



wwPDB EM Validation Summary Report ⓘ

Sep 9, 2026 – 03:10 am BST

PDB ID : 7AR7 / pdb_00007ar7
EMDB ID : EMD-11875
Title : Cryo-EM structure of Arabidopsis thaliana complex-I (open conformation)
Authors : Klusch, N.; Kuelbrandt, W.
Deposited on : 2020-10-23
Resolution : 3.72 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:

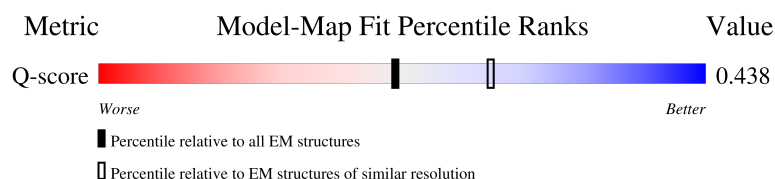
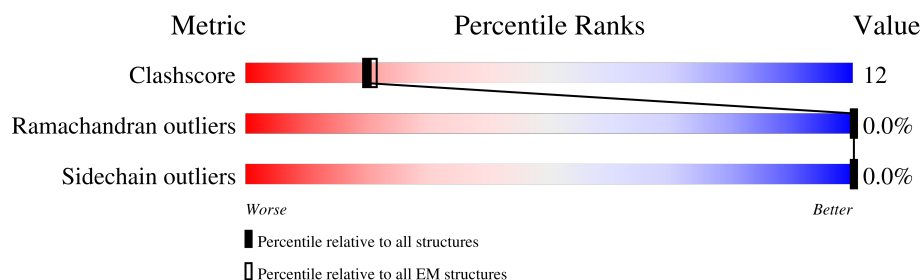
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 3.72 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	10474 (3.22 - 4.22)

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	16% 55% 23% 23%
2	B	157	76% 24%
3	C	185	74% 26%
4	D	385	68% 32%

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Mol	Chain	Length	Quality of chain
5	E	192	
6	F	434	
7	G	688	
8	H	324	
9	I	169	
10	J	205	
11	K	88	
12	L	615	
13	M	487	
14	N	488	
15	P	331	
16	Q	119	
17	R	62	
18	S	93	
19	T	84	
20	U	83	
21	V	140	
22	W	133	
23	X	96	
24	Z	125	
25	a	58	
26	b	40	
27	c	76	
28	d	75	
29	e	64	

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Mol	Chain	Length	Quality of chain
30	f	100	
31	g	72	
32	i	85	
33	j	51	
34	k	47	
35	l	46	
36	m	67	
37	n	109	
38	o	80	
39	p	93	
40	q	63	
41	r	10	
42	u	30	
43	v	30	
44	x	214	
45	y	268	
46	z	233	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
47	SF4	B	500	-	-	X	-
47	SF4	F	501	-	-	X	-
48	FES	E	500	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 60606 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 [ubiquinone] iron-sulfur protein 2.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	70	LEU	SER	conflict	UNP P93306
D	227	SER	PRO	conflict	UNP P93306
D	309	LEU	SER	conflict	UNP P93306
D	363	SER	LEU	conflict	UNP P93306

- 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		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	126	ARG	TRP	conflict	UNP P92558

- 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-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	88	Total	C	N	O	S	0	0
			692	466	107	112	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	SER	conflict	UNP Q04614

- 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 are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	91	PHE	SER	conflict	UNP P29388
L	288	PHE	SER	conflict	UNP P29388
L	537	LEU	PRO	conflict	UNP P29388

- 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 are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	146	PHE	PRO	conflict	UNP P93313
M	326	LEU	PRO	conflict	UNP P93313
M	383	PHE	SER	conflict	UNP P93313

- 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 NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	331	Total	C	N	O	S	0	0
			2556	1641	438	462	15		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

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

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

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

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	93	Total	C	N	O	S	0	0
			728	459	129	134	6		

- Molecule 19 is a protein called Acyl carrier protein 1, mitochondrial.

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

- Molecule 20 is a protein called Acyl carrier protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	83	Total	C	N	O	S	0	0
			650	411	103	135	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	108	Total	C	N	O	S	0	0
			880	563	156	158	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	96	Total	C	N	O	S	0	0
			763	478	131	142	12		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	125	Total	C	N	O	S	0	0
			997	640	175	177	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	58	Total	C	N	O	S	0	0
			470	302	84	79	5		

- Molecule 26 is a protein called At2g46540/F11C10.23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	40	Total	C	N	O	S	0	0
			295	195	48	49	3		

- Molecule 27 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	76	Total	C	N	O	S	0	0
			617	396	115	100	6		

- Molecule 28 is a protein called Excitatory amino acid transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	75	Total	C	N	O	S	0	0
			592	382	106	99	5		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-A.

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

- Molecule 30 is a protein called At4g16450.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	100	Total	C	N	O	S	0	0
			752	484	122	141	5		

- Molecule 31 is a protein called ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	72	Total	C	N	O	S	0	0
			586	379	100	104	3		

- Molecule 32 is a protein called At1g67350.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	85	Total	C	N	O	S	0	0
			737	466	135	131	5		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2.

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

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3-A.

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

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

8, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	l	46	Total	C	N	O	0	0
			360	241	57	62		

- Molecule 36 is a protein called AT2G31490 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	67	Total	C	N	O	S	0	0
			565	364	104	95	2		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	80	Total	C	N	O	S	0	0
			657	413	115	119	10		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10-B.

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

- Molecule 40 is a protein called Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	q	63	Total	C	N	O	0	0
			520	332	92	96		

- Molecule 41 is a protein called B14.5a.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	r	10	Total	C	N	O	0	0
			87	58	17	12		

- Molecule 42 is a protein called unknown.

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

- Molecule 43 is a protein called Uncharacterized protein At2g27730, mitochondrial.

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

- Molecule 44 is a protein called Gamma carbonic anhydrase-like 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	x	214	Total	C	N	O	S	0	0
			1659	1063	285	306	5		

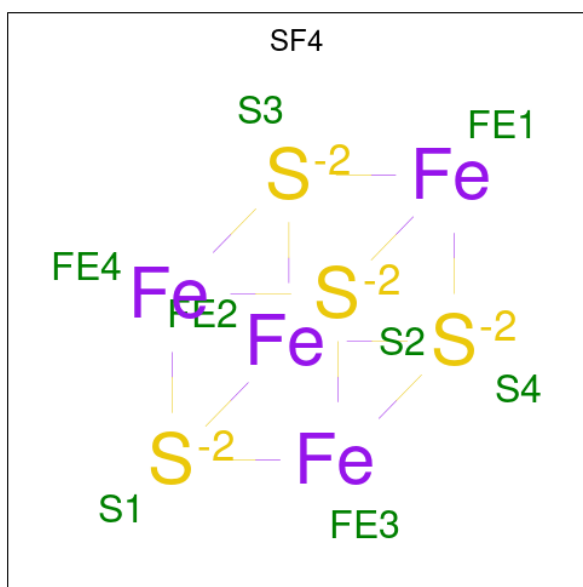
- Molecule 45 is a protein called Gamma carbonic anhydrase 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	y	268	Total	C	N	O	S	0	0
			2032	1271	363	391	7		

- Molecule 46 is a protein called Gamma carbonic anhydrase 1, mitochondrial.

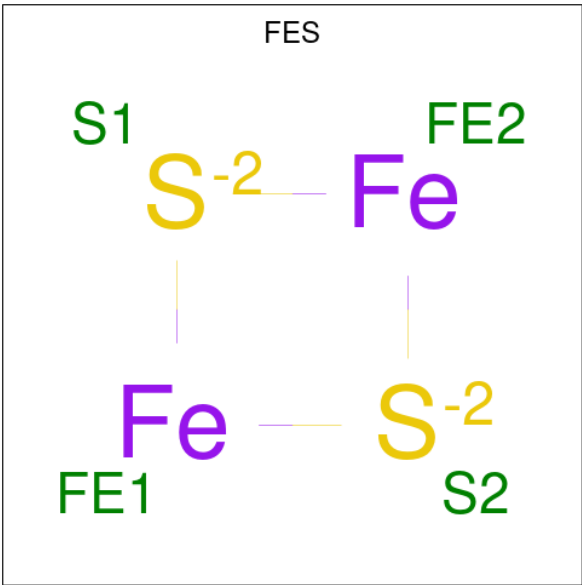
Mol	Chain	Residues	Atoms					AltConf	Trace
46	z	233	Total	C	N	O	S	0	0
			1772	1111	325	330	6		

- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



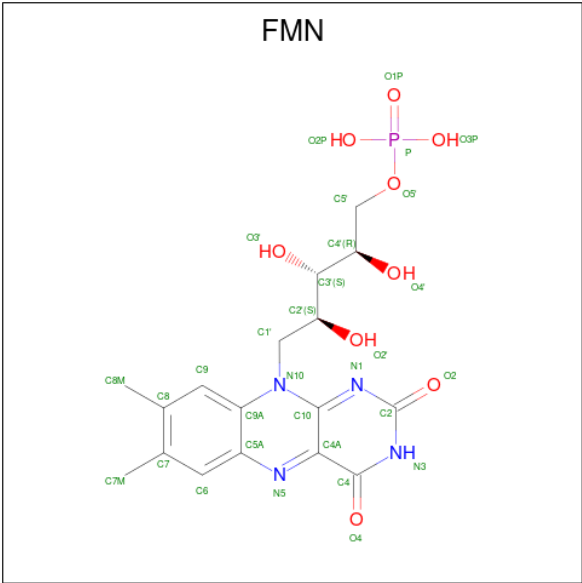
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

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



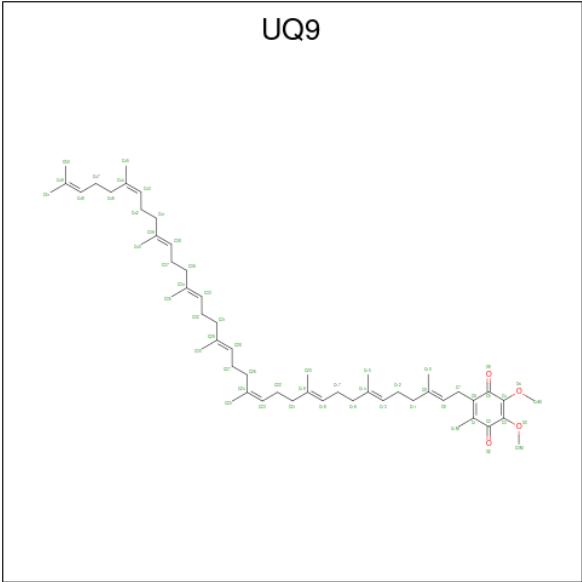
Mol	Chain	Residues	Atoms			AltConf
48	E	1	Total	Fe	S	0
			4	2	2	
48	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 49 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



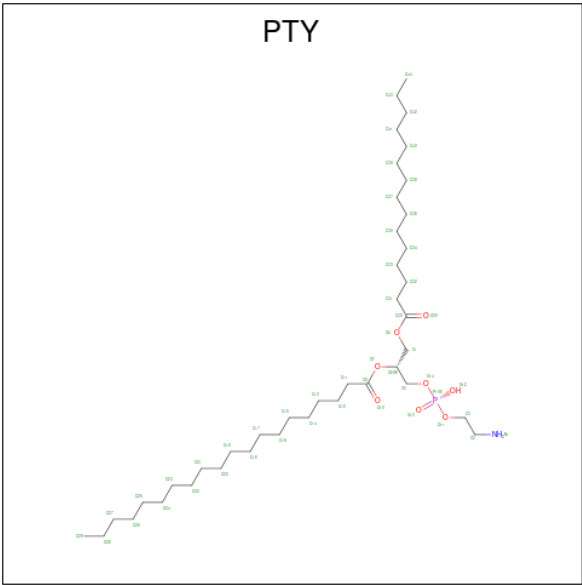
Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 50 is Ubiquinone-9 (CCD ID: UQ9) (formula: C₅₄H₈₂O₄).



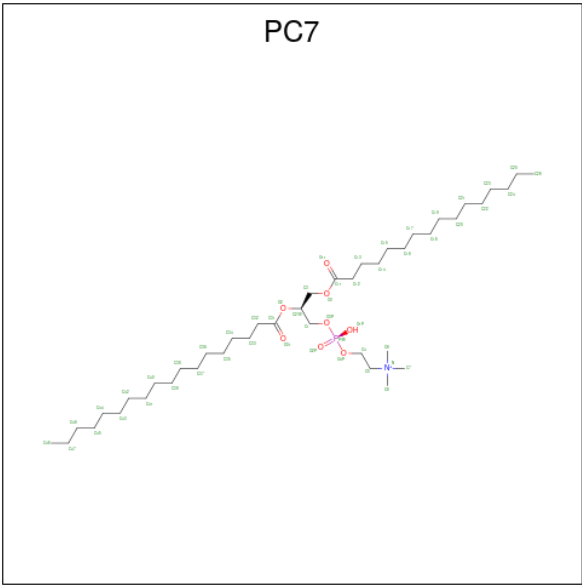
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
50	H	1	35	31	4	0

- Molecule 51 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



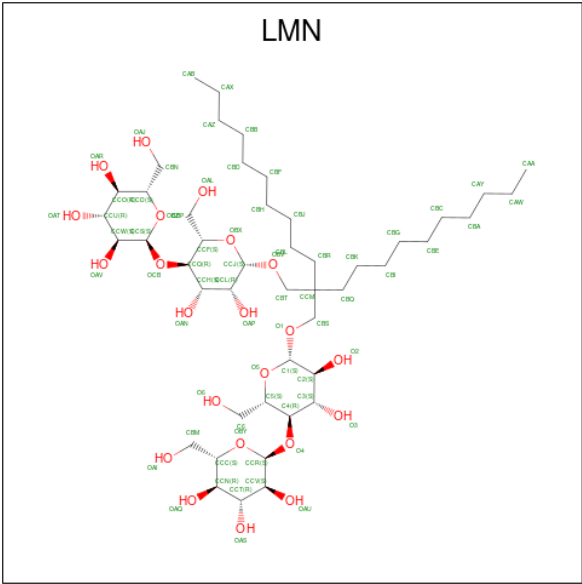
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
51	I	1	50	40	1	8	1	0
51	M	1	50	40	1	8	1	0
51	N	1	50	40	1	8	1	0

- Molecule 52 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).



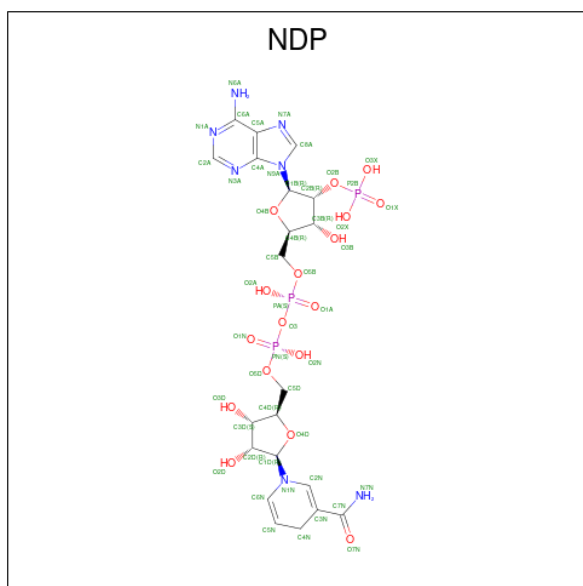
Mol	Chain	Residues	Atoms					AltConf
52	M	1	Total	C	N	O	P	0
			52	42	1	8	1	
52	f	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 53 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: C₄₇H₈₈O₂₂).



Mol	Chain	Residues	Atoms			AltConf
53	M	1	Total	C	O	0
			69	47	22	

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

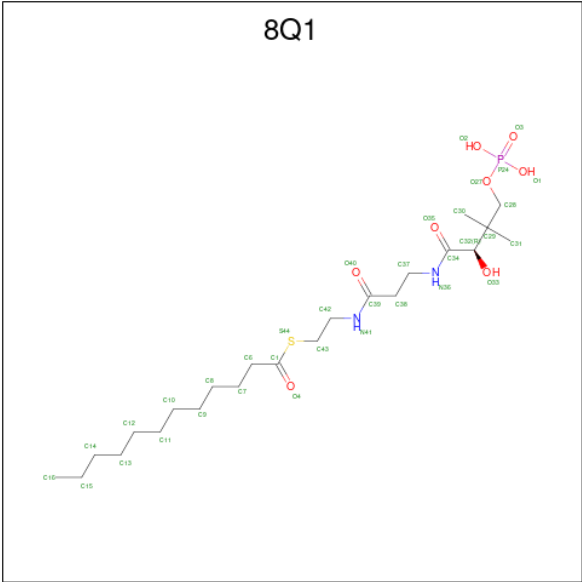


Mol	Chain	Residues	Atoms					AltConf
54	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

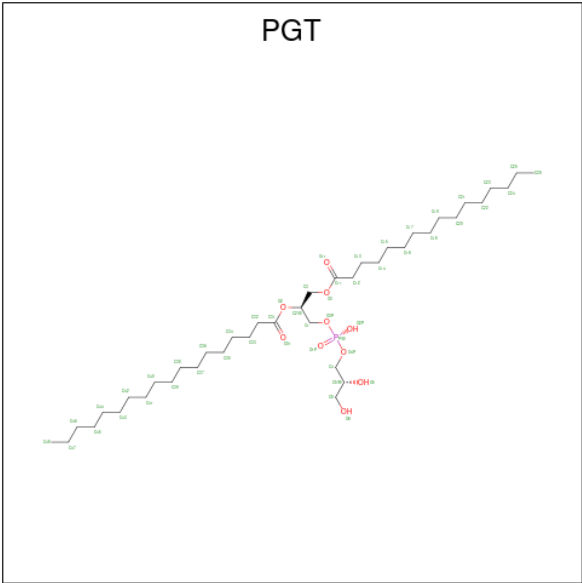
Mol	Chain	Residues	Atoms		AltConf
55	R	1	Total	Zn	0
			1	1	
55	y	1	Total	Zn	0
			1	1	

- Molecule 56 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).



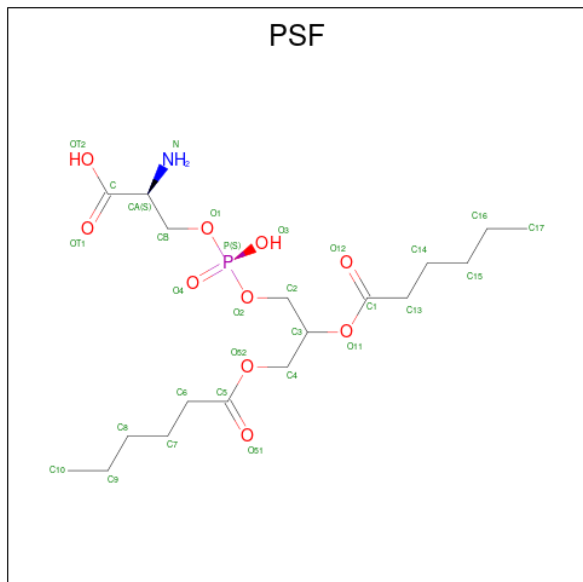
Mol	Chain	Residues	Atoms						AltConf
56	W	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
56	n	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 57 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



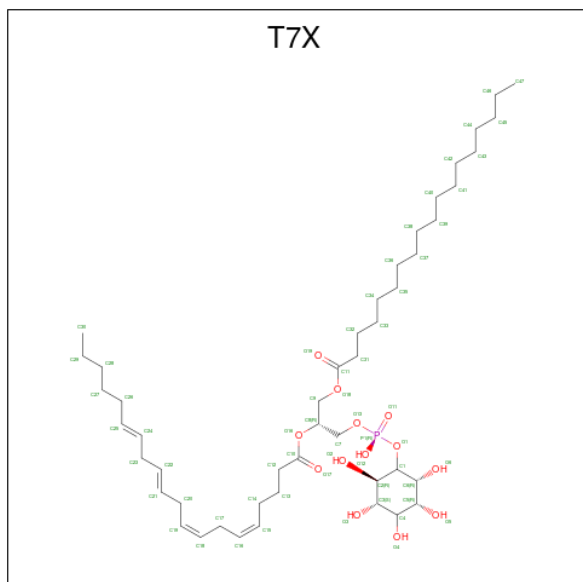
Mol	Chain	Residues	Atoms				AltConf
57	y	1	Total	C	O	P	0
			41	30	10	1	

- Molecule 58 is 1,2-DICAPROYL-SN-PHOSPHATIDYL-L-SERINE (CCD ID: PSF) (formula: $C_{18}H_{34}NO_{10}P$).



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

- Molecule 59 is Phosphatidylinositol (CCD ID: T7X) (formula: $C_{47}H_{83}O_{13}P$).

