



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 02:50 am GMT

PDB ID : 7AQQ
EMDB ID : EMD-11872
Title : Cryo-EM structure of Arabidopsis thaliana Complex-I (membrane core)
Authors : Klusch, N.; Kuehlbrandt, W.; Yildiz, O.
Deposited on : 2020-10-22
Resolution : 3.06 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 : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

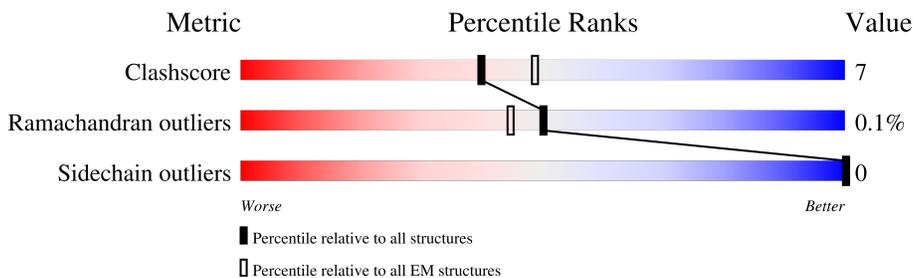
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.06 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.



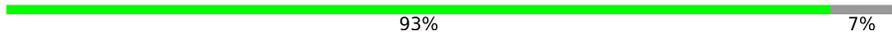
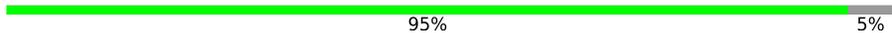
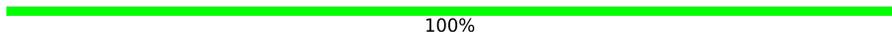
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	119	
2	H	325	
3	J	205	
4	K	100	
5	L	669	
6	M	495	
7	N	499	
8	O	159	
9	X	106	

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Mol	Chain	Length	Quality of chain
10	Z	143	 57% 11% 31%
11	a	65	 89% 11%
12	b	65	 62% 38%
13	d	81	 93% 7%
14	e	83	 78% 22%
15	f	106	 95% 5%
16	i	98	 71% 29%
17	u	30	 100%
18	v	113	 27% 73%
19	x	256	 84% 16%
20	y	278	 96% 4%
21	z	275	 85% 15%

2 Entry composition i

There are 30 unique types of molecules in this entry. The entry contains 23281 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	92	779	553	105	117	4	0	0

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	311	2439	1659	372	393	15	0	0

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	147	1162	784	179	191	8	0	0

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	L	26	208	133	37	38	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	M	262	2126	1457	319	339	11	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	326	LEU	PRO	conflict	UNP B5TM93
M	378	PHE	SER	conflict	UNP B5TM93

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 8 is a protein called AT3G07480.1.

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

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

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

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	Z	98	798	514	137	142	5	0	0

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

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

- Molecule 12 is a protein called At2g46540/F11C10.23.

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

- Molecule 13 is a protein called Excitatory amino acid transporter.

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

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	e	65	Total	C	N	O	S	0	0
			557	344	106	100	7		

- Molecule 15 is a protein called At4g16450.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	f	101	Total	C	N	O	S	0	0
			763	490	126	142	5		

- Molecule 16 is a protein called P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	i	70	Total	C	N	O	S	0	0
			614	384	116	111	3		

- Molecule 17 is a protein called unknown.

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

- Molecule 18 is a protein called Uncharacterized protein At2g27730, mitochondrial.

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

- Molecule 19 is a protein called Gamma carbonic anhydrase-like 2, mitochondrial.

