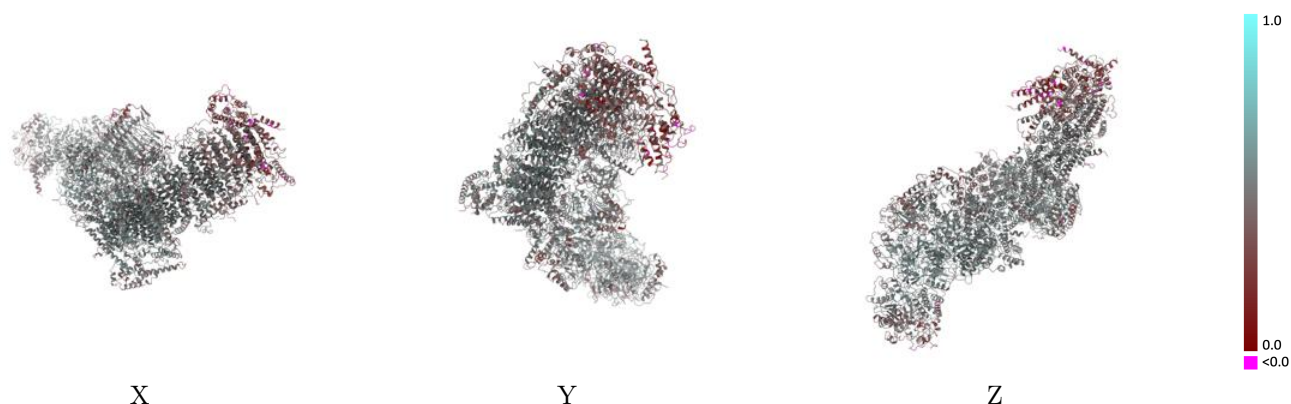
Y



Z

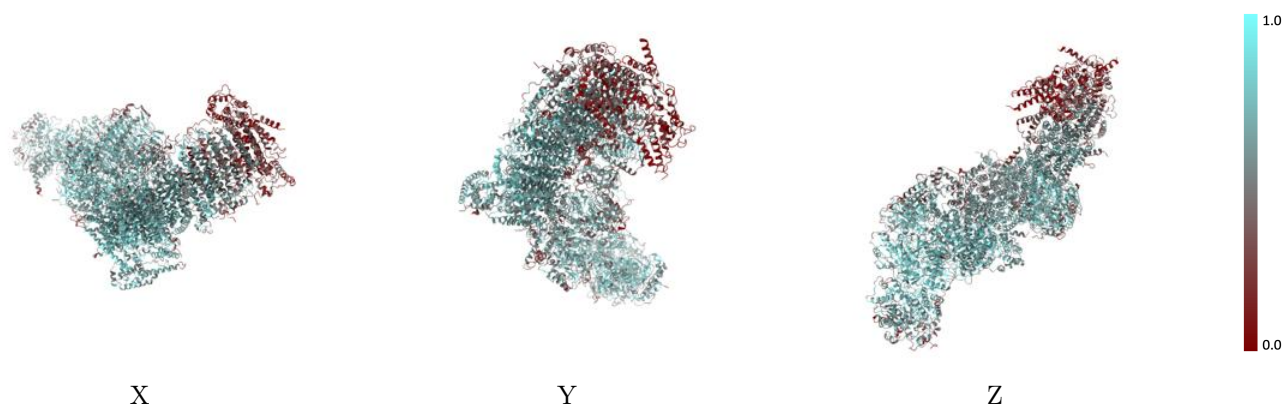
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