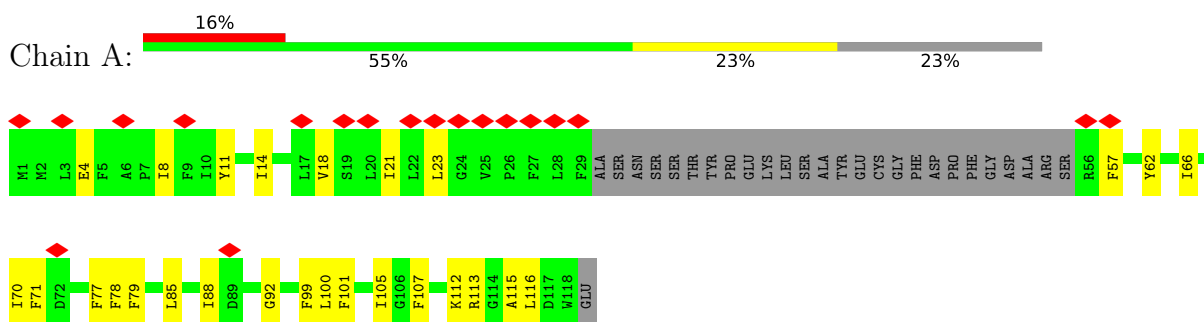


Mol	Chain	Residues	Atoms				AltConf
59	z	1	Total	C	O	P	0
			61	47	13	1	

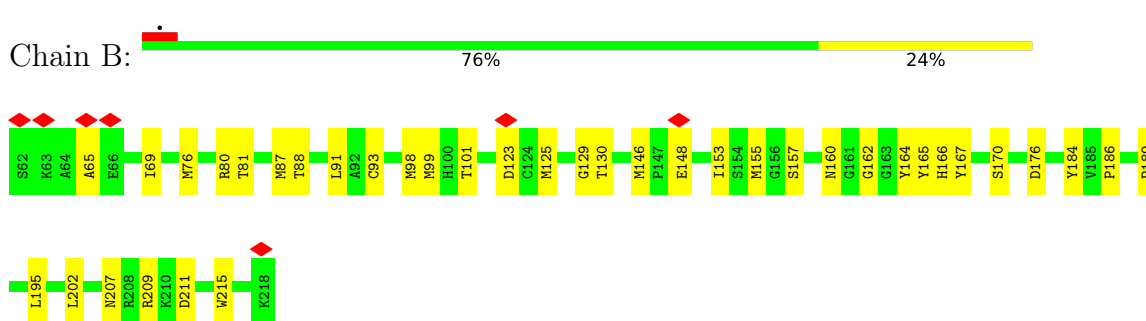
3 Residue-property plots [i](#)

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

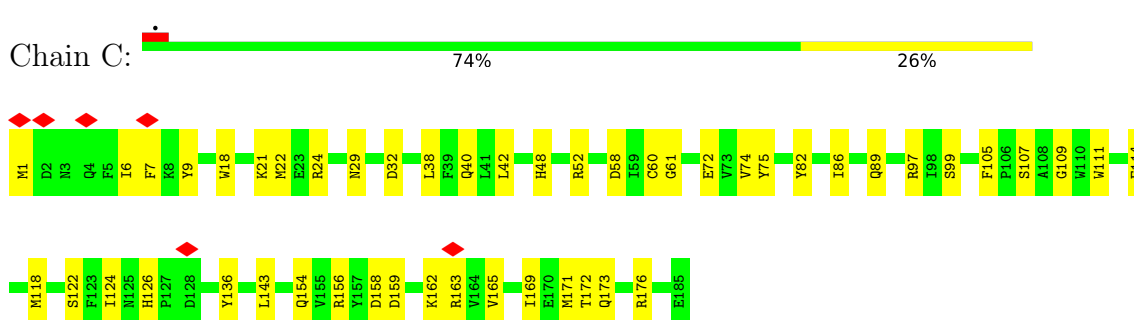
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



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

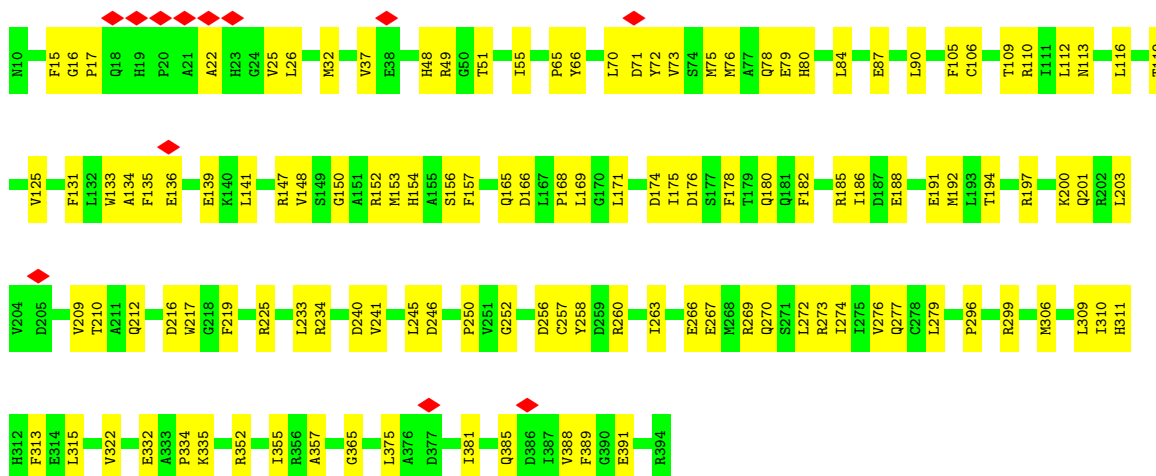


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3

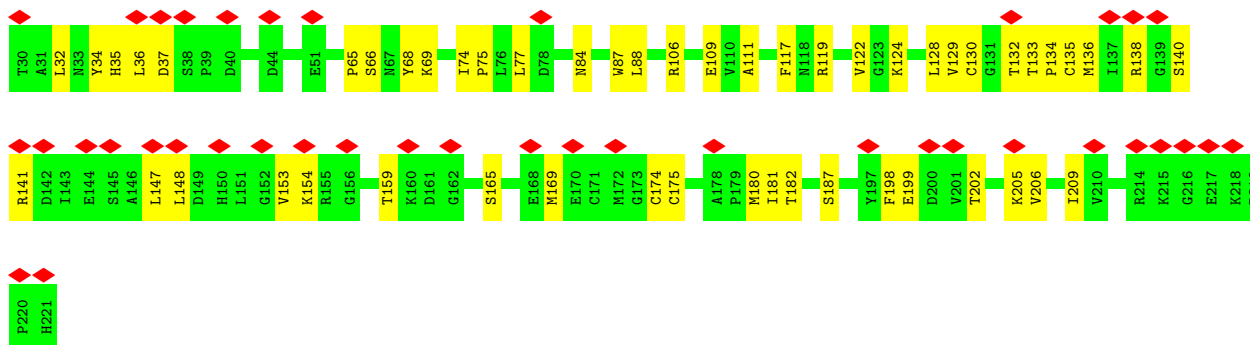


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2

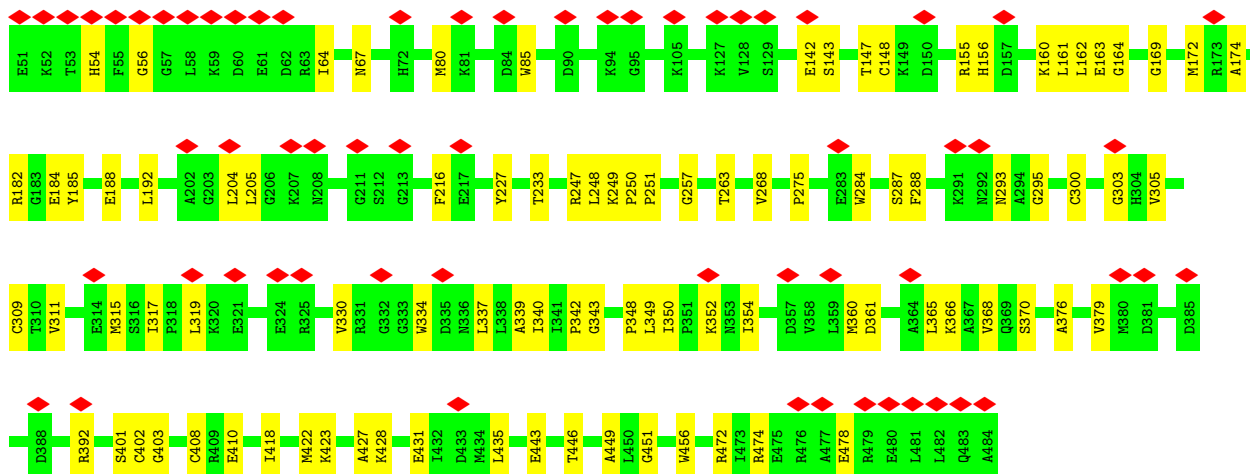
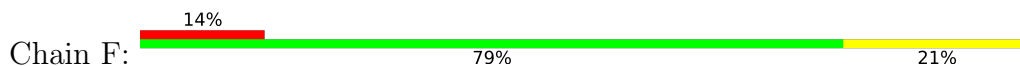




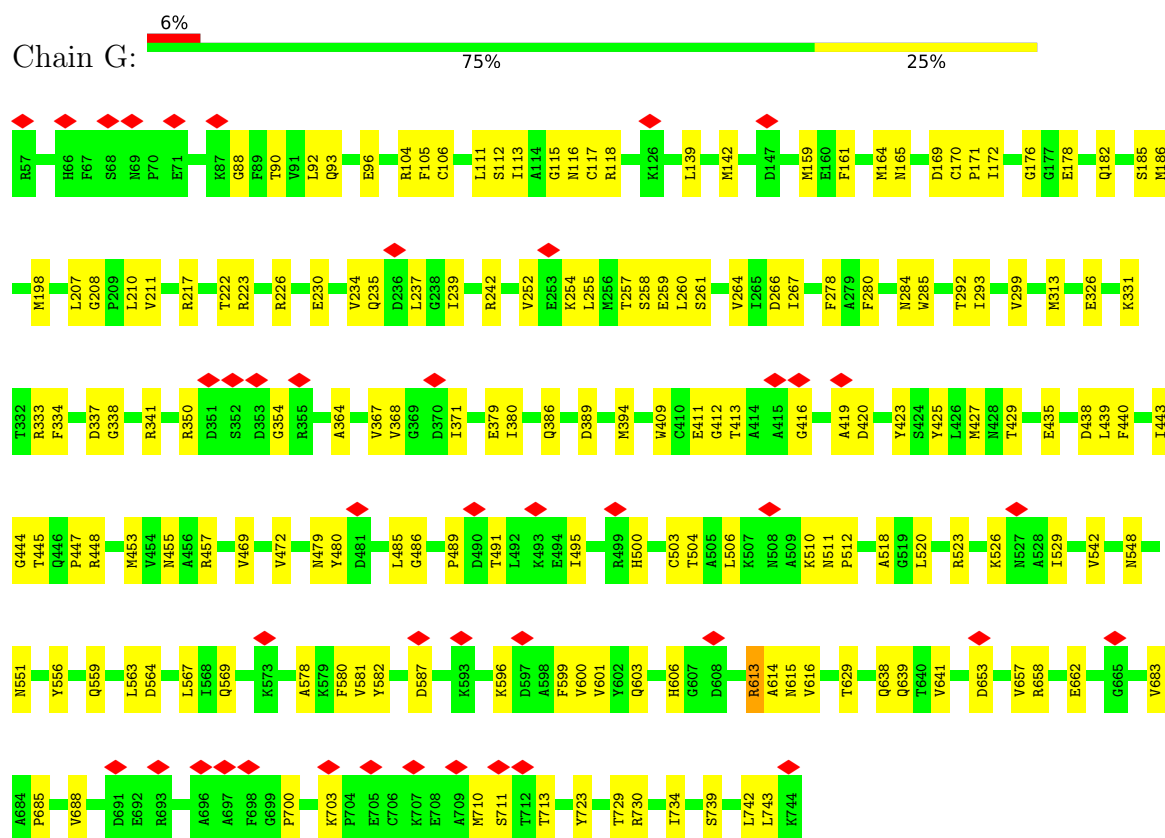
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



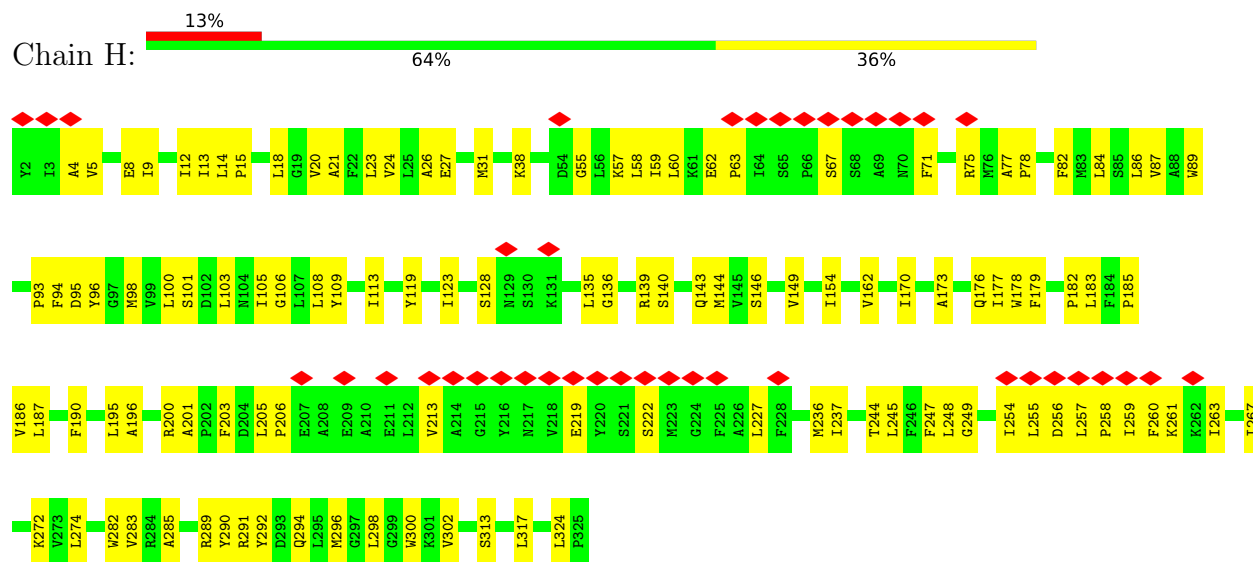
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



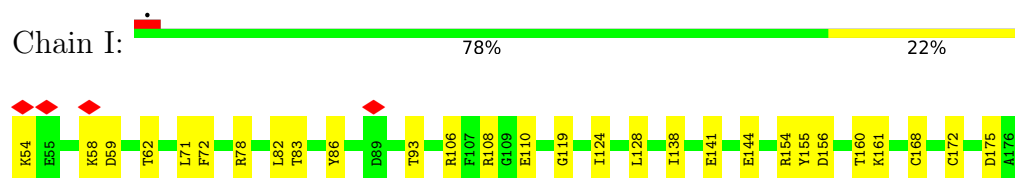
- Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 1, mitochondrial



• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

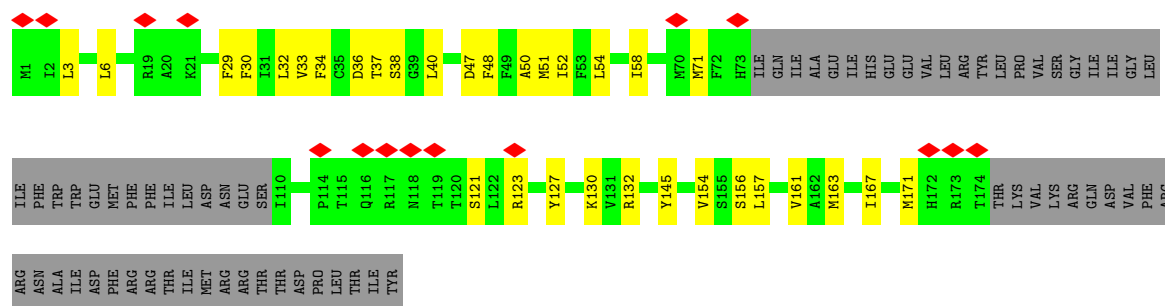


• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8-A, mitochondrial

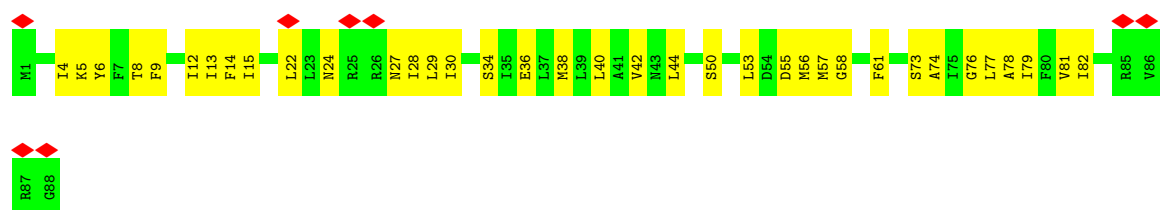




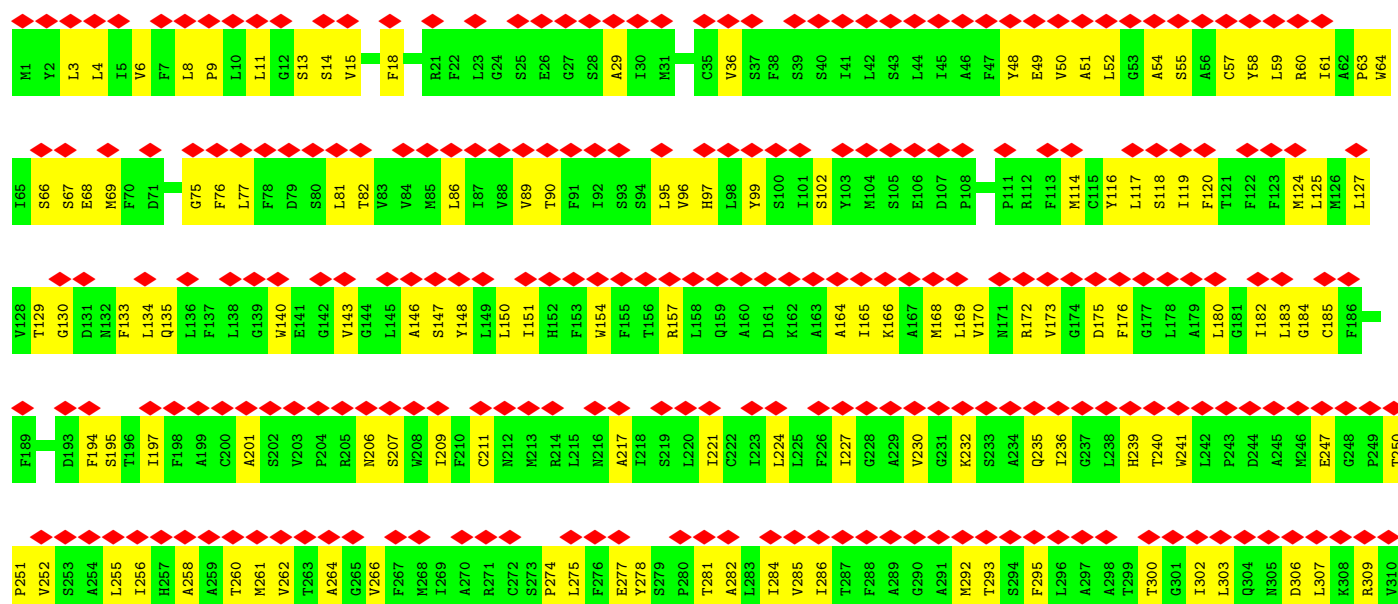
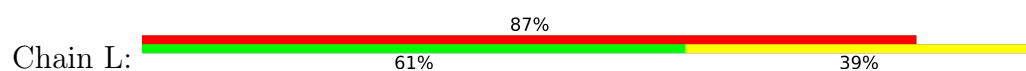
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