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

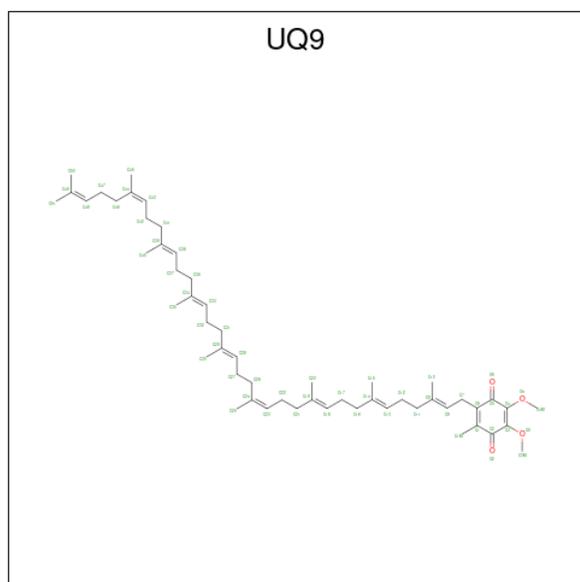
- Molecule 20 is a protein called Gamma carbonic anhydrase 2, mitochondrial.

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

- Molecule 21 is a protein called Gamma carbonic anhydrase 1, mitochondrial.

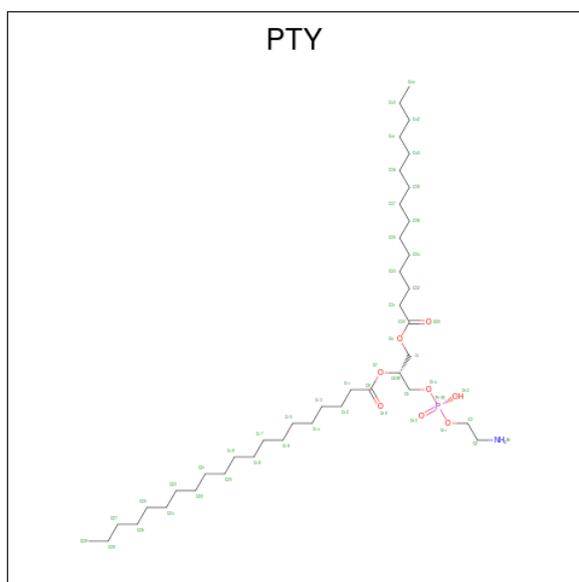
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	z	233	1772	1111	325	330	6	0	0

- Molecule 22 is Ubiquinone-9 (three-letter code: UQ9) (formula: $C_{54}H_{82}O_4$).



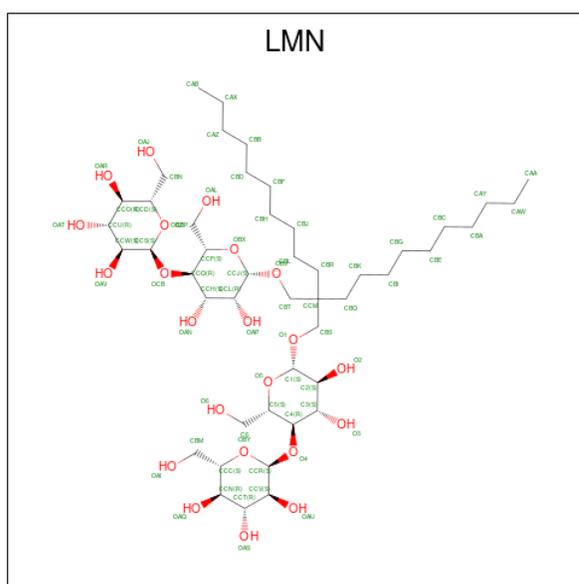
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
22	H	1	35	31	4	0

- Molecule 23 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



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

- Molecule 24 is Lauryl Maltose Neopentyl Glycol (three-letter code: LMN) (formula: $C_{47}H_{88}O_{22}$).