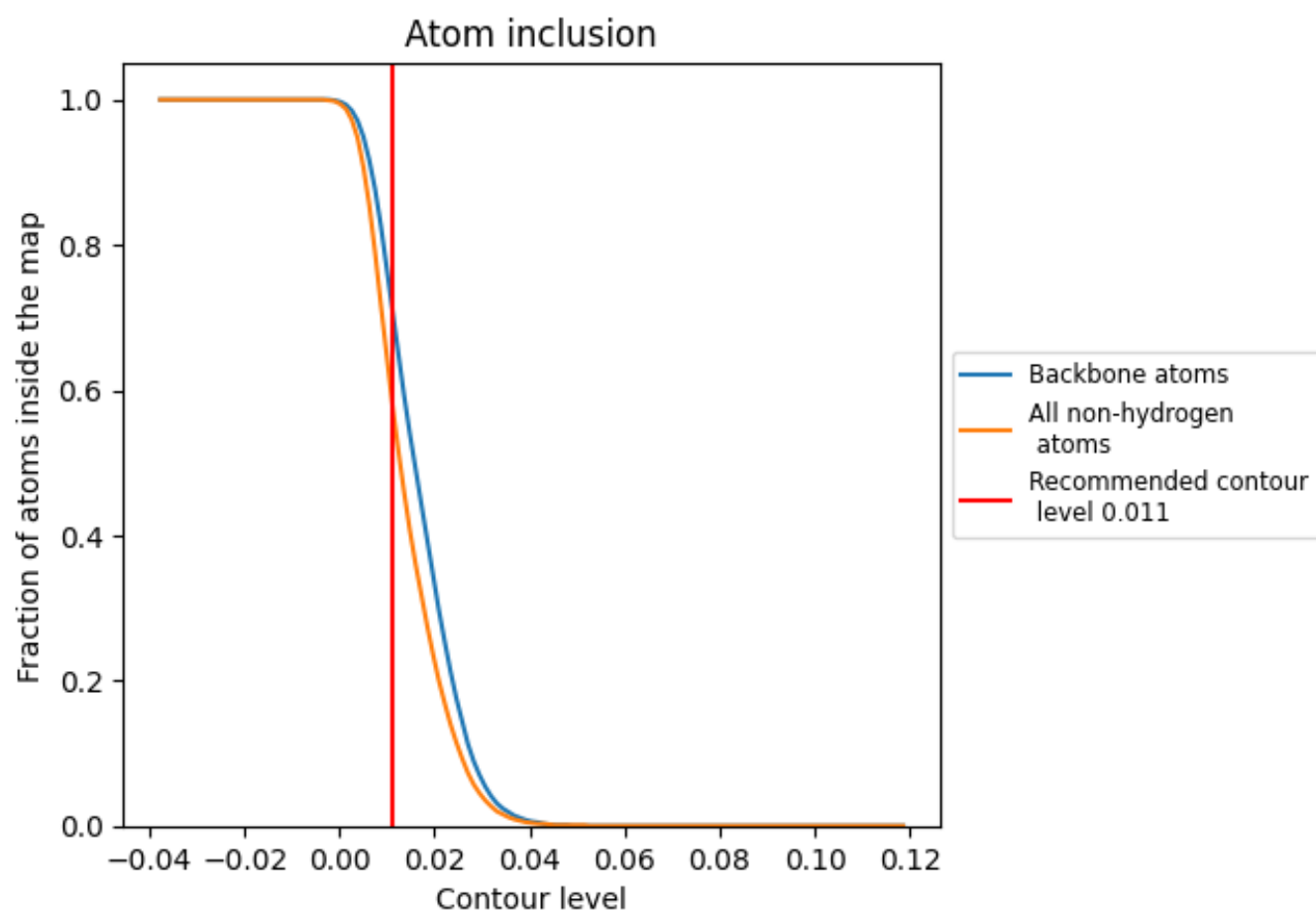
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.011).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 59% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5870	 0.4640
A	 0.6700	 0.5110
B	 0.7650	 0.5270
C	 0.7620	 0.5250
D	 0.7500	 0.5250
E	 0.5860	 0.4300
F	 0.5990	 0.4480
G	 0.7110	 0.5020
H	 0.6770	 0.5050
I	 0.7680	 0.5280
J	 0.6760	 0.5080
K	 0.6240	 0.4950
L	 0.3420	 0.3860
M	 0.6240	 0.4920
N	 0.6950	 0.5120
O	 0.4660	 0.4690
P	 0.5330	 0.4380
Q	 0.6830	 0.5180
R	 0.6970	 0.5130
S	 0.6250	 0.4400
T	 0.0590	 0.2200
U	 0.3630	 0.3910
V	 0.6280	 0.4660
W	 0.5370	 0.4540
X	 0.6330	 0.4640
Z	 0.6400	 0.4780
a	 0.6570	 0.4830
b	 0.6300	 0.4860
c	 0.4270	 0.4000
d	 0.6560	 0.4880
e	 0.7320	 0.4950
f	 0.7370	 0.5050
g	 0.4710	 0.4420
i	 0.6290	 0.4670
j	 0.1910	 0.3270



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Chain	Atom inclusion	Q-score
k	 0.1020	 0.2430
l	 0.1520	 0.2900
m	 0.3430	 0.4120
n	 0.1850	 0.2900
o	 0.2330	 0.3210
p	 0.4750	 0.4170
q	 0.1940	 0.4040
r	 0.1930	 0.3340
u	 0.6670	 0.4100
v	 0.5640	 0.4920
x	 0.6510	 0.4940
y	 0.6020	 0.4610
z	 0.6100	 0.4680