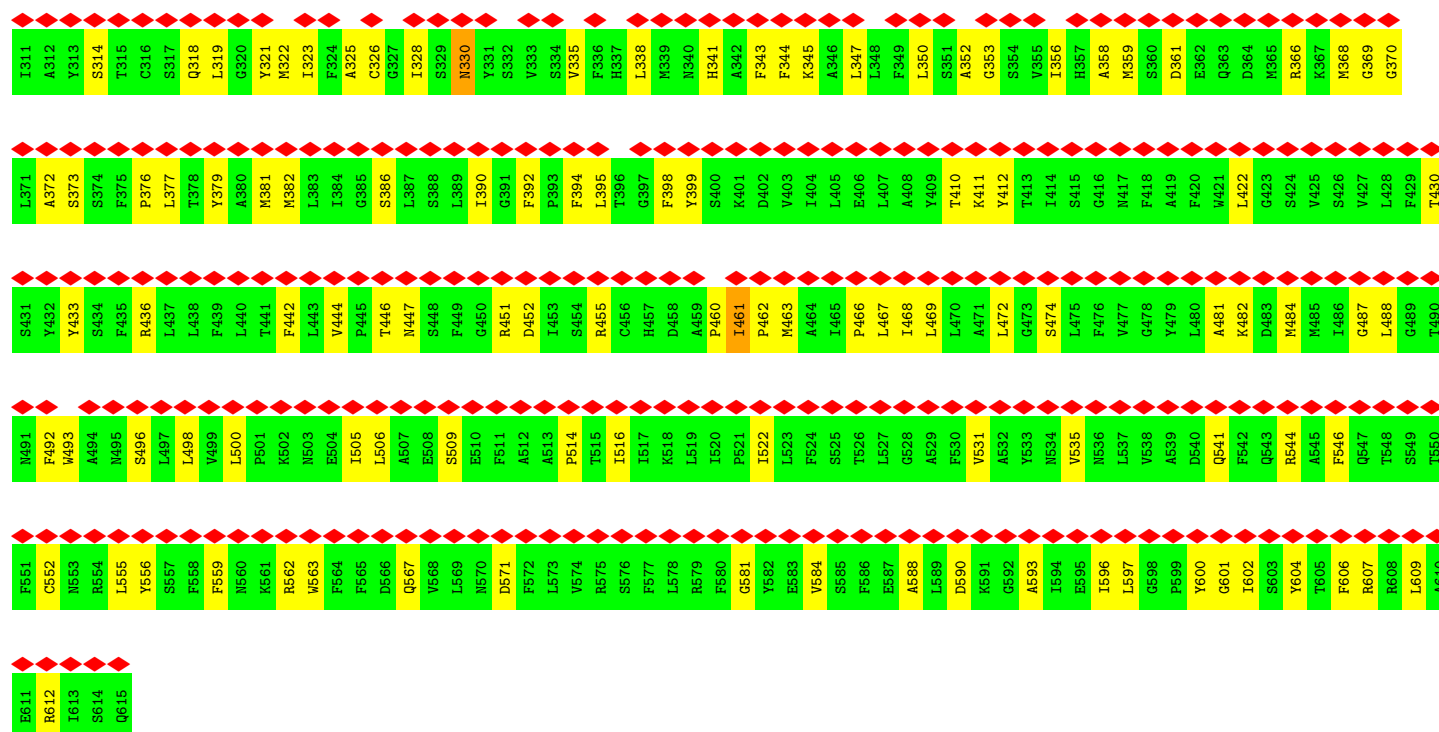


- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

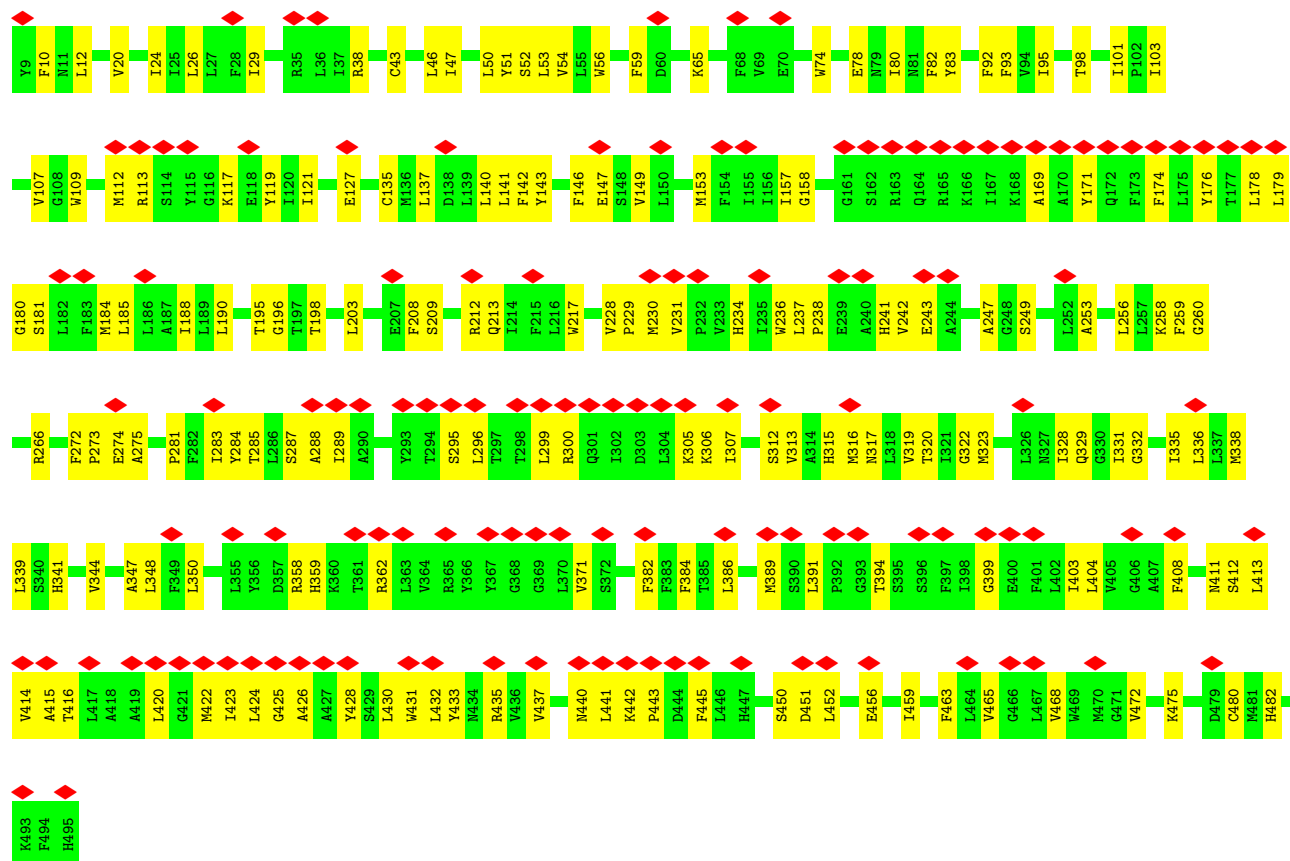


- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

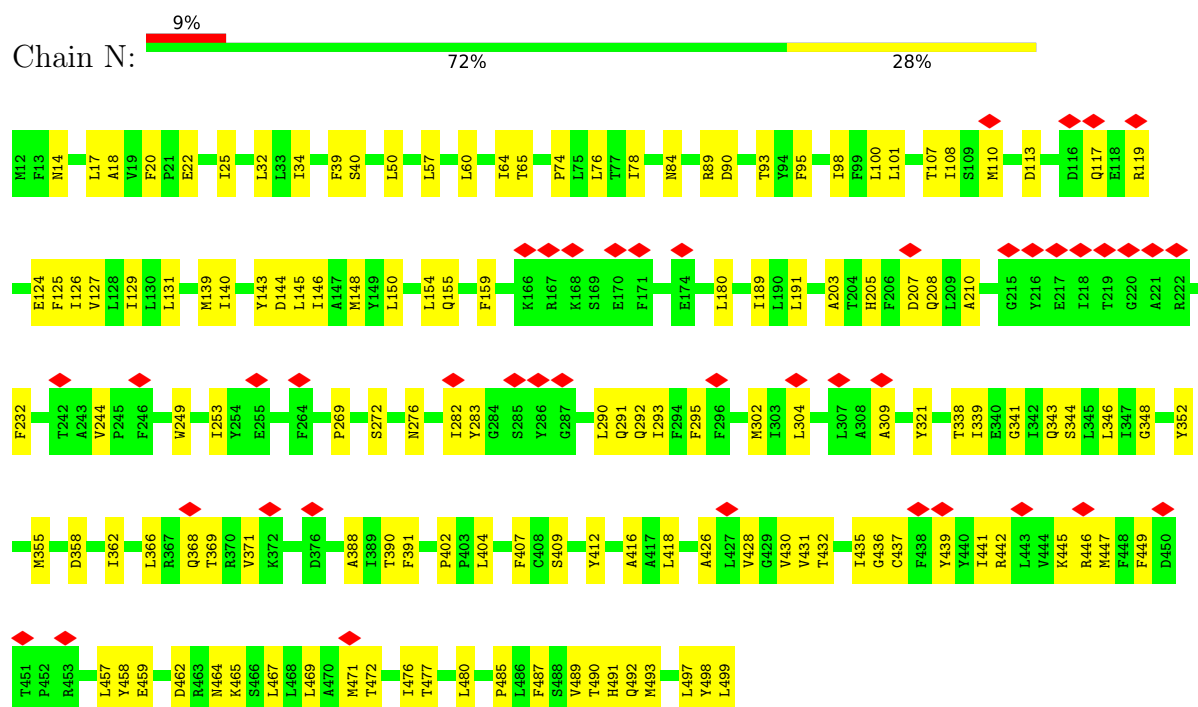




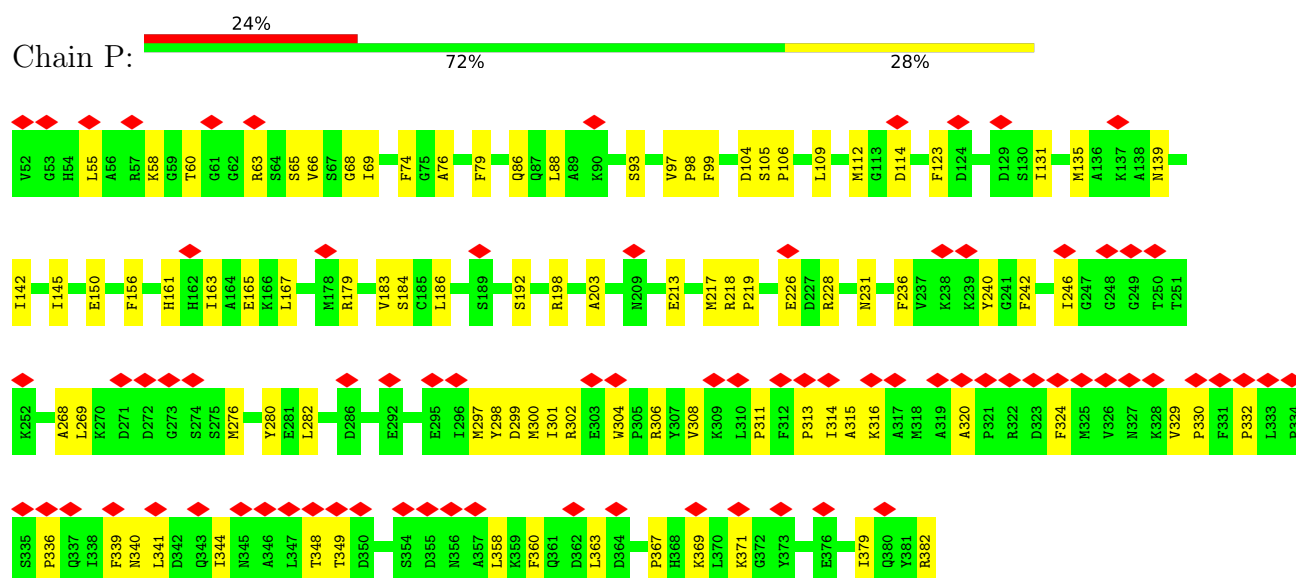
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



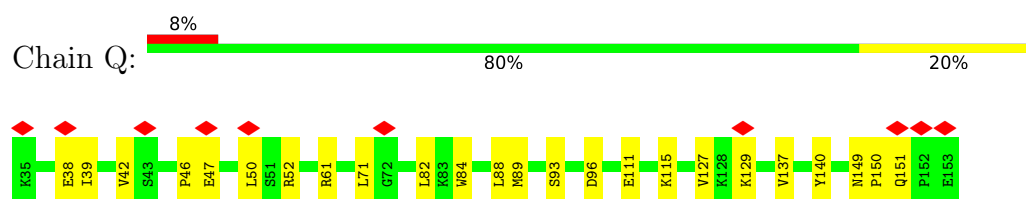
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2



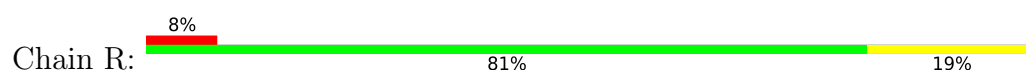
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



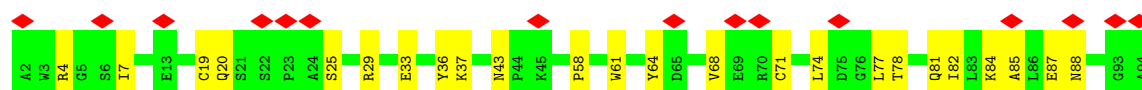
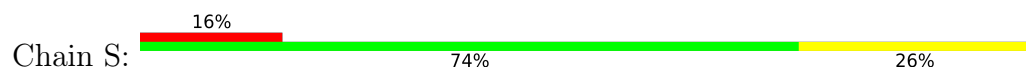
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



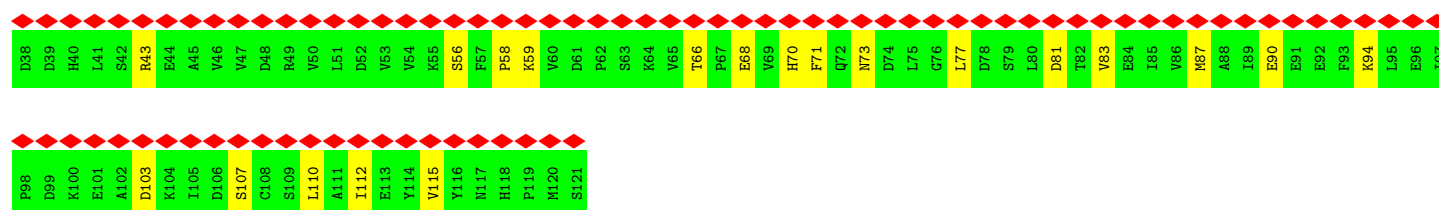
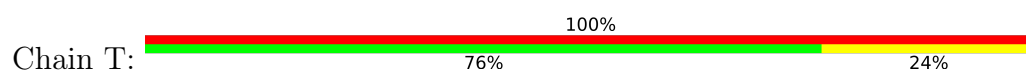
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



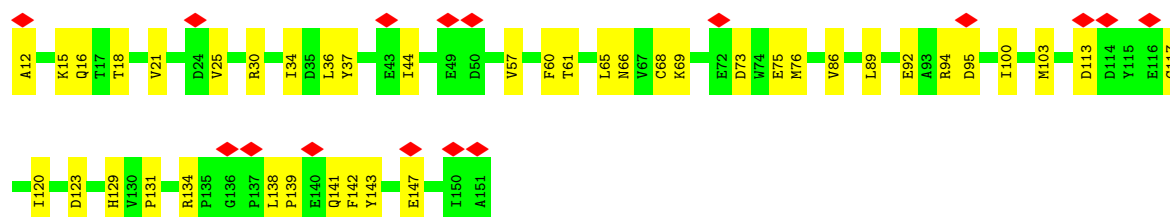
- Molecule 19: Acyl carrier protein 1, mitochondrial



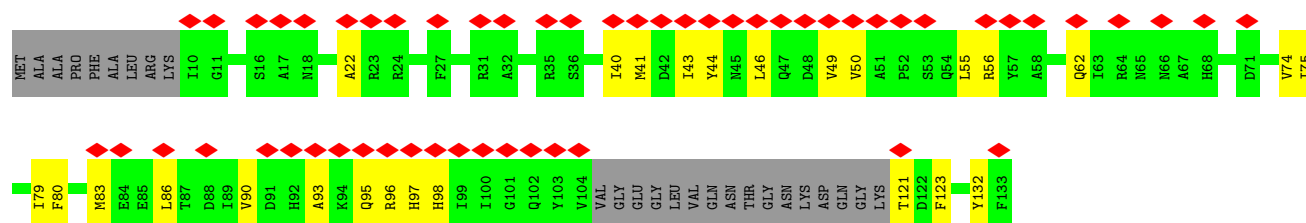
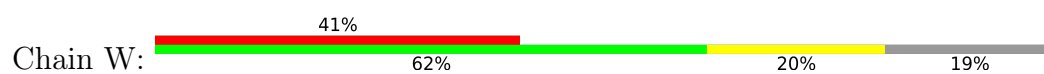
- Molecule 20: Acyl carrier protein 2, mitochondrial



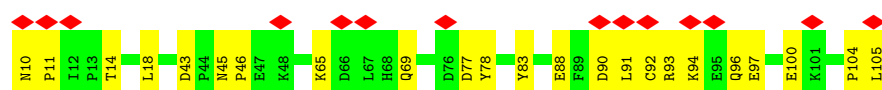
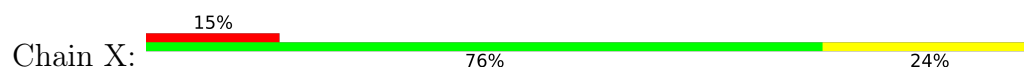
- Molecule 21: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial



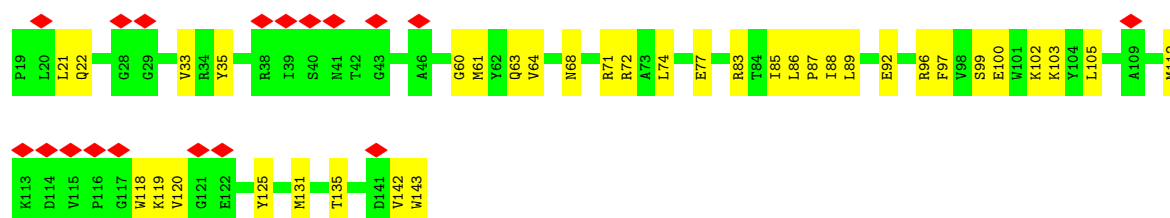
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



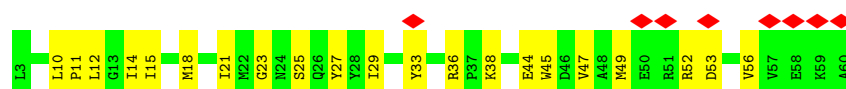
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A



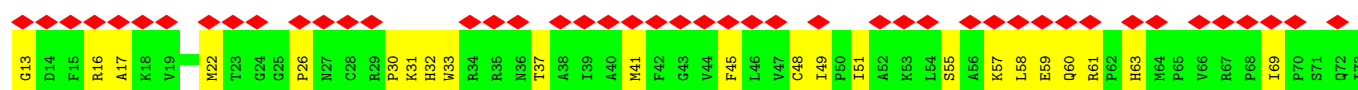
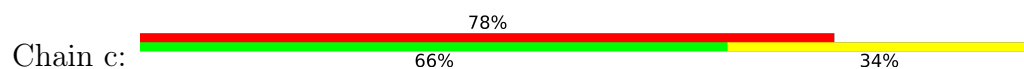
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

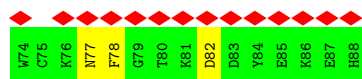


- Molecule 26: At2g46540/F11C10.23

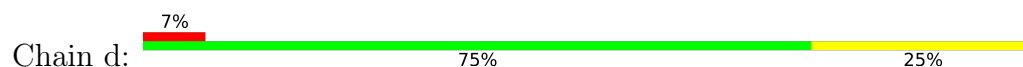


- Molecule 27: Transmembrane protein

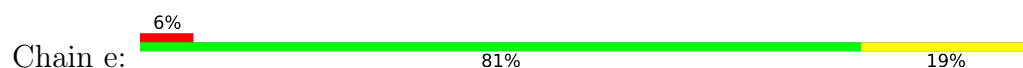




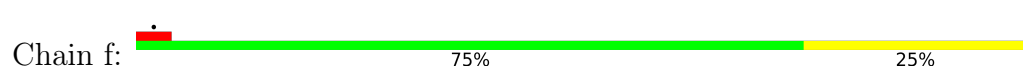
- Molecule 28: Excitatory amino acid transporter



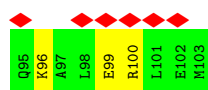
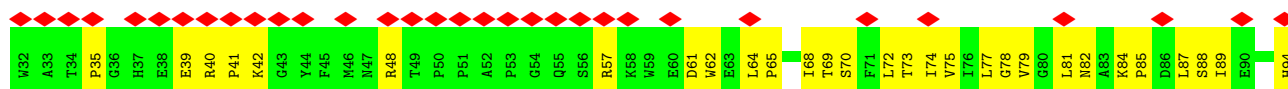
- Molecule 29: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-A



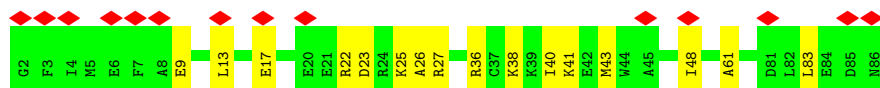
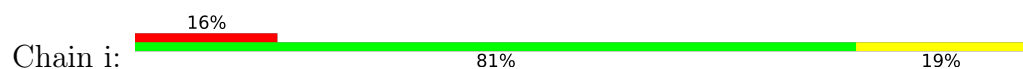
- Molecule 30: At4g16450



- Molecule 31: ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein



- Molecule 32: At1g67350

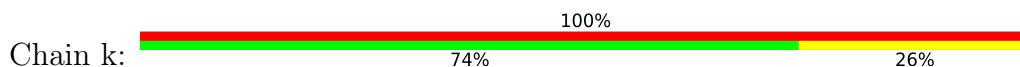


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2

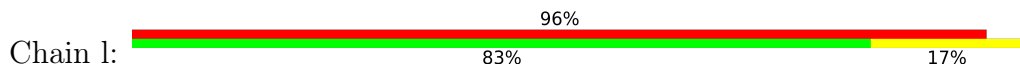




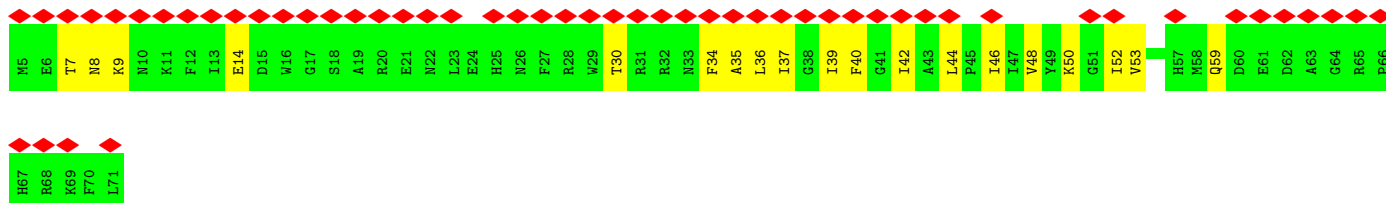
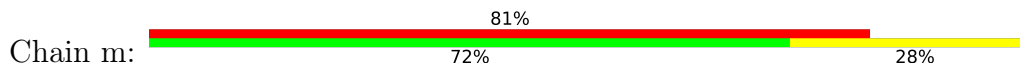
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3-A



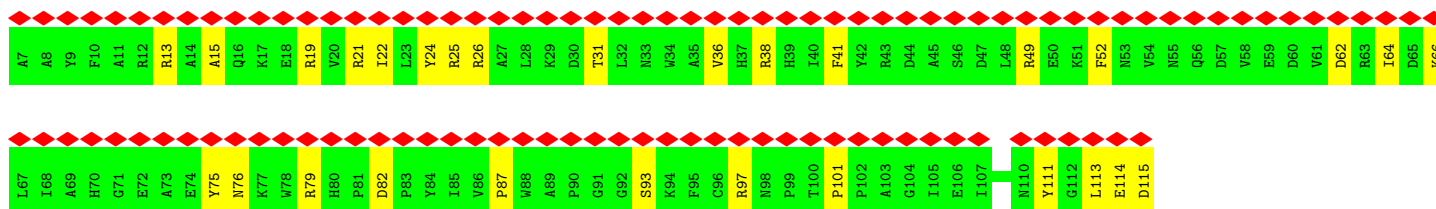
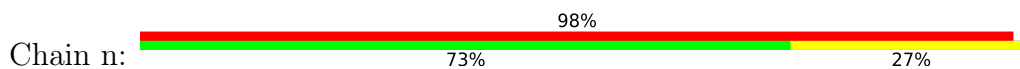
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