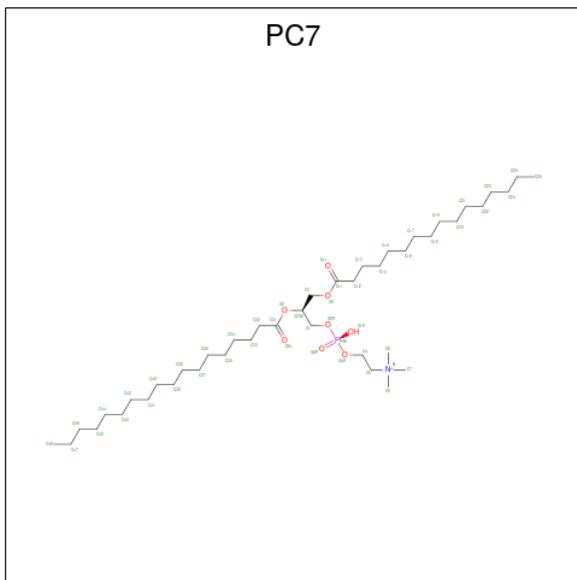


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	M	1	69	47	22	0

- Molecule 25 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 26 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PC7) (formula: C₄₂H₈₅NO₈P).

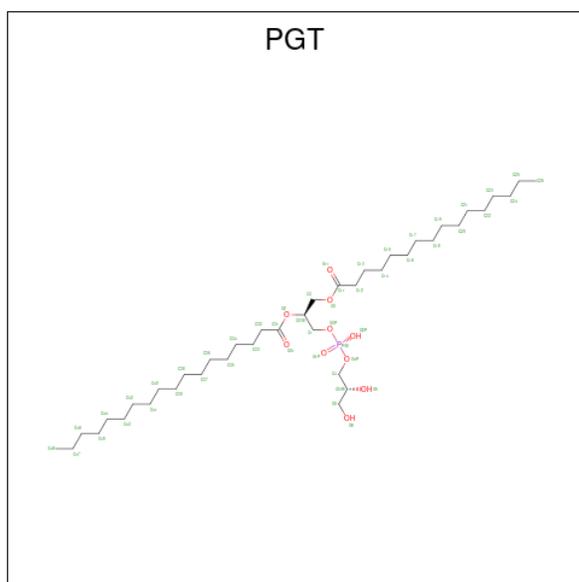


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
26	v	1	52	42	1	8	1	0

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

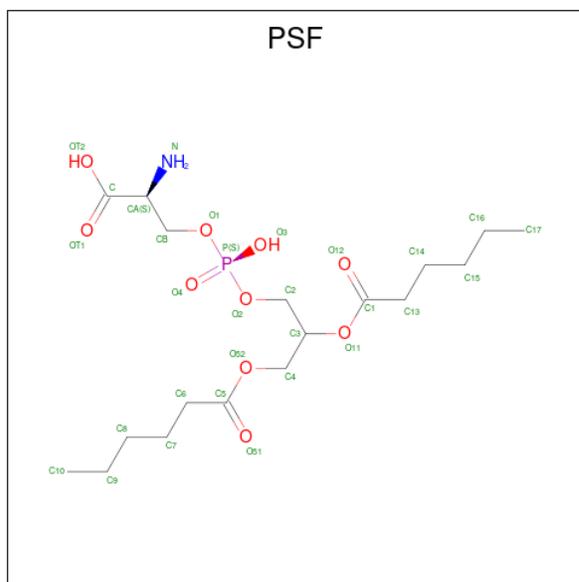
Mol	Chain	Residues	Atoms		AltConf
27	y	1	Total	Zn	0
			1	1	

- Molecule 28 is (1S)-2-[[[(2R)-2,3-DIHYDROXYPROPYL]OXY](HYDROXY)PHOSPHORYL]OXY-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: C₄₀H₇₉O₁₀P).