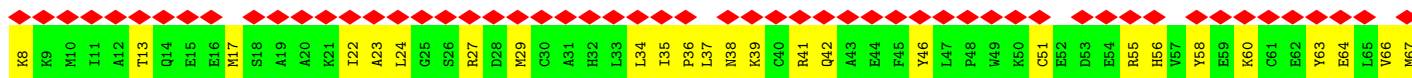
- Molecule 36: AT2G31490 protein



- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

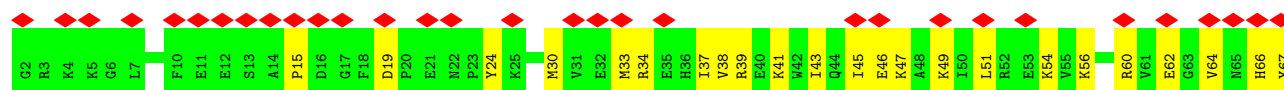


- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

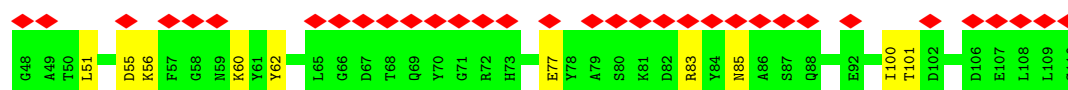
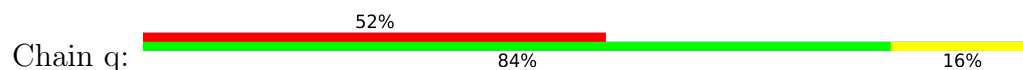




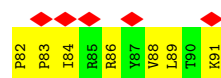
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10-B



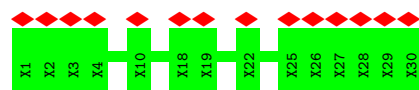
- Molecule 40: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 41: B14.5a



- Molecule 42: unknown

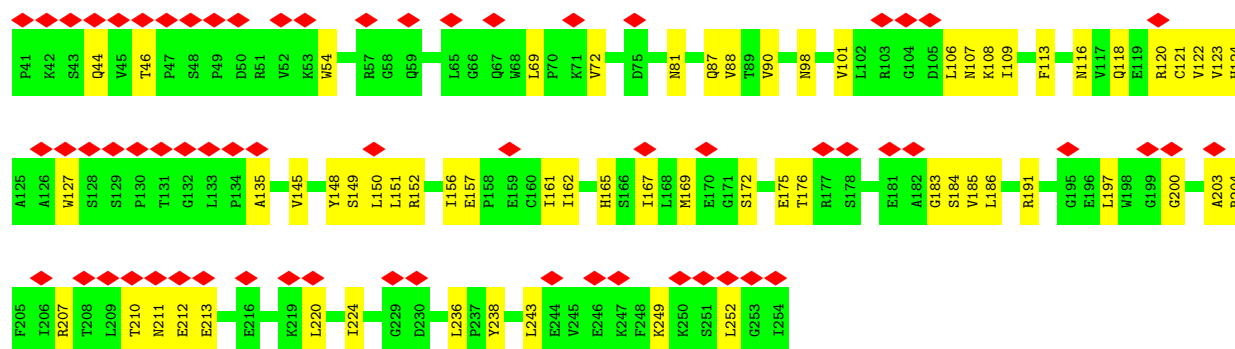


- Molecule 43: Uncharacterized protein At2g27730, mitochondrial

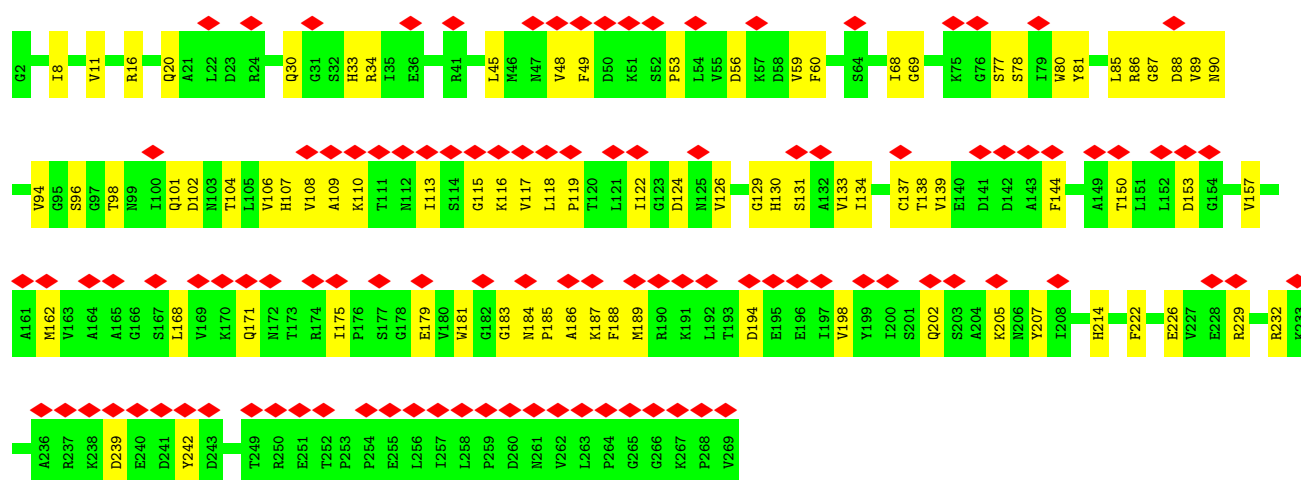
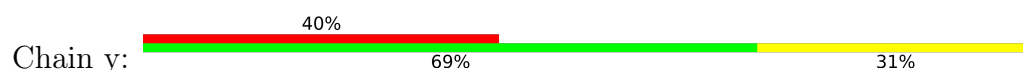


- Molecule 44: Gamma carbonic anhydrase-like 2, mitochondrial

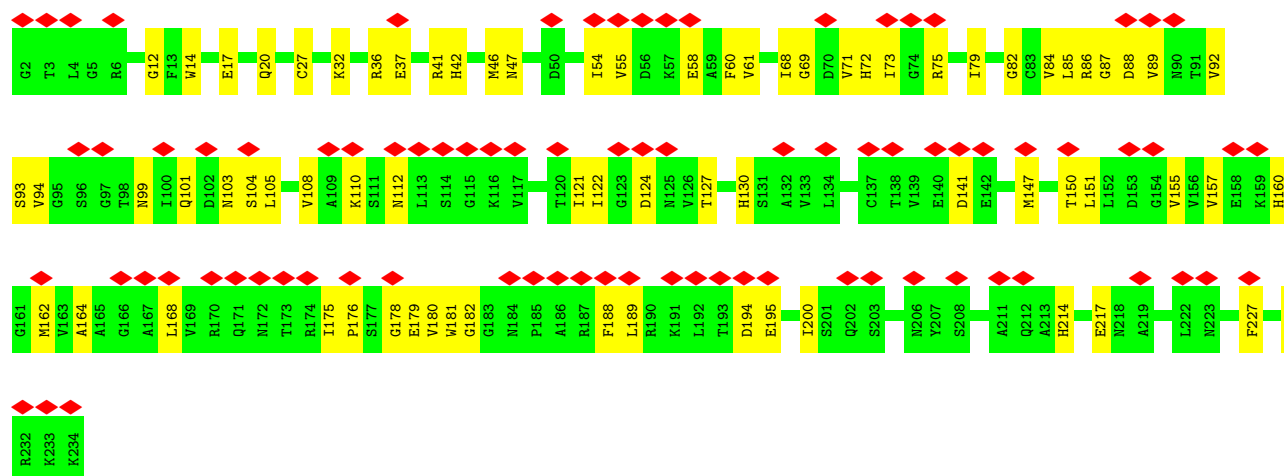




• Molecule 45: Gamma carbonic anhydrase 2, mitochondrial



• Molecule 46: 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	48933	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	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.011	Depositor
Map size ($\text{\AA}$)	502.2, 502.2, 502.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.837, 0.837, 0.837	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, UQ9, PTY, SF4, PSF, PC7, FES, FMN, LMN, T7X, PGT, 8Q1, ZN

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	0.15	0/813	0.33	0/1103
2	B	0.14	0/1279	0.28	0/1734
3	C	0.13	0/1629	0.30	0/2207
4	D	0.15	0/3147	0.33	0/4256
5	E	0.13	0/1535	0.36	0/2084
6	F	0.12	0/3441	0.32	0/4641
7	G	0.12	0/5347	0.31	0/7242
8	H	0.17	0/2609	0.42	0/3553
9	I	0.15	0/1410	0.33	0/1904
10	J	0.14	0/1118	0.30	0/1523
11	K	0.15	0/702	0.35	0/948
12	L	0.14	0/4938	0.39	1/6706 (0.0%)
13	M	0.15	0/3996	0.36	0/5431
14	N	0.14	0/3924	0.33	0/5327
15	P	0.14	0/2613	0.37	0/3539
16	Q	0.15	0/966	0.34	1/1305 (0.1%)
17	R	0.11	0/493	0.28	0/668
18	S	0.13	0/740	0.34	0/996
19	T	0.11	0/679	0.30	0/922
20	U	0.14	0/660	0.38	0/892
21	V	0.14	0/1146	0.33	0/1555
22	W	0.13	0/899	0.37	0/1218
23	X	0.14	0/777	0.42	0/1044
24	Z	0.14	0/1027	0.38	0/1392
25	a	0.15	0/482	0.40	0/646
26	b	0.14	0/300	0.34	0/407
27	c	0.11	0/637	0.34	0/860
28	d	0.15	0/605	0.36	0/815
29	e	0.11	0/559	0.27	0/745
30	f	0.15	0/768	0.35	0/1038
31	g	0.12	0/606	0.35	0/826
32	i	0.14	0/757	0.35	0/1019

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	j	0.13	0/433	0.31	0/592
34	k	0.13	0/384	0.39	0/515
35	l	0.09	0/370	0.23	0/504
36	m	0.11	0/580	0.30	0/778
37	n	0.10	0/938	0.30	0/1273
38	o	0.17	0/666	0.52	0/886
39	p	0.13	0/799	0.33	0/1074
40	q	0.10	0/537	0.30	0/728
41	r	0.21	0/89	0.73	0/119
43	v	0.09	0/230	0.22	0/311
44	x	0.13	0/1700	0.34	0/2320
45	y	0.11	0/2066	0.31	0/2800
46	z	0.12	0/1804	0.32	0/2441
All	All	0.14	0/61198	0.34	2/82887 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	46	PRO	CA-N-CD	-6.63	102.72	112.00
12	L	461	ILE	CB-CA-C	-5.92	108.07	114.35

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	785	0	807	24	0
2	B	1244	0	1231	36	0
3	C	1581	0	1529	38	0
4	D	3077	0	3043	92	0
5	E	1500	0	1472	41	0
6	F	3368	0	3353	64	0
7	G	5252	0	5241	118	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	2536	0	2641	104	0
9	I	1381	0	1328	38	0
10	J	1093	0	1171	35	0
11	K	692	0	753	28	0
12	L	4807	0	4847	204	0
13	M	3887	0	4037	143	0
14	N	3820	0	3925	107	0
15	P	2556	0	2598	64	0
16	Q	939	0	928	19	0
17	R	482	0	478	7	0
18	S	728	0	759	18	0
19	T	667	0	648	14	0
20	U	650	0	635	17	0
21	V	1123	0	1112	33	0
22	W	880	0	873	16	0
23	X	763	0	761	19	0
24	Z	997	0	979	32	0
25	a	470	0	472	21	0
26	b	295	0	322	7	0
27	c	617	0	619	24	0
28	d	592	0	610	18	0
29	e	546	0	512	8	0
30	f	752	0	754	21	0
31	g	586	0	572	24	0
32	i	737	0	705	13	0
33	j	415	0	406	16	0
34	k	374	0	369	20	0
35	l	360	0	364	8	0
36	m	565	0	555	15	0
37	n	911	0	879	27	0
38	o	657	0	671	29	0
39	p	778	0	768	30	0
40	q	520	0	478	6	0
41	r	87	0	98	13	0
42	u	150	0	34	0	0
43	v	226	0	235	1	0
44	x	1659	0	1673	46	0
45	y	2032	0	2044	64	0
46	z	1772	0	1768	60	0
47	B	8	0	0	2	0
47	F	8	0	0	2	0
47	G	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	I	16	0	0	1	0
48	E	4	0	0	2	0
48	G	4	0	0	0	0
49	F	31	0	19	2	0
50	H	35	0	40	5	0
51	I	50	0	77	7	0
51	M	50	0	79	3	0
51	N	50	0	79	4	0
52	M	52	0	77	6	0
52	f	52	0	82	3	0
53	M	69	0	88	6	0
54	P	48	0	22	0	0
55	R	1	0	0	0	0
55	y	1	0	0	0	0
56	W	35	0	0	1	0
56	n	35	0	0	0	0
57	y	41	0	52	1	0
58	z	30	0	32	1	0
59	z	61	0	0	0	0
All	All	60606	0	60704	1504	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 12.

The worst 5 of 1504 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:M:389:MET:HE1	13:M:430:LEU:HG	1.54	0.89
7:G:596:LYS:HA	7:G:613:ARG:NH2	1.89	0.88
41:r:86:ARG:HH12	41:r:88:VAL:HG22	1.40	0.87
13:M:38:ARG:HH21	13:M:112:MET:HB2	1.40	0.86
12:L:369:GLY:HA3	12:L:446:THR:HA	1.58	0.85

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	155/157 (99%)	142 (92%)	13 (8%)	0	100	100
3	C	183/185 (99%)	174 (95%)	9 (5%)	0	100	100
4	D	383/385 (100%)	356 (93%)	27 (7%)	0	100	100
5	E	190/192 (99%)	170 (90%)	20 (10%)	0	100	100
6	F	432/434 (100%)	408 (94%)	24 (6%)	0	100	100
7	G	686/688 (100%)	637 (93%)	49 (7%)	0	100	100
8	H	322/324 (99%)	291 (90%)	31 (10%)	0	100	100
9	I	167/169 (99%)	162 (97%)	5 (3%)	0	100	100
10	J	134/205 (65%)	131 (98%)	3 (2%)	0	100	100
11	K	86/88 (98%)	85 (99%)	0	1 (1%)	10	39
12	L	613/615 (100%)	559 (91%)	54 (9%)	0	100	100
13	M	485/487 (100%)	465 (96%)	20 (4%)	0	100	100
14	N	486/488 (100%)	466 (96%)	20 (4%)	0	100	100
15	P	329/331 (99%)	309 (94%)	20 (6%)	0	100	100
16	Q	117/119 (98%)	109 (93%)	8 (7%)	0	100	100
17	R	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
18	S	91/93 (98%)	82 (90%)	9 (10%)	0	100	100
19	T	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
20	U	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
21	V	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
22	W	104/133 (78%)	100 (96%)	4 (4%)	0	100	100
23	X	94/96 (98%)	89 (95%)	5 (5%)	0	100	100
24	Z	123/125 (98%)	114 (93%)	8 (6%)	1 (1%)	16	47
25	a	56/58 (97%)	56 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	b	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
27	c	74/76 (97%)	59 (80%)	15 (20%)	0	100	100
28	d	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
29	e	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
30	f	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
31	g	70/72 (97%)	65 (93%)	5 (7%)	0	100	100
32	i	83/85 (98%)	77 (93%)	6 (7%)	0	100	100
33	j	49/51 (96%)	45 (92%)	4 (8%)	0	100	100
34	k	45/47 (96%)	39 (87%)	6 (13%)	0	100	100
35	l	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
36	m	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
37	n	107/109 (98%)	98 (92%)	9 (8%)	0	100	100
38	o	78/80 (98%)	70 (90%)	8 (10%)	0	100	100
39	p	91/93 (98%)	86 (94%)	5 (6%)	0	100	100
40	q	61/63 (97%)	53 (87%)	8 (13%)	0	100	100
41	r	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
43	v	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
44	x	212/214 (99%)	196 (92%)	16 (8%)	0	100	100
45	y	266/268 (99%)	239 (90%)	27 (10%)	0	100	100
46	z	231/233 (99%)	212 (92%)	19 (8%)	0	100	100
All	All	7468/7683 (97%)	6980 (94%)	486 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	28	ILE
24	Z	120	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	132/132 (100%)	132 (100%)	0	100	100
3	C	175/175 (100%)	175 (100%)	0	100	100
4	D	331/331 (100%)	331 (100%)	0	100	100
5	E	166/166 (100%)	166 (100%)	0	100	100
6	F	353/353 (100%)	353 (100%)	0	100	100
7	G	571/571 (100%)	570 (100%)	1 (0%)	87	86
8	H	271/271 (100%)	271 (100%)	0	100	100
9	I	151/151 (100%)	151 (100%)	0	100	100
10	J	123/186 (66%)	123 (100%)	0	100	100
11	K	76/76 (100%)	76 (100%)	0	100	100
12	L	518/518 (100%)	517 (100%)	1 (0%)	87	86
13	M	426/426 (100%)	426 (100%)	0	100	100
14	N	406/406 (100%)	406 (100%)	0	100	100
15	P	273/273 (100%)	273 (100%)	0	100	100
16	Q	100/100 (100%)	100 (100%)	0	100	100
17	R	55/55 (100%)	55 (100%)	0	100	100
18	S	82/82 (100%)	82 (100%)	0	100	100
19	T	79/79 (100%)	79 (100%)	0	100	100
20	U	75/75 (100%)	75 (100%)	0	100	100
21	V	123/123 (100%)	123 (100%)	0	100	100
22	W	96/114 (84%)	96 (100%)	0	100	100
23	X	87/87 (100%)	87 (100%)	0	100	100
24	Z	100/100 (100%)	100 (100%)	0	100	100
25	a	48/48 (100%)	48 (100%)	0	100	100
26	b	33/33 (100%)	33 (100%)	0	100	100
27	c	66/66 (100%)	66 (100%)	0	100	100
28	d	60/60 (100%)	60 (100%)	0	100	100
29	e	59/59 (100%)	59 (100%)	0	100	100
30	f	80/80 (100%)	80 (100%)	0	100	100
31	g	62/62 (100%)	62 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	i	77/77 (100%)	77 (100%)	0	100	100
33	j	42/42 (100%)	42 (100%)	0	100	100
34	k	38/38 (100%)	38 (100%)	0	100	100
35	l	37/37 (100%)	37 (100%)	0	100	100
36	m	58/58 (100%)	58 (100%)	0	100	100
37	n	92/92 (100%)	92 (100%)	0	100	100
38	o	70/70 (100%)	70 (100%)	0	100	100
39	p	83/83 (100%)	83 (100%)	0	100	100
40	q	52/52 (100%)	52 (100%)	0	100	100
41	r	10/10 (100%)	10 (100%)	0	100	100
43	v	23/23 (100%)	23 (100%)	0	100	100
44	x	183/183 (100%)	183 (100%)	0	100	100
45	y	223/223 (100%)	223 (100%)	0	100	100
46	z	188/188 (100%)	188 (100%)	0	100	100
All	All	6437/6540 (98%)	6435 (100%)	2 (0%)	100	100

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

Mol	Chain	Res	Type
7	G	613	ARG
12	L	330	ASN

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	S	57	GLN
25	a	42	HIS
46	z	47	ASN
18	S	81	GLN
22	W	66	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 24 ligands modelled in this entry, 2 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$
54	NDP	P	500	15	49,52,52	2.22	5 (10%)	66,80,80	1.67	12 (18%)
56	8Q1	W	200	-	31,34,34	1.70	6 (19%)	40,43,43	1.52	4 (10%)
48	FES	G	801	7	0,4,4	-	-	-	-	-
58	PSF	z	301	46	28,29,29	1.18	4 (14%)	32,36,36	1.24	2 (6%)
47	SF4	F	501	6	0,12,12	-	-	-	-	-
52	PC7	f	201	30	51,51,51	0.96	4 (7%)	57,59,59	1.03	2 (3%)
47	SF4	B	500	2	0,12,12	-	-	-	-	-
48	FES	E	500	5	0,4,4	-	-	-	-	-
51	PTY	I	303	9	49,49,49	0.87	4 (8%)	52,54,54	1.08	2 (3%)
51	PTY	M	502	13	49,49,49	0.88	4 (8%)	52,54,54	1.10	2 (3%)
56	8Q1	n	200	37	31,34,34	1.71	6 (19%)	40,43,43	1.50	5 (12%)
53	LMN	M	503	-	72,72,72	1.67	13 (18%)	96,98,98	1.11	4 (4%)
47	SF4	I	302	9	0,12,12	-	-	-	-	-
49	FMN	F	500	-	33,33,33	1.08	2 (6%)	48,50,50	1.22	8 (16%)
51	PTY	N	501	14	49,49,49	0.87	4 (8%)	52,54,54	1.08	2 (3%)
47	SF4	G	802	7	0,12,12	-	-	-	-	-
50	UQ9	H	500	8	35,35,58	2.55	12 (34%)	42,45,73	1.59	9 (21%)
57	PGT	y	302	-	40,40,50	1.17	3 (7%)	43,46,56	1.09	2 (4%)
59	T7X	z	302	-	61,61,61	0.84	4 (6%)	71,73,73	1.04	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	SF4	I	301	9	0,12,12	-	-	-		
47	SF4	G	803	7	0,12,12	-	-	-		
52	PC7	M	501	13,12	51,51,51	0.96	4 (7%)	57,59,59	1.09	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
54	NDP	P	500	15	-	4/34/77/77	0/5/5/5
56	8Q1	W	200	-	-	21/41/41/41	-
48	FES	G	801	7	-	-	0/1/1/1
58	PSF	z	301	46	-	11/35/35/35	-
47	SF4	F	501	6	-	-	0/6/5/5
52	PC7	f	201	30	-	26/55/55/55	-
47	SF4	B	500	2	-	-	0/6/5/5
48	FES	E	500	5	-	-	0/1/1/1
51	PTY	I	303	9	-	22/53/53/53	-
51	PTY	M	502	13	-	24/53/53/53	-
56	8Q1	n	200	37	-	7/41/41/41	-
53	LMN	M	503	-	-	35/50/130/130	0/4/4/4
47	SF4	I	302	9	-	-	0/6/5/5
49	FMN	F	500	-	-	7/18/18/18	0/3/3/3
51	PTY	N	501	14	-	27/53/53/53	-
59	T7X	z	302	-	-	24/56/80/80	0/1/1/1
50	UQ9	H	500	8	-	4/30/54/81	0/1/1/1
57	PGT	y	302	-	-	27/45/45/55	-
47	SF4	G	802	7	-	-	0/6/5/5
47	SF4	I	301	9	-	-	0/6/5/5
47	SF4	G	803	7	-	-	0/6/5/5
52	PC7	M	501	13,12	-	20/55/55/55	-

The worst 5 of 75 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	P	500	NDP	P2B-O2B	12.51	1.82	1.59
50	H	500	UQ9	C6-C1	10.23	1.53	1.35
56	W	200	8Q1	C34-N36	5.55	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	n	200	8Q1	C34-N36	5.52	1.45	1.33
56	n	200	8Q1	C39-N41	5.38	1.45	1.33

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	P	500	NDP	PN-O3-PA	-7.18	108.20	132.83
56	n	200	8Q1	C6-C1-S44	5.55	119.92	113.46
56	W	200	8Q1	C6-C1-S44	5.43	119.78	113.46
50	H	500	UQ9	C7-C8-C9	-4.16	119.86	126.79
59	z	302	T7X	O16-C10-C12	4.13	120.41	111.50

There are no chirality outliers.