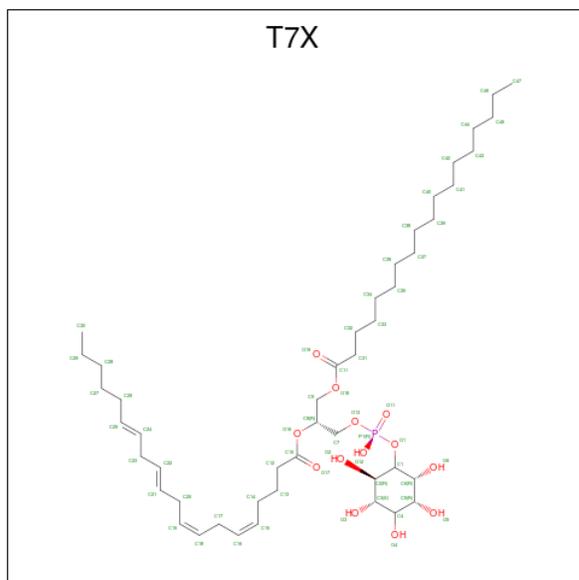
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
28	y	1	41	30	10	1	0

- Molecule 29 is 1,2-DICAPROYL-SN-PHOSPHATIDYL-L-SERINE (three-letter code: PSF) (formula: $C_{18}H_{34}NO_{10}P$).



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

- Molecule 30 is Phosphatidylinositol (three-letter code: T7X) (formula: $C_{47}H_{83}O_{13}P$).

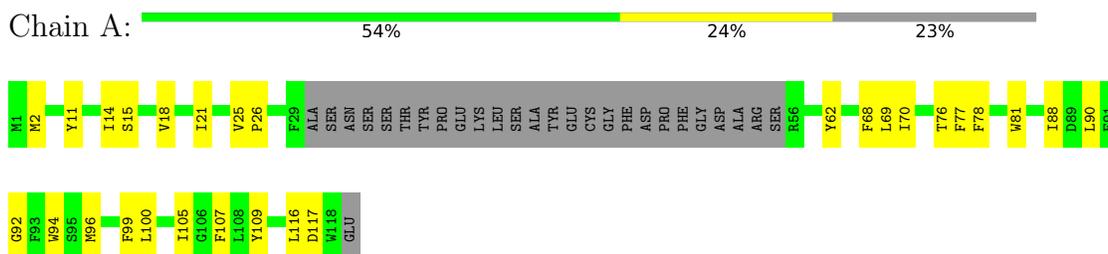


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
30	z	1	61	47	13	1	0

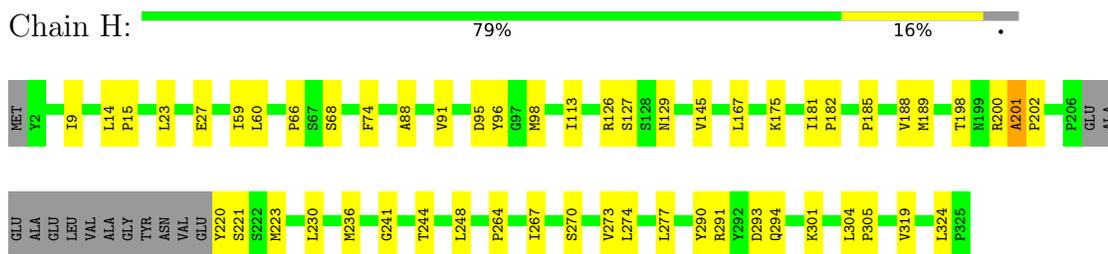
3 Residue-property plots [i](#)

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

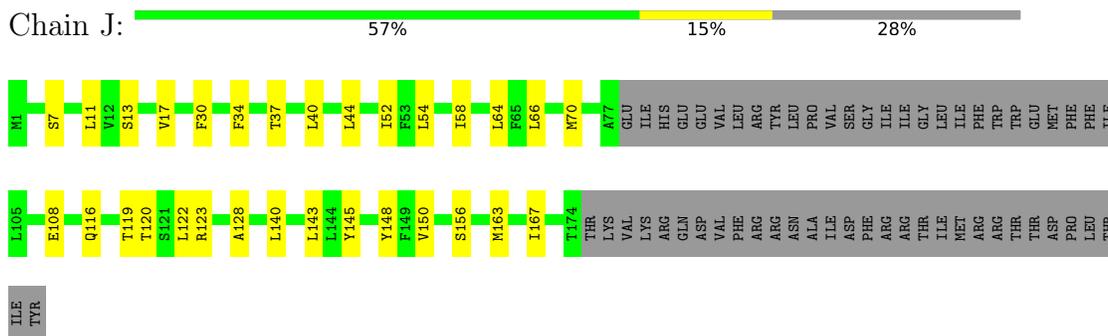
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