5 of 259 torsion outliers are listed below:

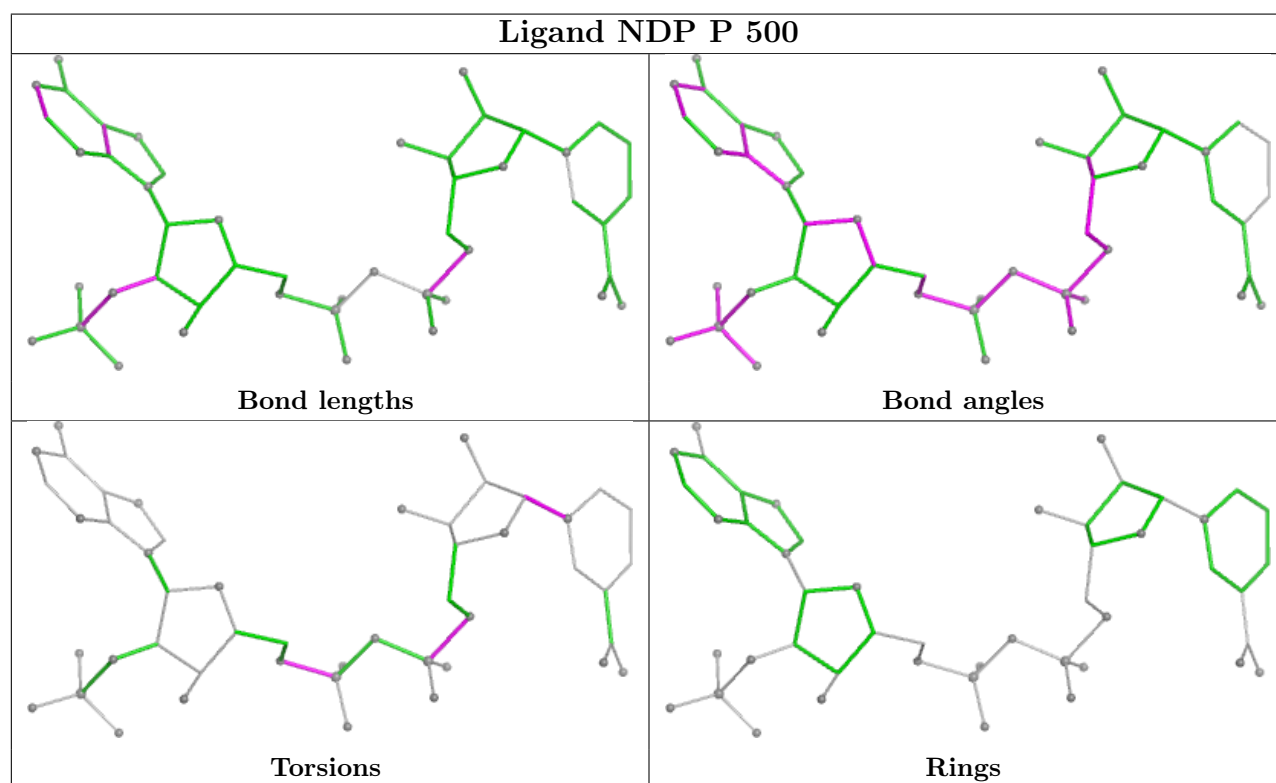
Mol	Chain	Res	Type	Atoms
49	F	500	FMN	N10-C1'-C2'-O2'
49	F	500	FMN	N10-C1'-C2'-C3'
49	F	500	FMN	C1'-C2'-C3'-O3'
49	F	500	FMN	C1'-C2'-C3'-C4'
50	H	500	UQ9	C9-C11-C12-C13

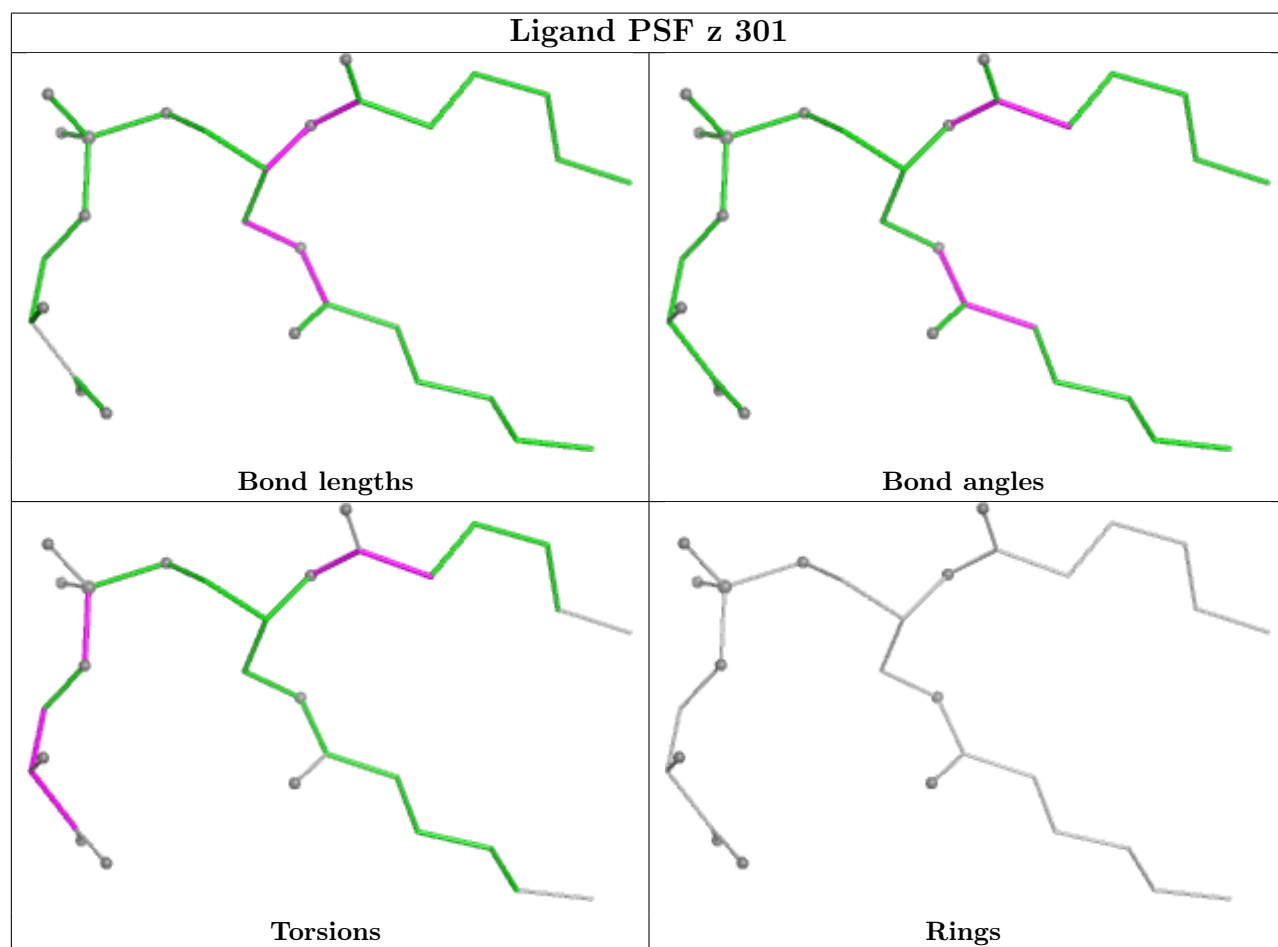
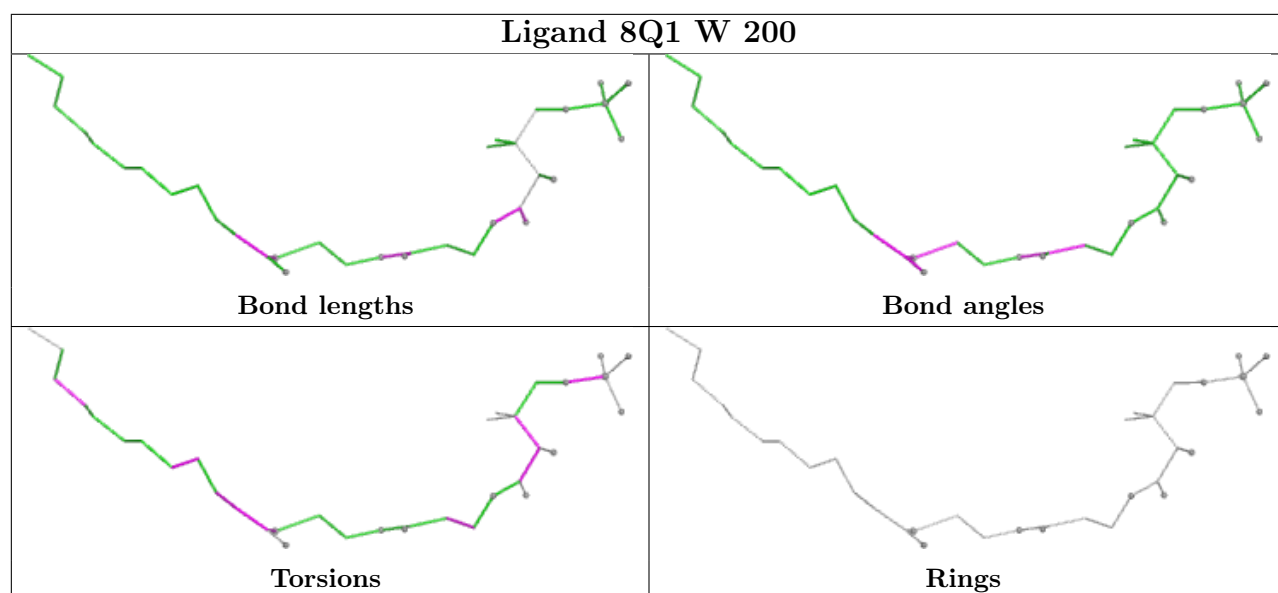
There are no ring outliers.

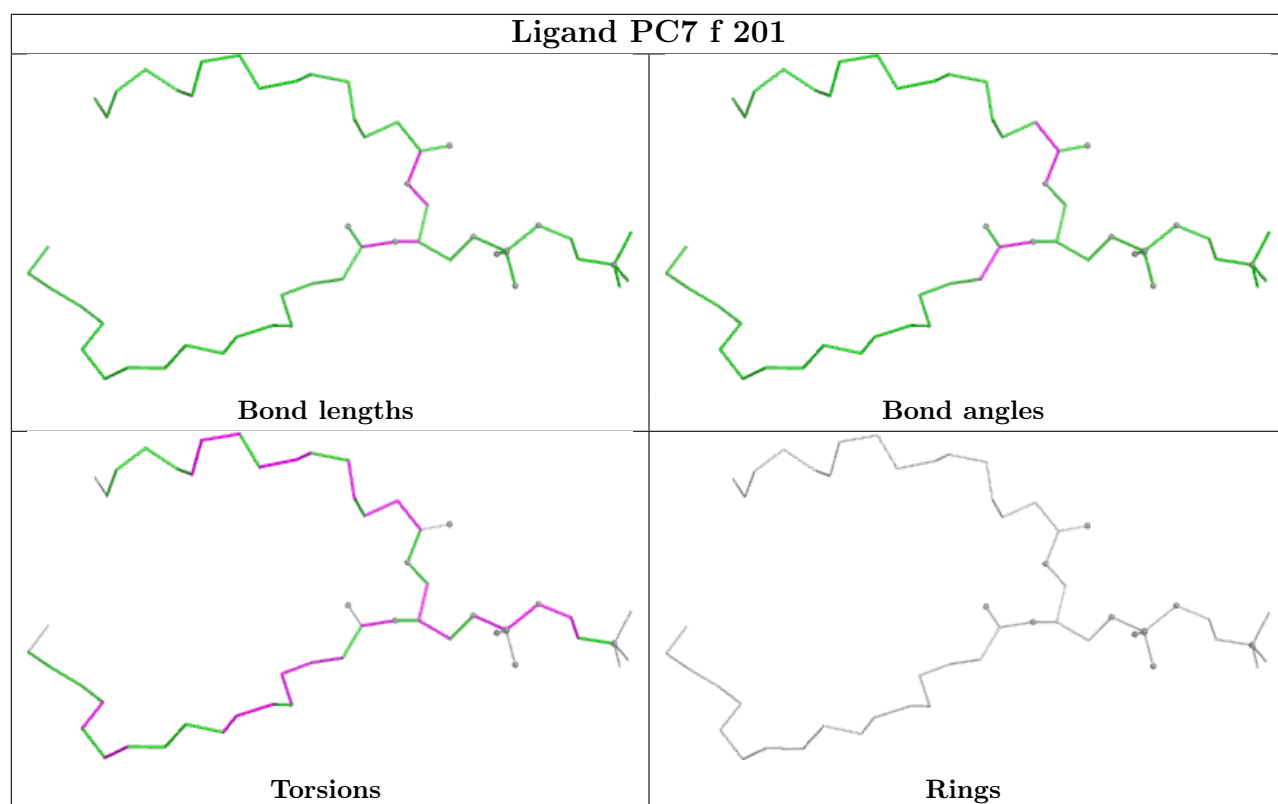
15 monomers are involved in 45 short contacts:

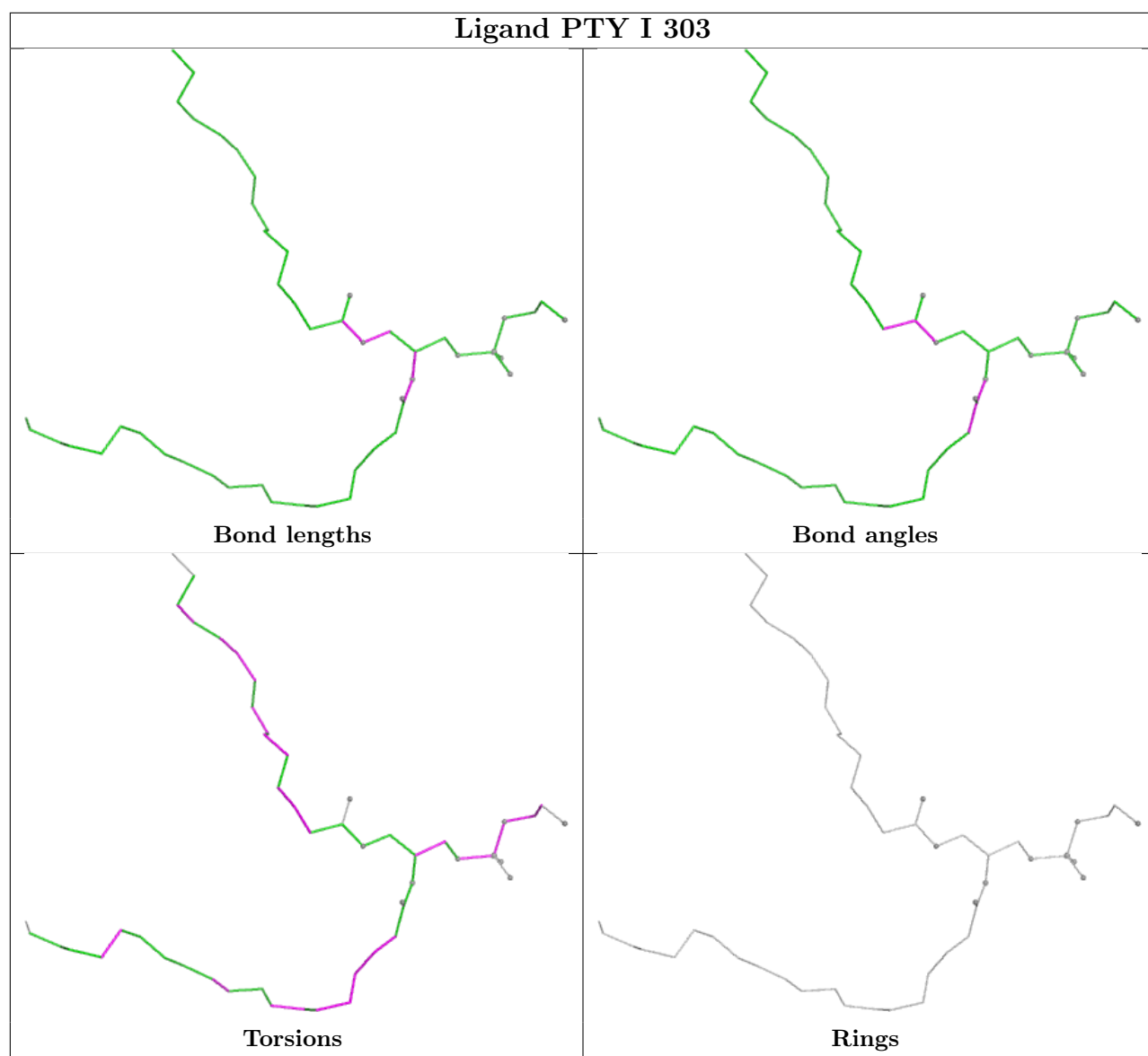
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	W	200	8Q1	1	0
58	z	301	PSF	1	0
47	F	501	SF4	2	0
52	f	201	PC7	3	0
47	B	500	SF4	2	0
48	E	500	FES	2	0
51	I	303	PTY	7	0
51	M	502	PTY	3	0
53	M	503	LMN	6	0
49	F	500	FMN	2	0
51	N	501	PTY	4	0
50	H	500	UQ9	5	0
57	y	302	PGT	1	0
47	I	301	SF4	1	0
52	M	501	PC7	6	0

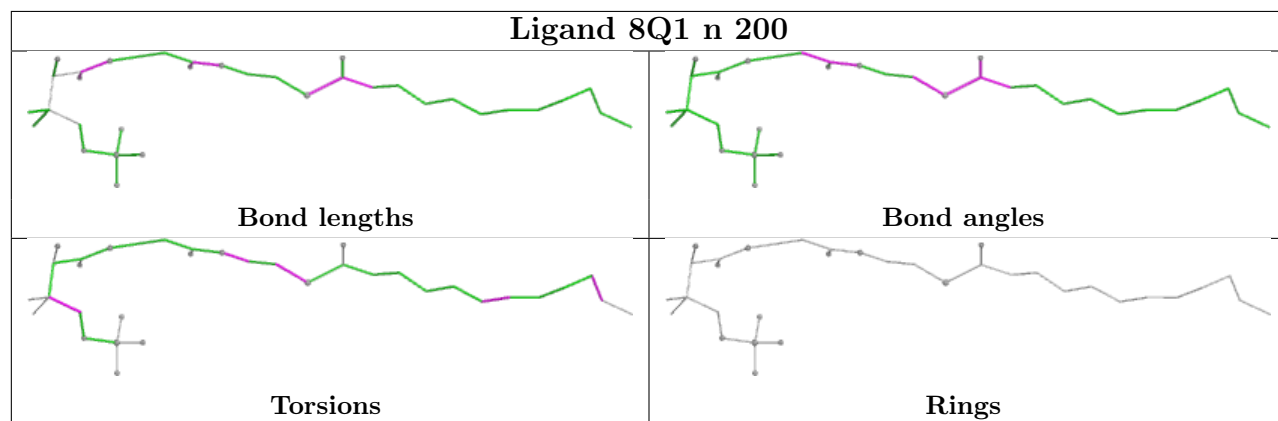
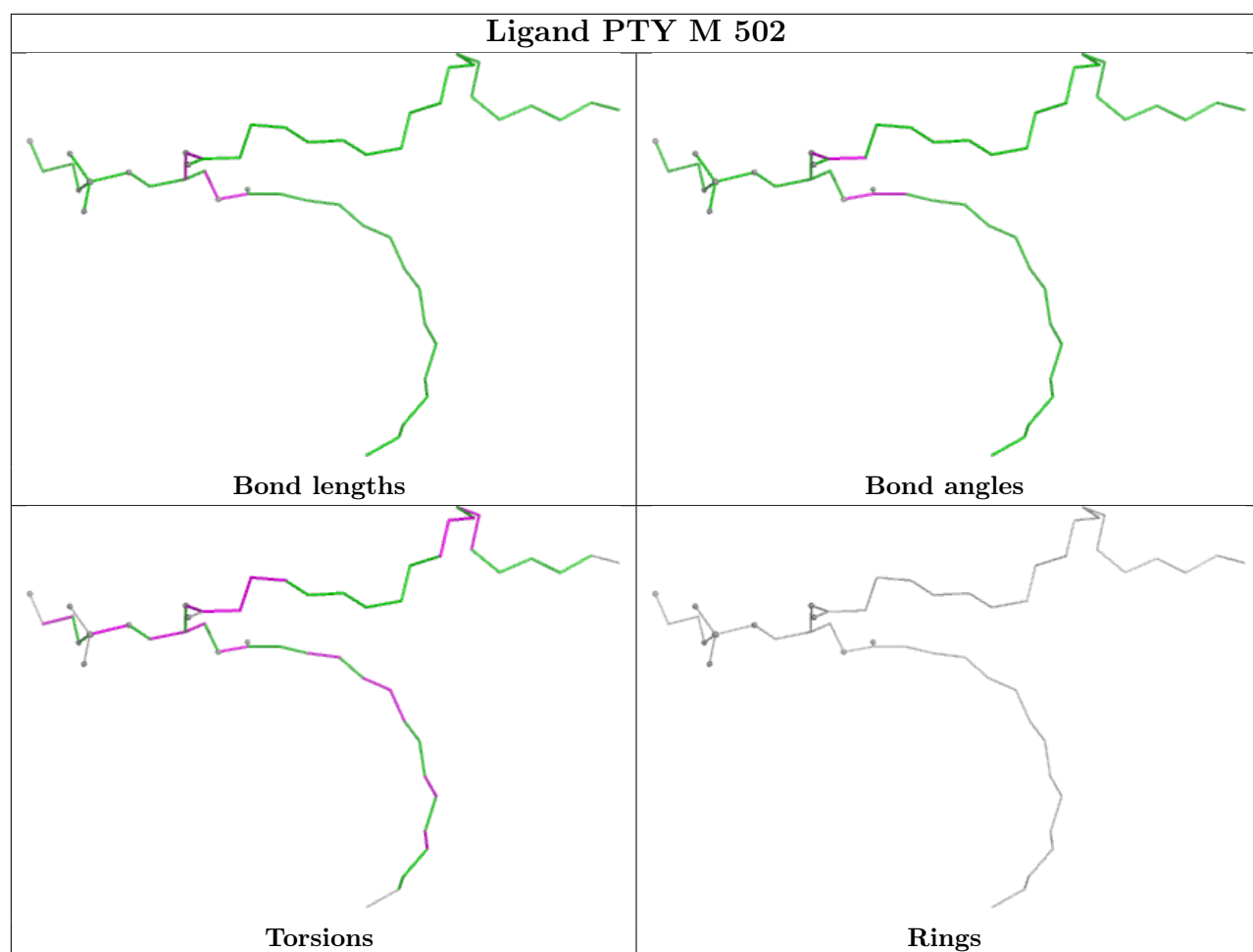
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

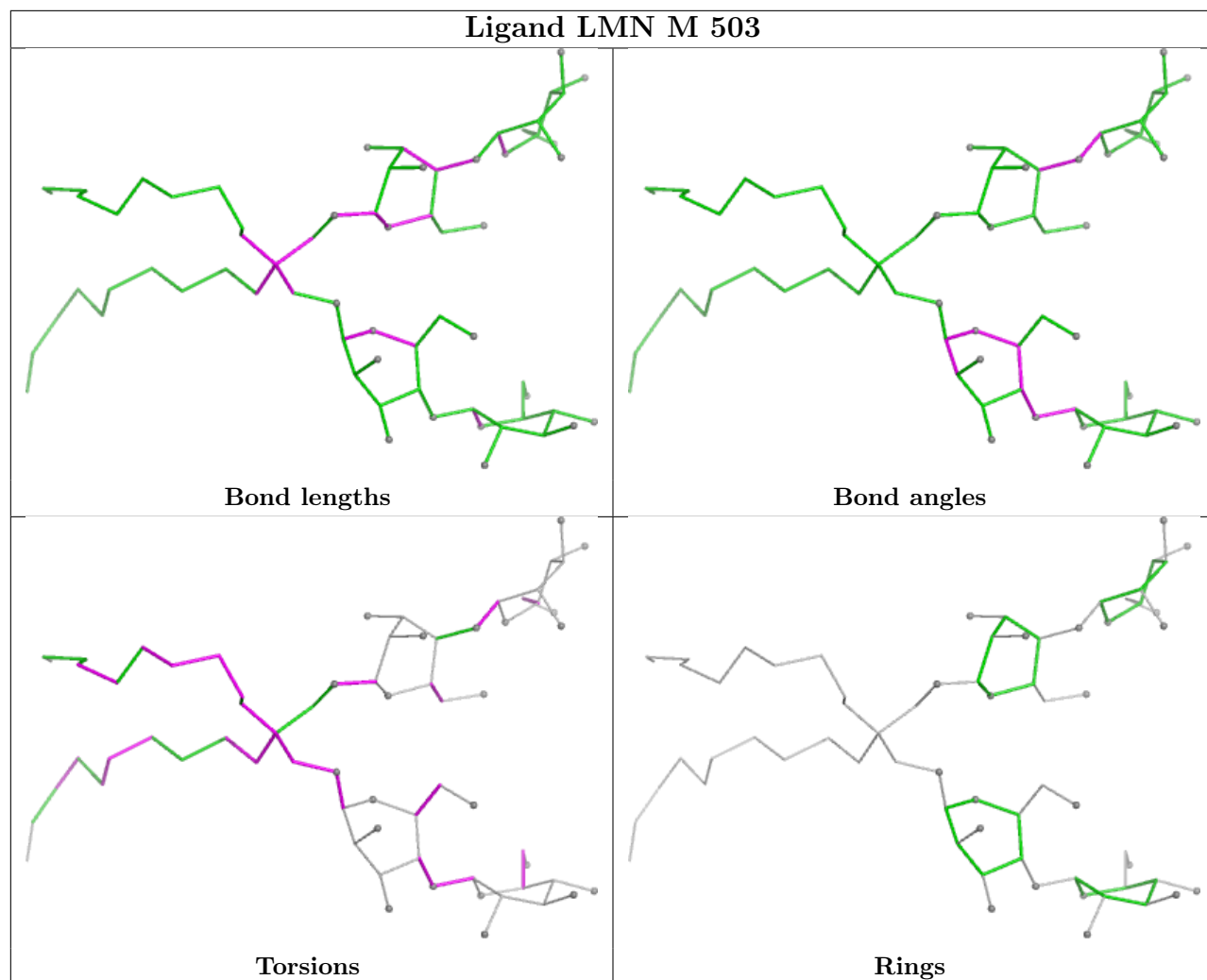


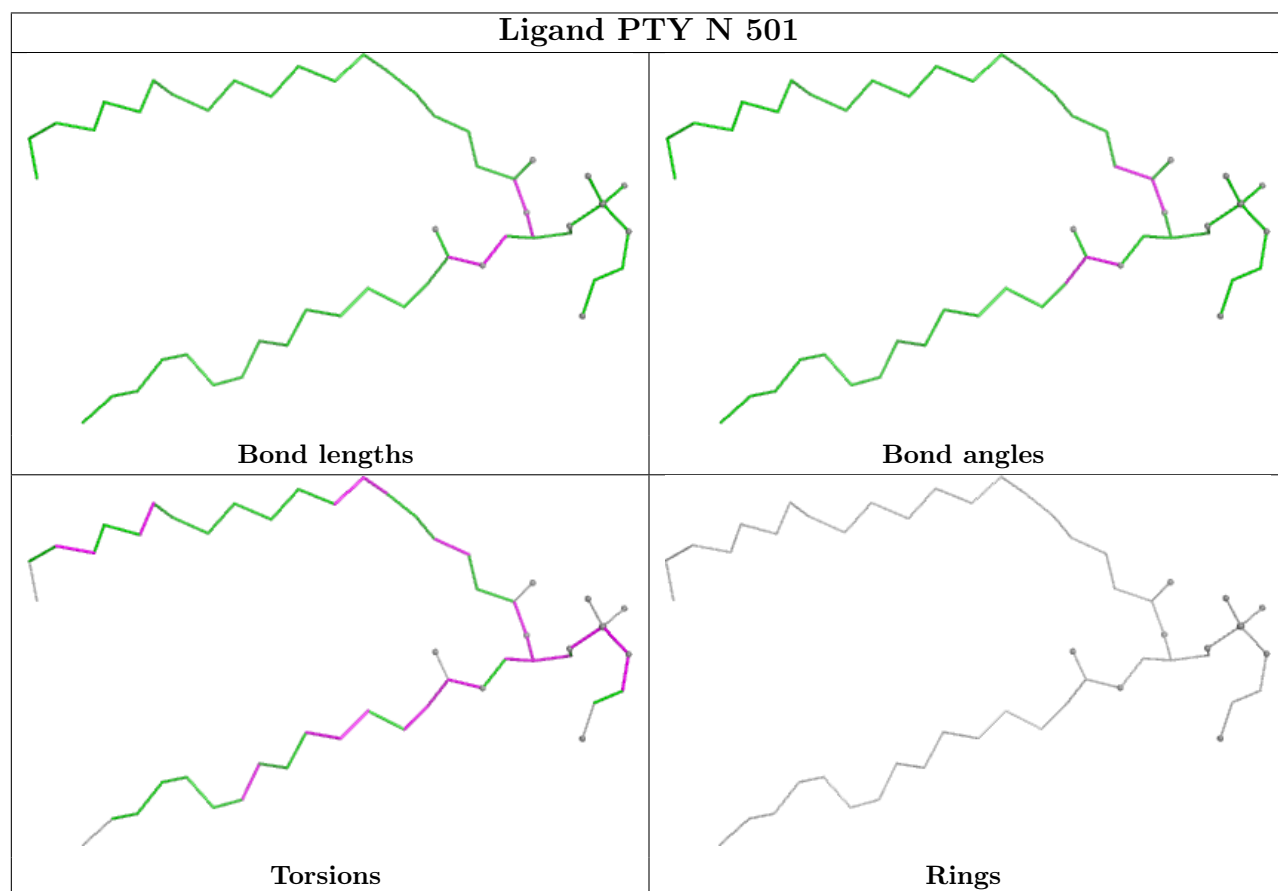
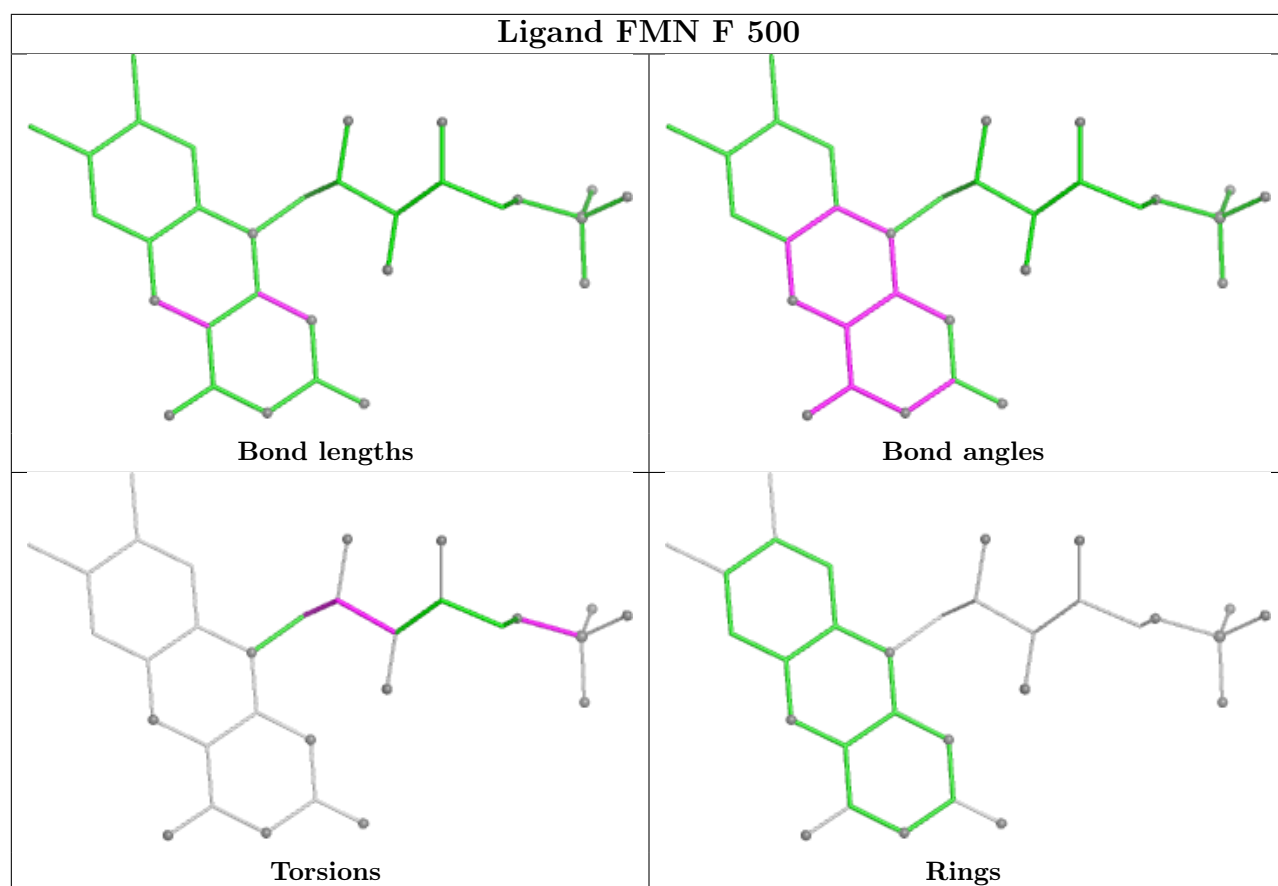


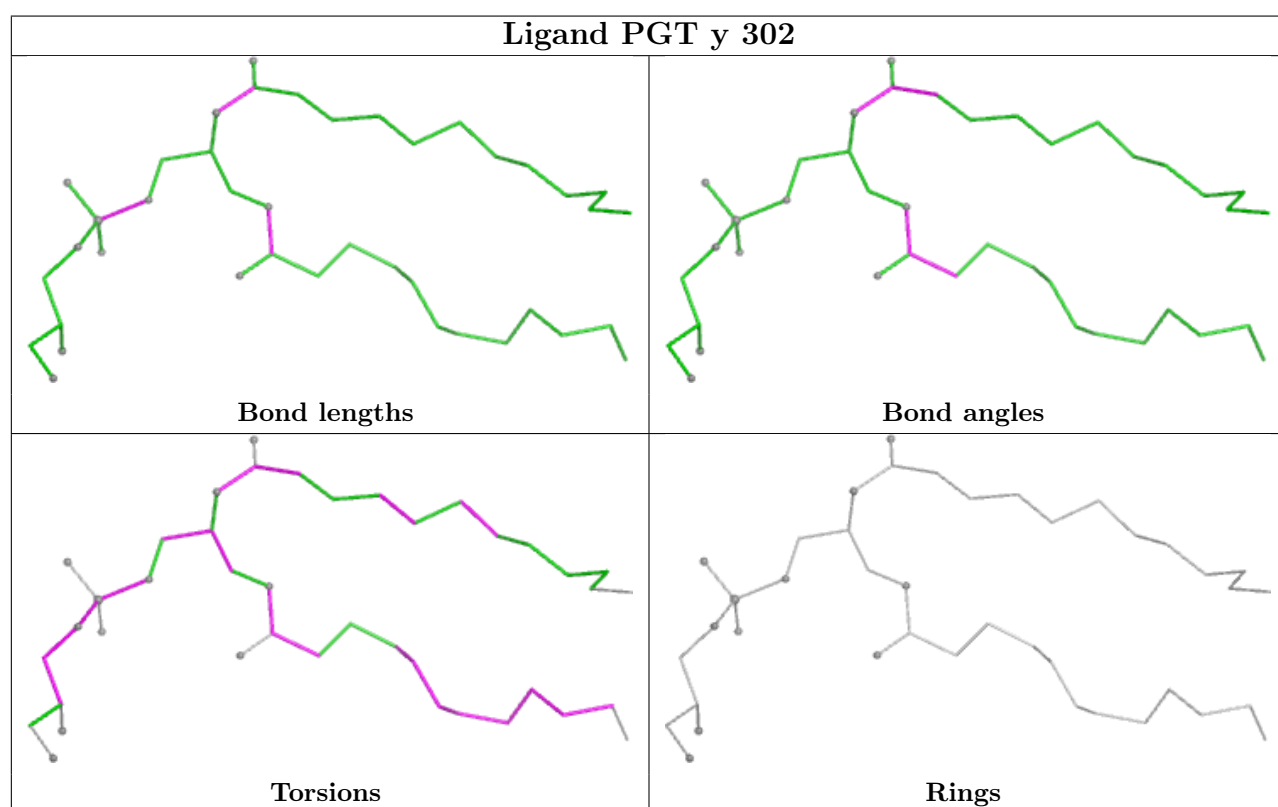
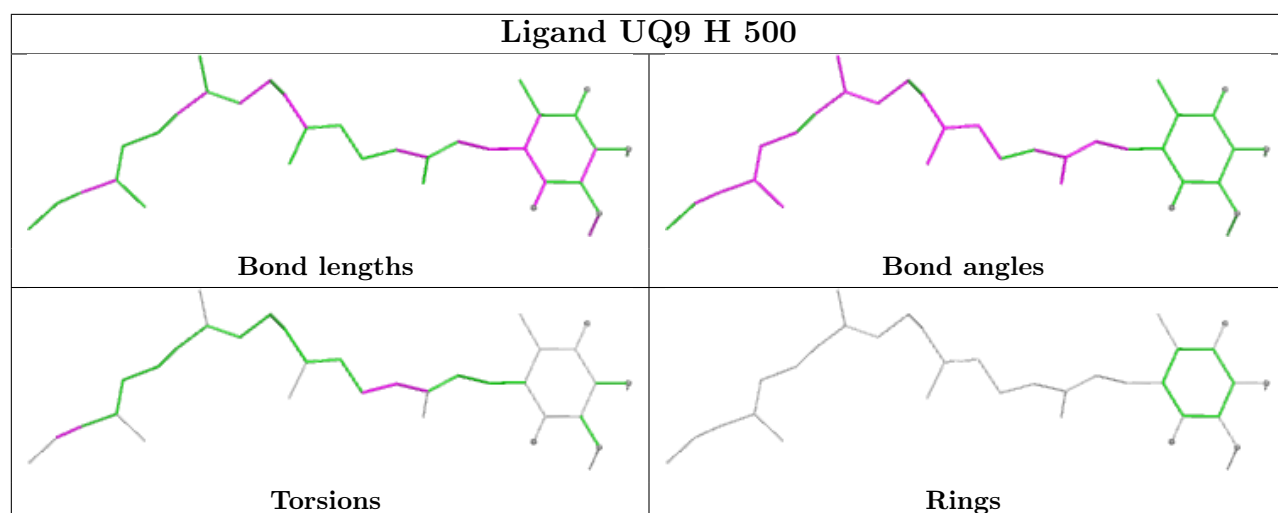


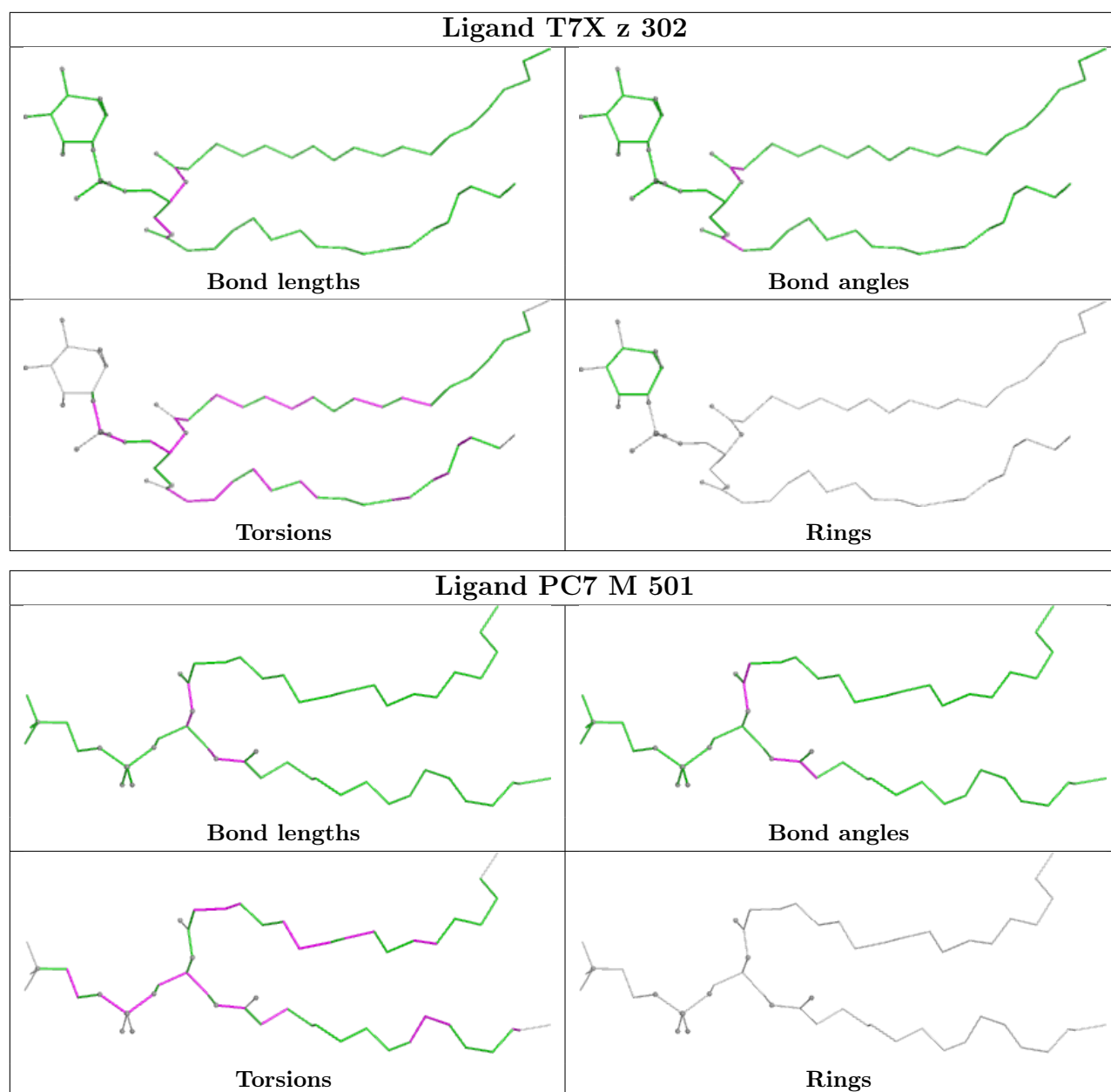












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

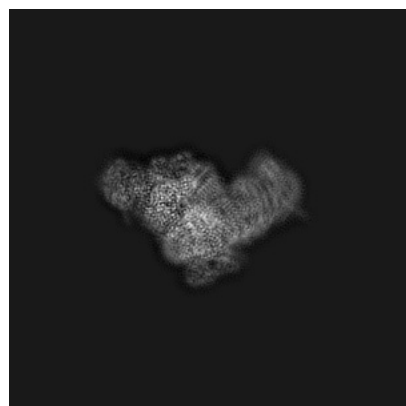
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11875. These allow visual inspection of the internal detail of the map and identification of artifacts.