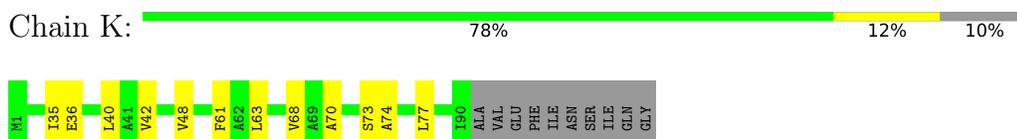
- Molecule 2: NADH-ubiquinone oxidoreductase chain 1

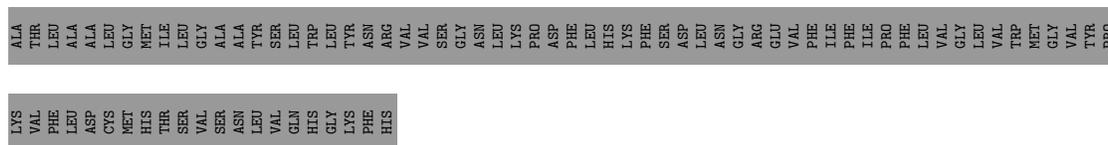


- Molecule 3: NADH-ubiquinone oxidoreductase chain 6



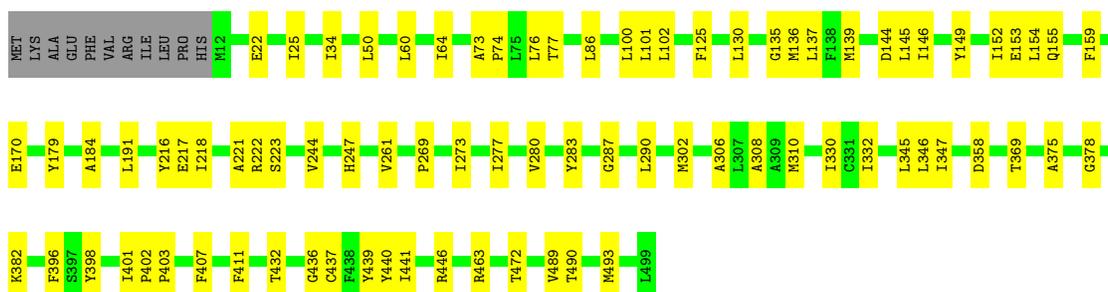
- Molecule 4: NADH dehydrogenase subunit 4L





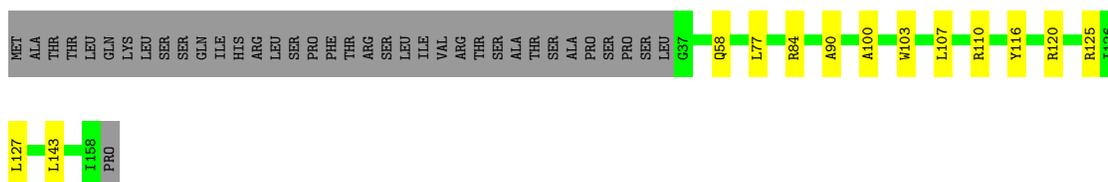
- Molecule 7: NADH-ubiquinone oxidoreductase chain 2

Chain N: 81% 16%



- Molecule 8: AT3G07480.1

Chain O: 69% 8% 23%



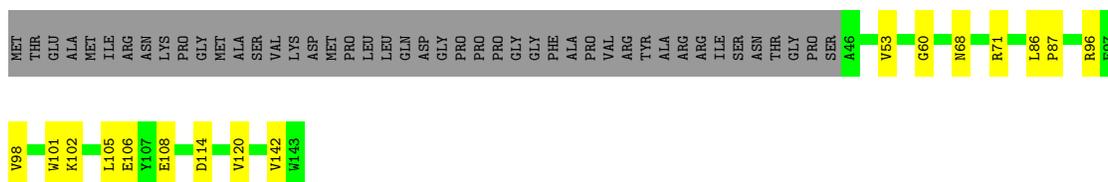
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B

Chain X: 80% 11% 8%



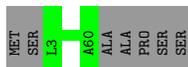
- Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A

Chain Z: 57% 11% 31%



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

Chain a: 89% 11%



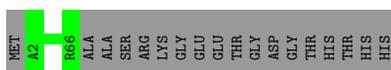
- Molecule 12: At2g46540/F11C10.23



- Molecule 13: Excitatory amino acid transporter



- Molecule 14: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-B



- Molecule 15: At4g16450



- Molecule 16: P1



- Molecule 17: unknown



There are no outlier residues recorded for this chain.

- Molecule 18: Uncharacterized protein At2g27730, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	459177	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

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: T7X, UQ9, PTY, ZN, LMN, FE, PSF, PC7, PGT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/807	0.44	0/1096
2	H	0.29	0/2510	0.49	0/3416
3	J	0.28	0/1187	0.47	0/1617
4	K	0.28	0/717	0.47	0/969
5	L	0.23	0/211	0.54	0/282
6	M	0.27	0/2188	0.44	0/2976
7	N	0.28	0/3924	0.46	0/5327
8	O	0.24	0/971	0.49	0/1314
9	X	0.26	0/781	0.45	0/1049
10	Z	0.28	0/820	0.51	0/1108
11	a	0.25	0/481	0.50	0/646
12	b	0.25	0/300	0.46	0/407
13	d	0.26	0/605	0.49	0/815
14	e	0.27	0/570	0.49	0/759
15	f	0.28	0/779	0.46	0/1052
16	i	0.26	0/632	0.50	0/852
18	v	0.24	0/230	0.39	0/311
19	x	0.28	0/1700	0.50	0/2320
20	y	0.27	0/2066	0.48	0/2800
21	z	0.27	0/1804	0.50	0/2441
All	All	0.27	0/23283	0.48	0/31557

There are no bond length outliers.

There are no bond angle outliers.

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	779	0	796	22	0
2	H	2439	0	2554	39	0
3	J	1162	0	1238	26	0
4	K	707	0	771	15	0
5	L	208	0	211	8	0
6	M	2126	0	2227	33	0
7	N	3820	0	3926	66	0
8	O	956	0	968	8	0
9	X	767	0	766	8	0
10	Z	798	0	780	12	0
11	a	469	0	472	0	0
12	b	295	0	322	0	0
13	d	592	0	610	0	0
14	e	557	0	525	0	0
15	f	763	0	767	0	0
16	i	614	0	577	0	0
17	u	150	0	34	0	0
18	v	226	0	235	0	0
19	x	1659	0	1673	0	0
20	y	2032	0	2044	0	0
21	z	1772	0	1771	0	0
22	H	35	0	43	2	0
23	H	50	0	79	4	0
23	N	50	0	79	5	0
24	M	69	0	88	1	0
25	O	1	0	0	0	0
26	v	52	0	84	0	0
27	y	1	0	0	0	0
28	y	41	0	52	0	0
29	z	30	0	32	0	0
30	z	61	0	0	0	0
All	All	23281	0	23724	198	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 198 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)
6:M:142:PHE:O	6:M:146:PHE:HB2	1.78	0.83
4:K:36:GLU:OE1	4:K:73:SER:OG	1.99	0.79
4:K:42:VAL:HG11	7:N:191:LEU:HG	1.66	0.76
3:J:37:THR:HG21	4:K:40:LEU:HD11	1.65	0.76
1:A:88:ILE:HD12	1:A:92:GLY:HA3	1.69	0.73