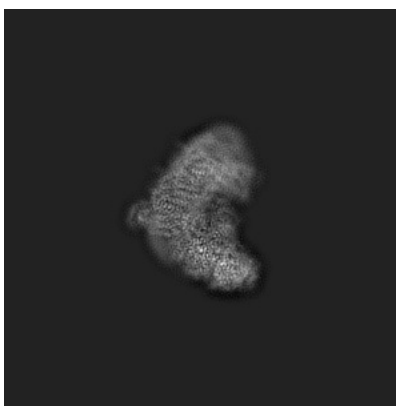
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

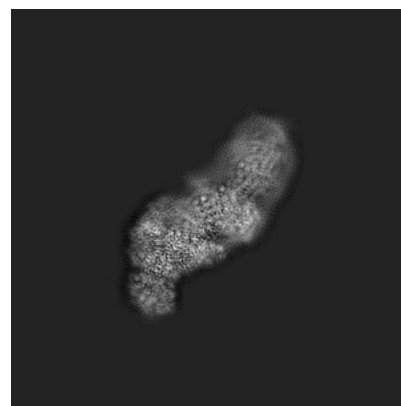
6.1.1 Primary map



X

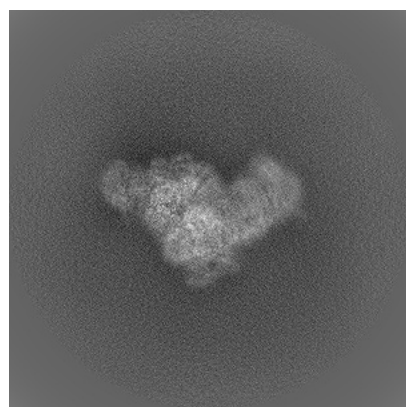


Y

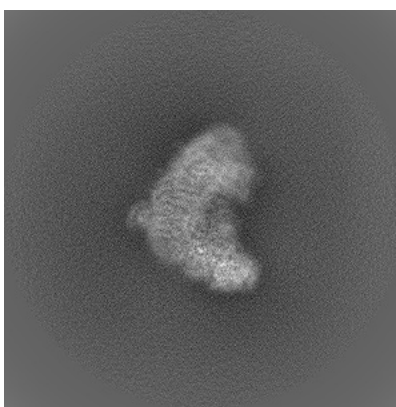


Z

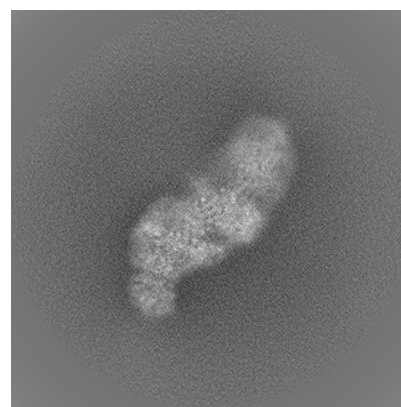
6.1.2 Raw map



X



Y

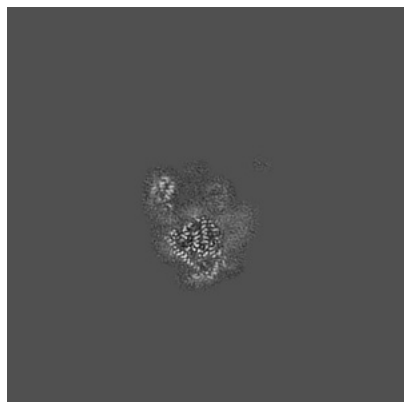


Z

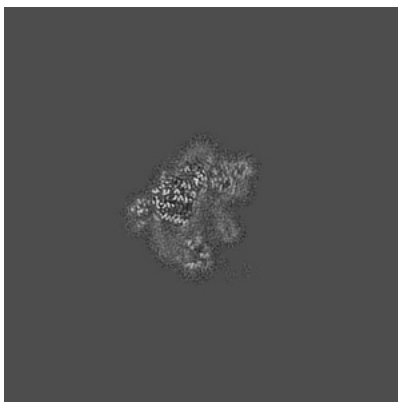
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 300

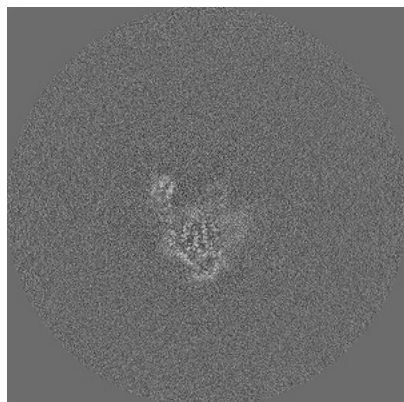


Y Index: 300

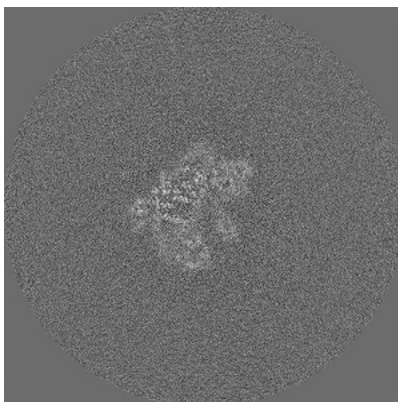


Z Index: 300

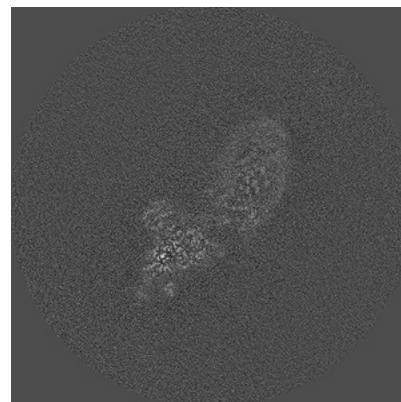
6.2.2 Raw map



X Index: 300



Y Index: 300

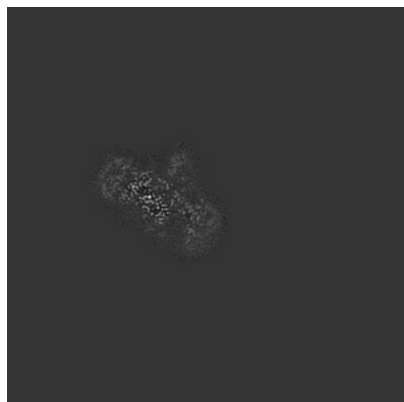


Z Index: 300

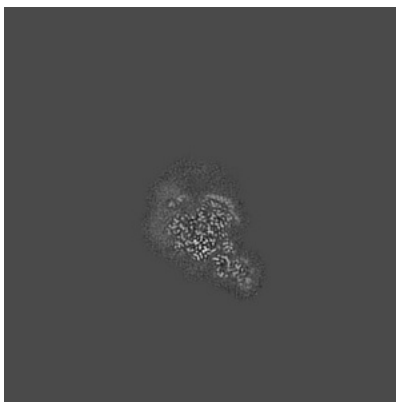
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 224

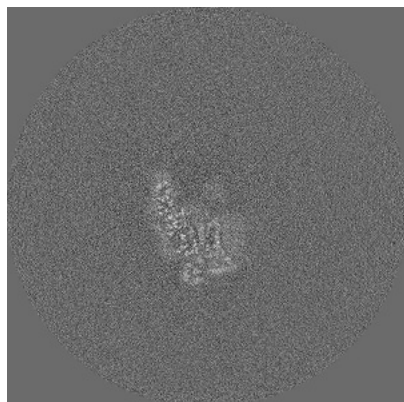


Y Index: 240

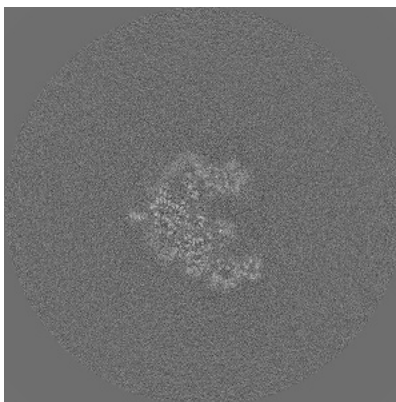


Z Index: 299

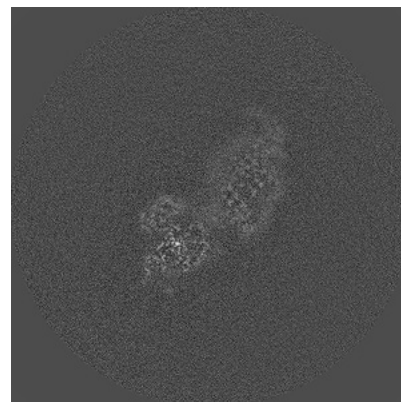
6.3.2 Raw map



X Index: 287



Y Index: 268

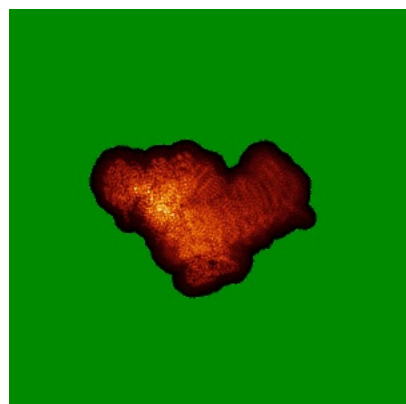


Z Index: 291

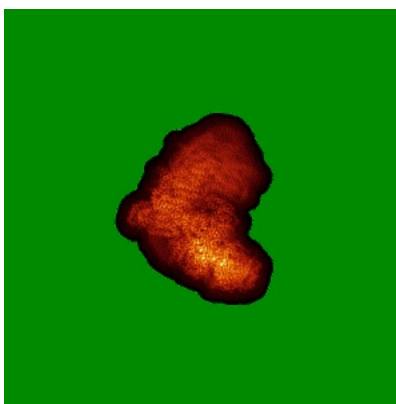
The images above show the largest variance slices of the map in three orthogonal directions.

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

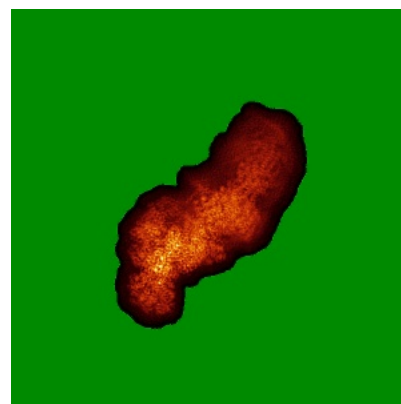
6.4.1 Primary map



X

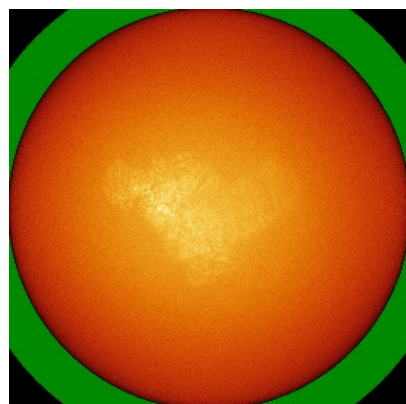


Y

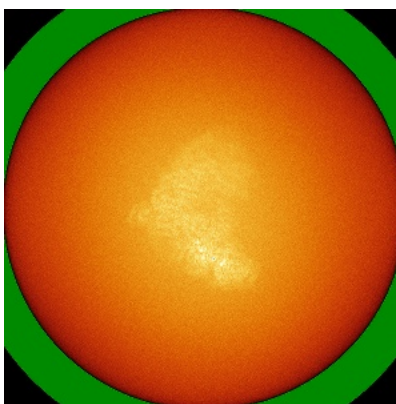


Z

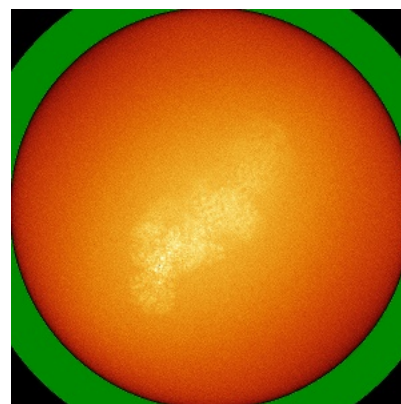
6.4.2 Raw map



X



Y

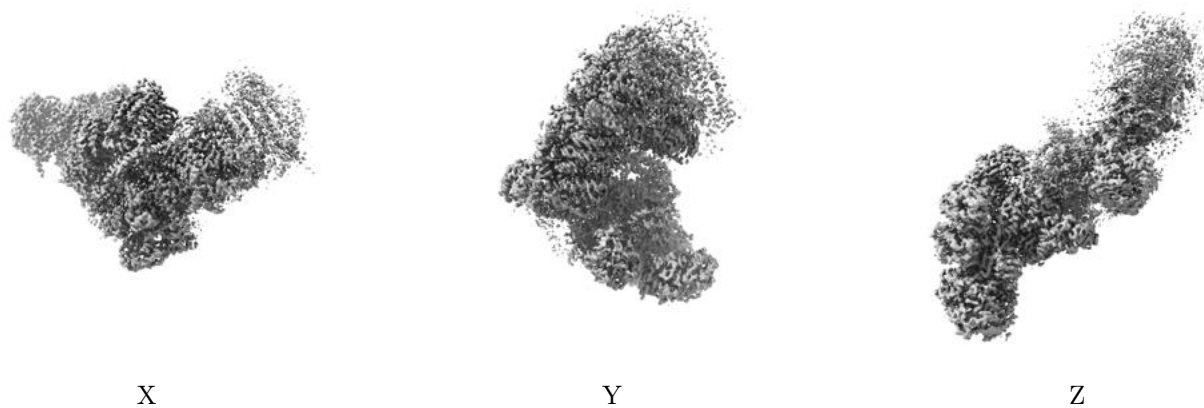


Z

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.

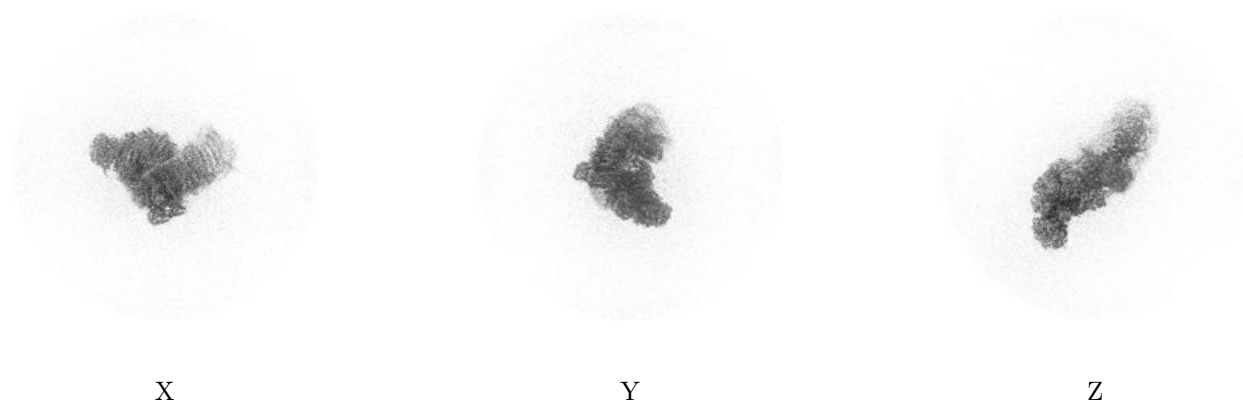
6.5 Orthogonal surface views [i](#)

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.

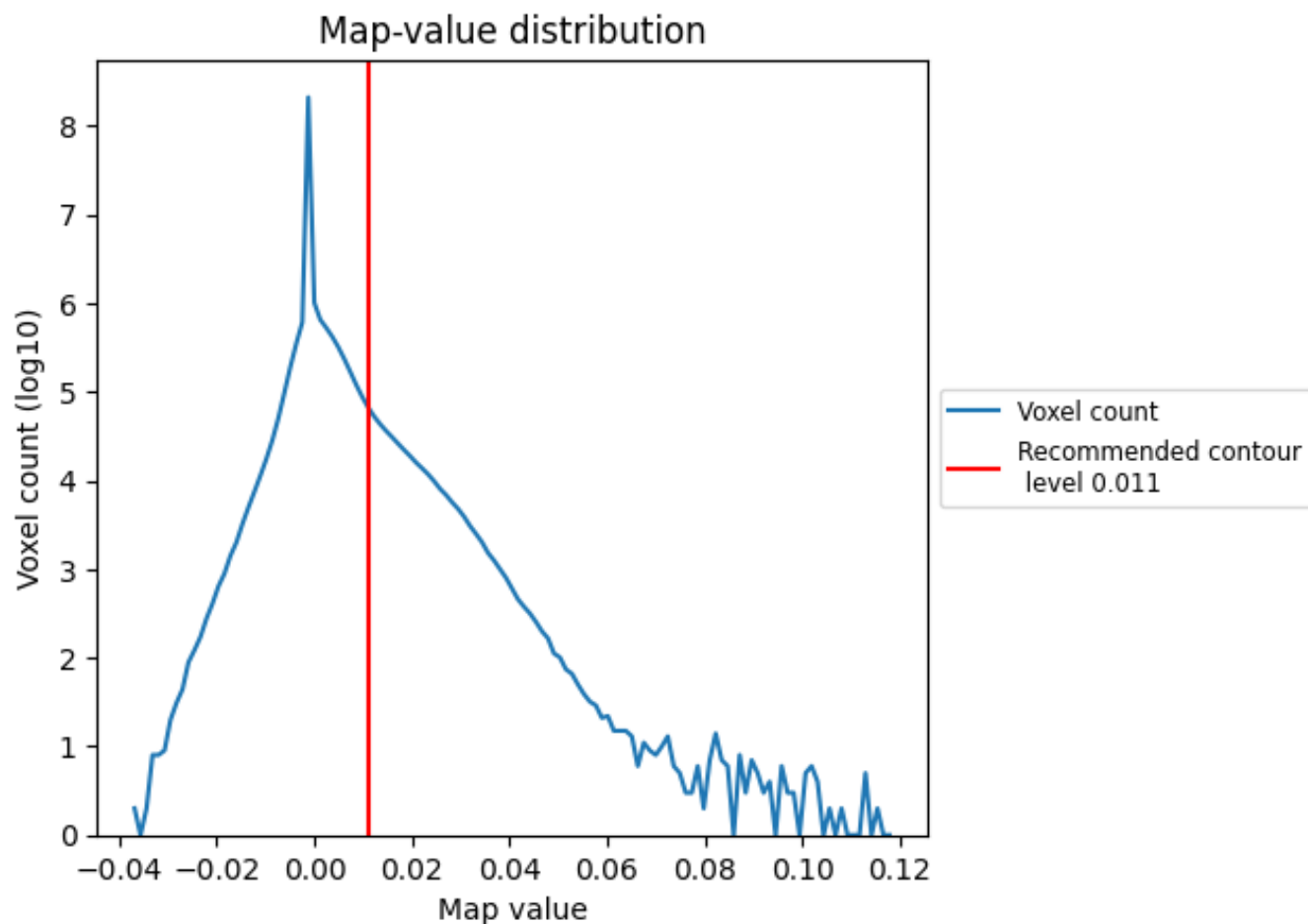
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

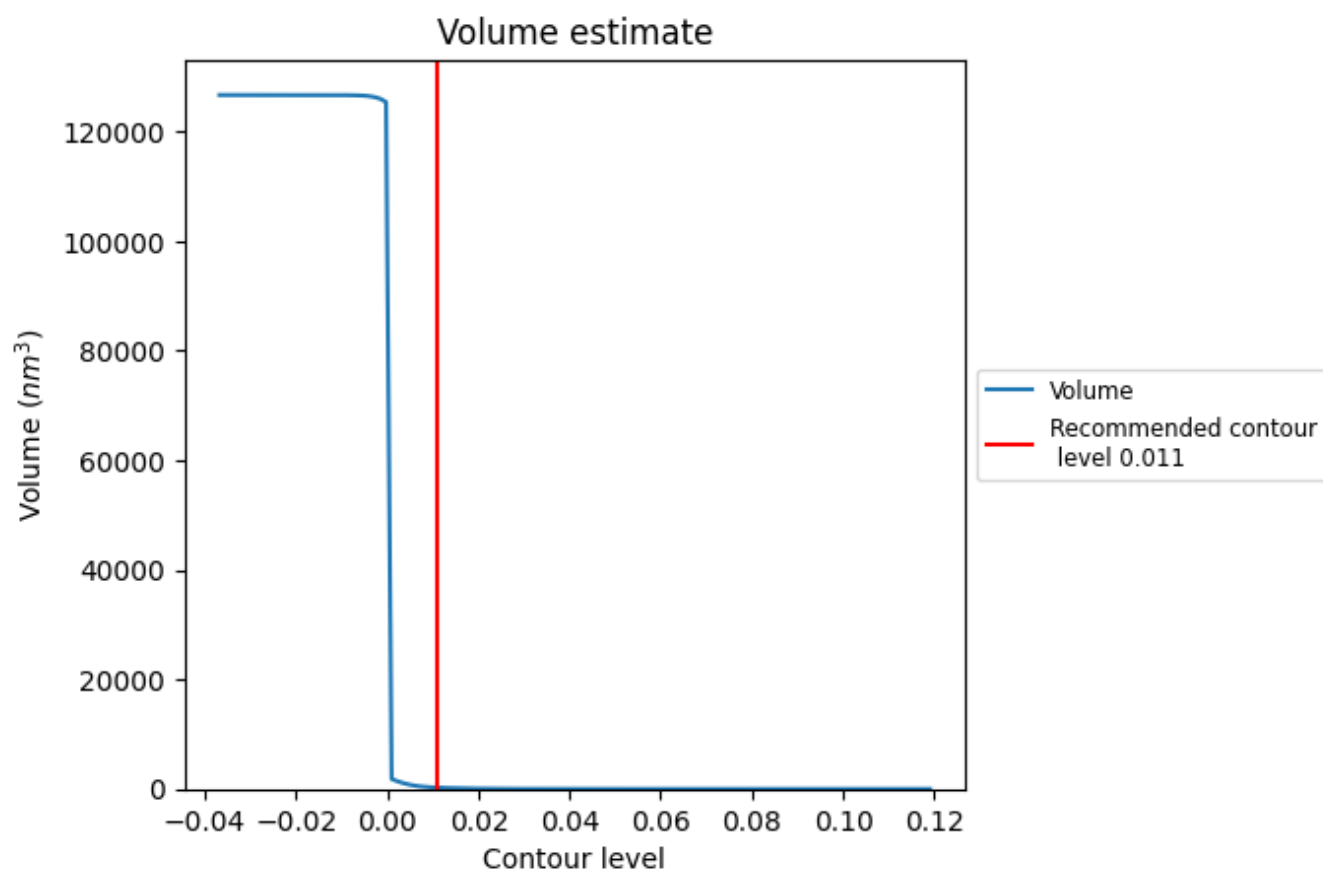
This section contains the results of statistical analysis of the map.

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.

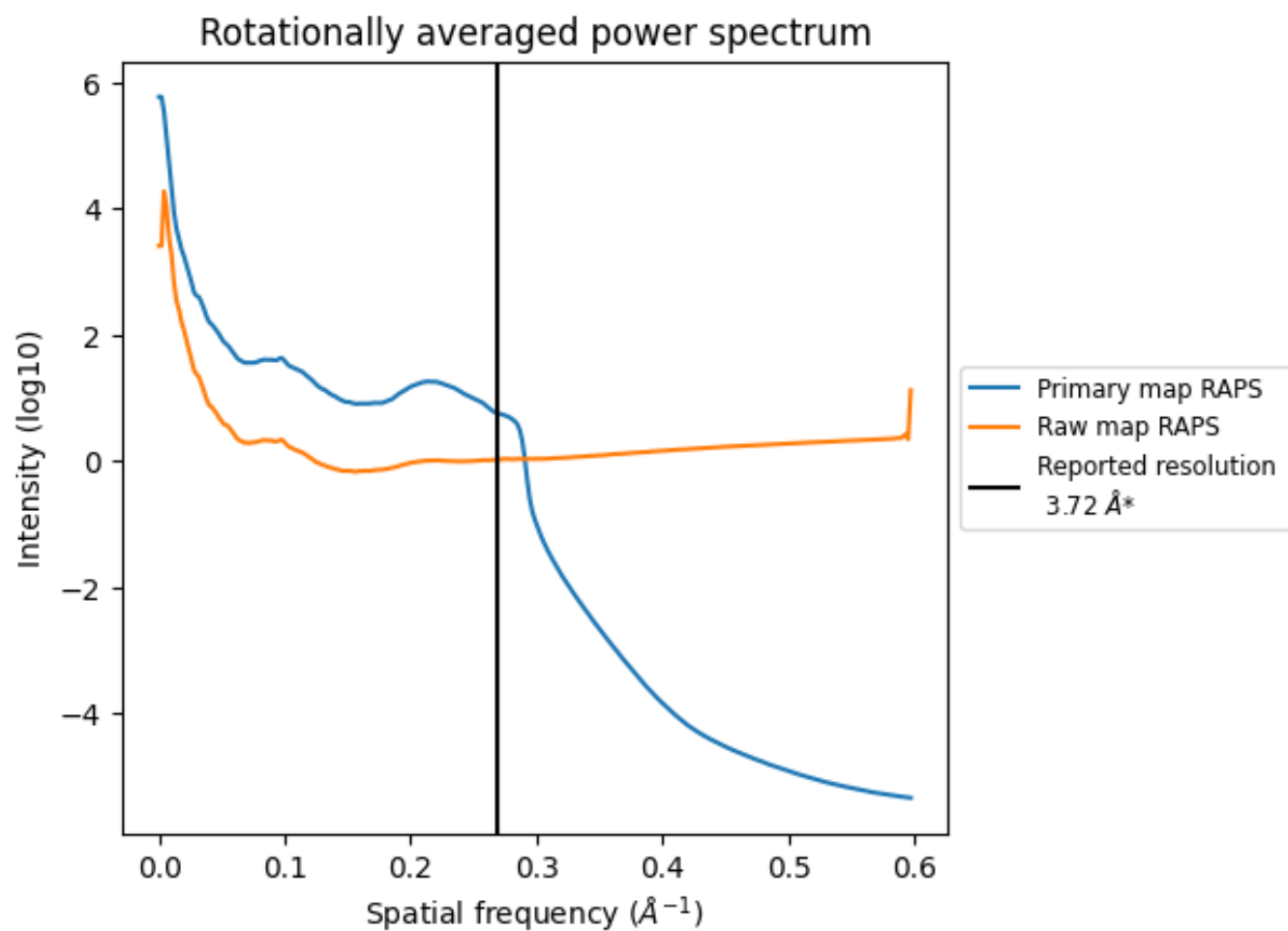
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 234 nm^3 ; this corresponds to an approximate mass of 211 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 ⓘ

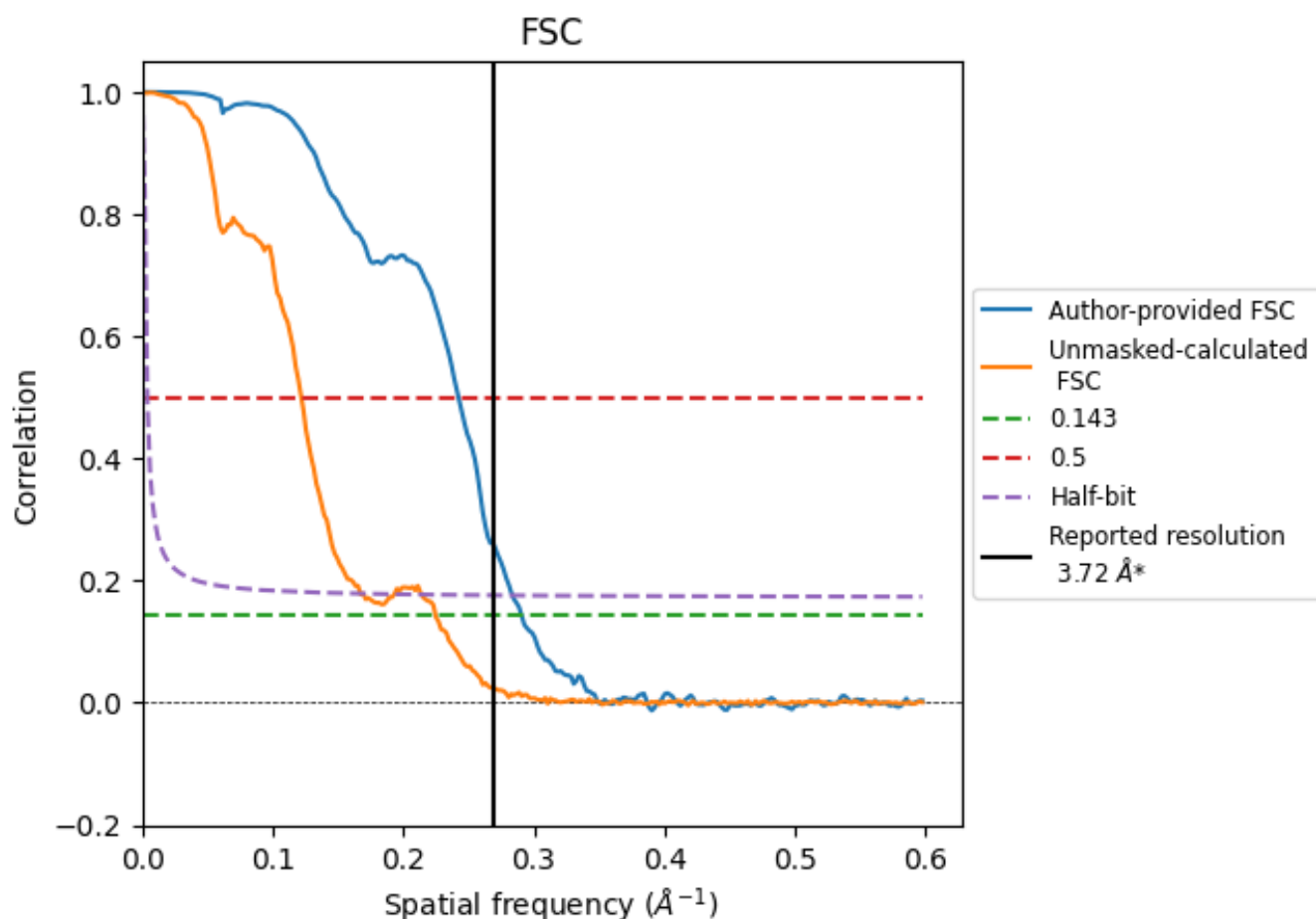


*Reported resolution corresponds to spatial frequency of 0.269 $\text{\AA}^{-1}$

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 0.269 Å⁻¹

8.2 Resolution estimates [i](#)

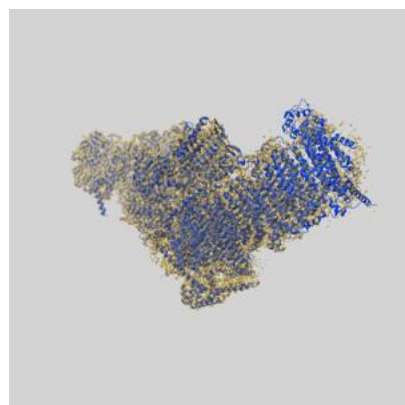
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.72	-	-
Author-provided FSC curve	3.44	4.13	3.53
Unmasked-calculated*	4.45	8.20	5.98

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.45 differs from the reported value 3.72 by more than 10 %

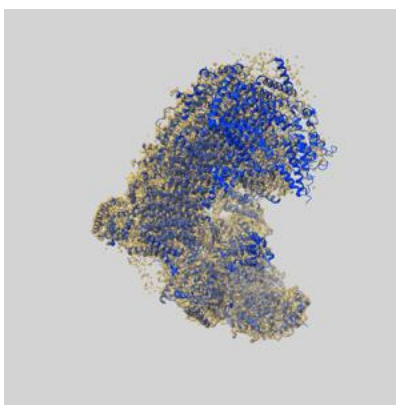
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11875 and PDB model 7AR7. Per-residue inclusion information can be found in section [3](#) on page [20](#).

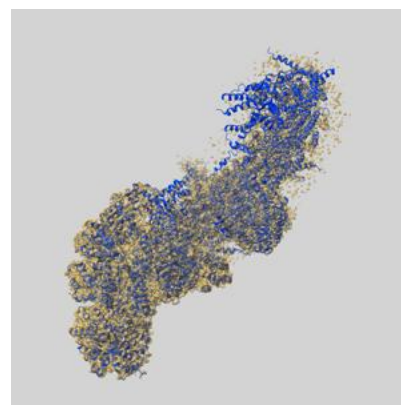
9.1 Map-model overlay [i](#)



X



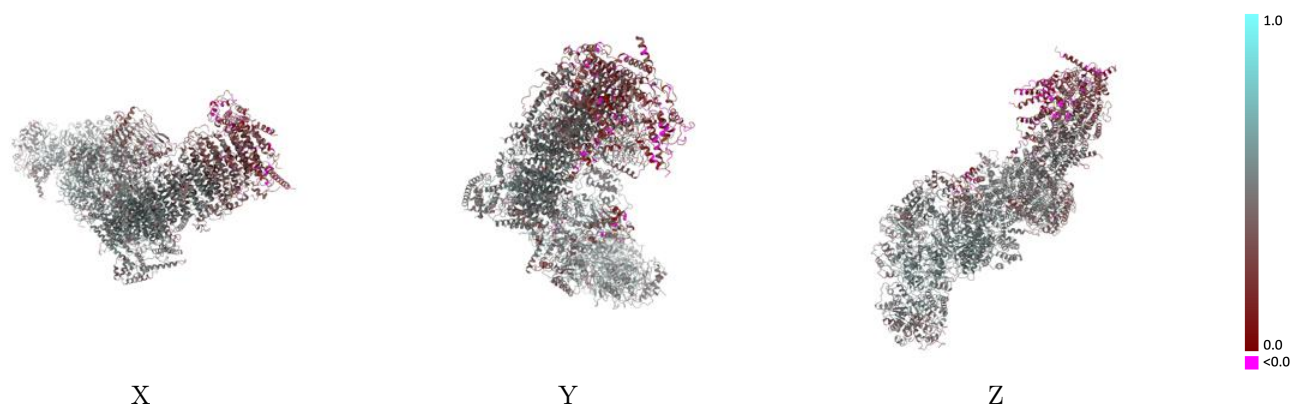
Y



Z

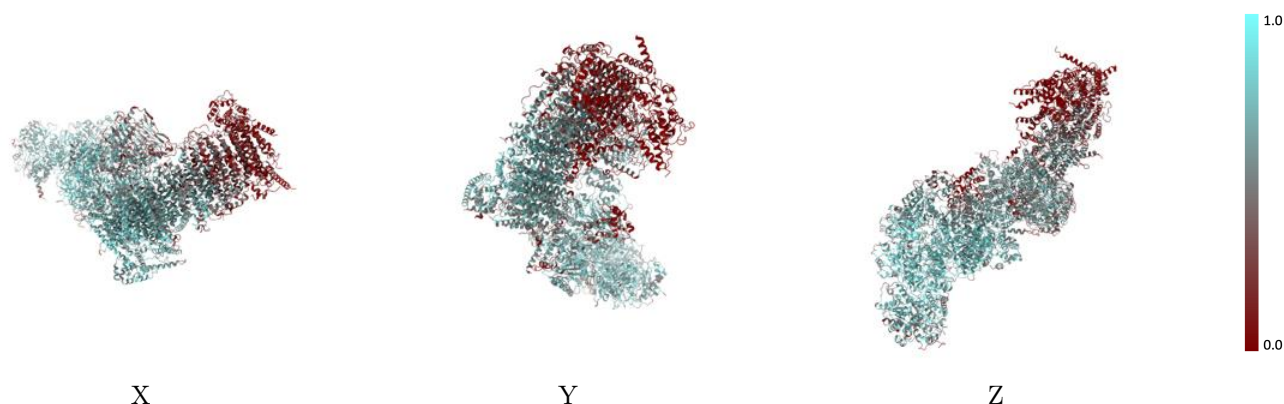
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



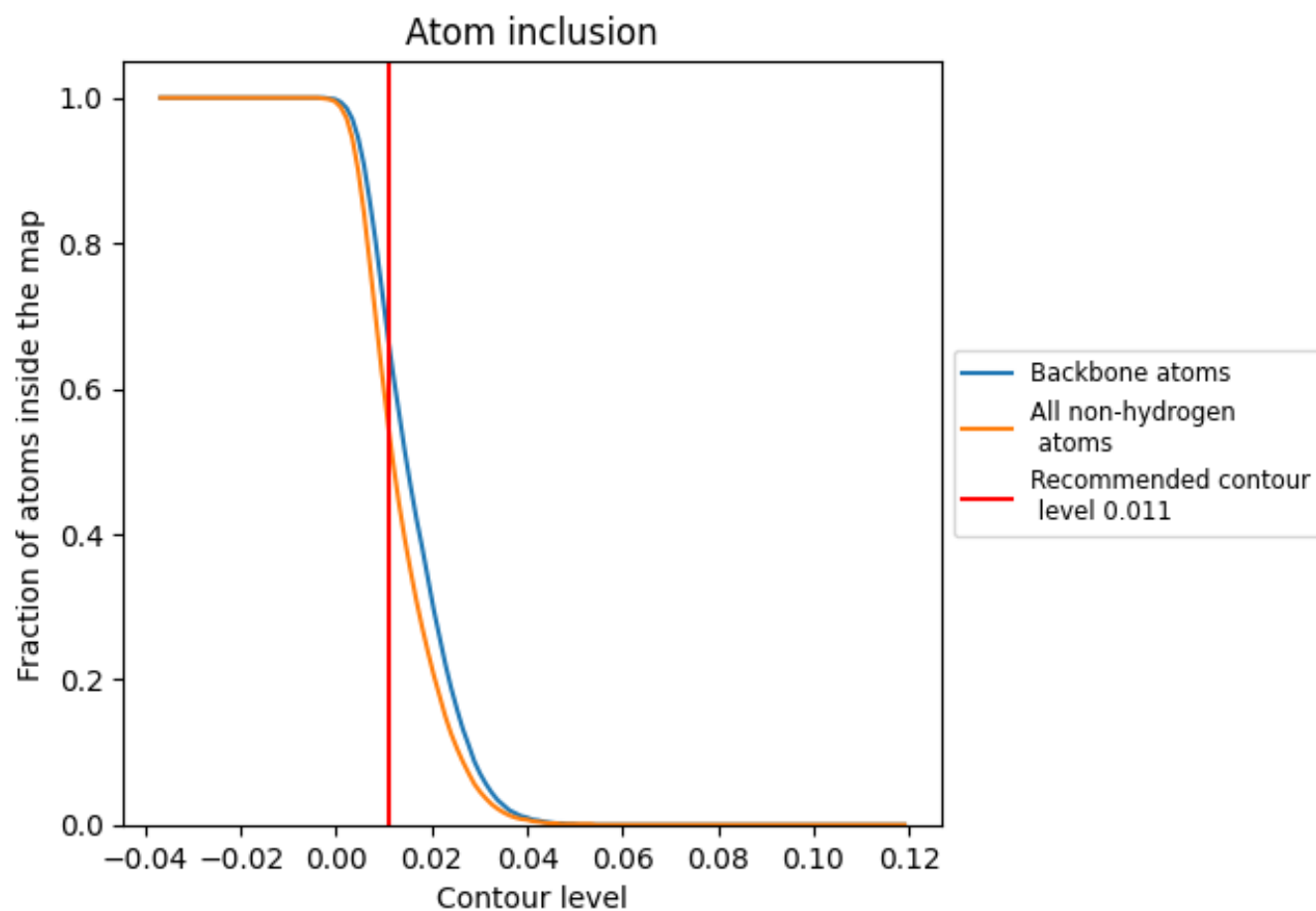
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 66% of all backbone atoms, 55% 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	 0.5450	 0.4380
A	 0.6350	 0.4980
B	 0.7590	 0.5290
C	 0.7650	 0.5350
D	 0.7750	 0.5320
E	 0.6190	 0.4410
F	 0.6440	 0.4680
G	 0.7300	 0.5110
H	 0.6610	 0.4930
I	 0.7860	 0.5380
J	 0.6460	 0.5010
K	 0.5980	 0.4920
L	 0.1770	 0.2760
M	 0.5100	 0.4500
N	 0.6410	 0.4990
P	 0.5620	 0.4460
Q	 0.6910	 0.5240
R	 0.7120	 0.5120
S	 0.6470	 0.4530
T	 0.0170	 0.1250
U	 0.0770	 0.2080
V	 0.6600	 0.4710
W	 0.4340	 0.3980
X	 0.6360	 0.4590
Z	 0.6590	 0.4850
a	 0.6560	 0.4840
b	 0.6320	 0.4870
c	 0.2450	 0.3200
d	 0.6380	 0.4850
e	 0.7020	 0.4760
f	 0.6750	 0.5020
g	 0.3900	 0.3800
i	 0.5980	 0.4490
j	 0.1090	 0.2500
k	 0.0640	 0.2160



Continued on next page...

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Chain	Atom inclusion	Q-score
l	 0.0770	 0.2590
m	 0.1760	 0.2650
n	 0.0490	 0.1900
o	 0.0980	 0.2180
p	 0.3820	 0.3740
q	 0.4030	 0.4550
r	 0.3420	 0.4450
u	 0.5130	 0.3280
v	 0.5750	 0.4650
x	 0.5150	 0.4390
y	 0.4450	 0.3960
z	 0.4980	 0.4200