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	88/119 (74%)	86 (98%)	2 (2%)	0	100	100
2	H	307/325 (94%)	287 (94%)	19 (6%)	1 (0%)	37	64
3	J	143/205 (70%)	136 (95%)	7 (5%)	0	100	100
4	K	88/100 (88%)	86 (98%)	2 (2%)	0	100	100
5	L	24/669 (4%)	21 (88%)	3 (12%)	0	100	100
6	M	260/495 (52%)	256 (98%)	3 (1%)	1 (0%)	30	58
7	N	486/499 (97%)	475 (98%)	11 (2%)	0	100	100
8	O	120/159 (76%)	114 (95%)	6 (5%)	0	100	100
9	X	95/106 (90%)	94 (99%)	1 (1%)	0	100	100
10	Z	96/143 (67%)	91 (95%)	4 (4%)	1 (1%)	13	38
11	a	56/65 (86%)	56 (100%)	0	0	100	100
12	b	38/65 (58%)	38 (100%)	0	0	100	100
13	d	73/81 (90%)	71 (97%)	2 (3%)	0	100	100
14	e	63/83 (76%)	63 (100%)	0	0	100	100
15	f	99/106 (93%)	96 (97%)	3 (3%)	0	100	100
16	i	68/98 (69%)	66 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	v	28/113 (25%)	27 (96%)	1 (4%)	0	100	100
19	x	212/256 (83%)	207 (98%)	5 (2%)	0	100	100
20	y	266/278 (96%)	252 (95%)	14 (5%)	0	100	100
21	z	231/275 (84%)	227 (98%)	4 (2%)	0	100	100
All	All	2841/4240 (67%)	2749 (97%)	89 (3%)	3 (0%)	50	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	201	ALA
6	M	231	VAL
10	Z	120	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	83/106 (78%)	83 (100%)	0	100	100
2	H	262/272 (96%)	262 (100%)	0	100	100
3	J	131/186 (70%)	131 (100%)	0	100	100
4	K	78/86 (91%)	78 (100%)	0	100	100
5	L	21/568 (4%)	21 (100%)	0	100	100
6	M	232/434 (54%)	232 (100%)	0	100	100
7	N	406/416 (98%)	406 (100%)	0	100	100
8	O	107/141 (76%)	107 (100%)	0	100	100
9	X	87/94 (93%)	87 (100%)	0	100	100
10	Z	79/115 (69%)	79 (100%)	0	100	100
11	a	48/53 (91%)	48 (100%)	0	100	100
12	b	33/53 (62%)	33 (100%)	0	100	100
13	d	60/66 (91%)	60 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	e	60/73 (82%)	60 (100%)	0	100	100
15	f	81/84 (96%)	81 (100%)	0	100	100
16	i	64/90 (71%)	64 (100%)	0	100	100
18	v	23/84 (27%)	23 (100%)	0	100	100
19	x	183/216 (85%)	183 (100%)	0	100	100
20	y	223/232 (96%)	223 (100%)	0	100	100
21	z	188/228 (82%)	188 (100%)	0	100	100
All	All	2449/3597 (68%)	2449 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
6	M	31	ASN
7	N	53	ASN
9	X	45	ASN
19	x	116	ASN
21	z	101	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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
28	PGT	y	302	-	40,40,50	1.16	3 (7%)	43,46,56	1.10	2 (4%)
26	PC7	v	201	-	51,51,51	0.95	4 (7%)	57,59,59	1.04	2 (3%)
30	T7X	z	302	-	61,61,61	0.84	4 (6%)	71,73,73	1.07	3 (4%)
23	PTY	N	501	-	49,49,49	0.86	4 (8%)	52,54,54	1.12	2 (3%)
23	PTY	H	402	-	49,49,49	0.87	4 (8%)	52,54,54	1.12	2 (3%)
24	LMN	M	501	-	72,72,72	1.65	14 (19%)	96,98,98	1.02	3 (3%)
29	PSF	z	301	-	28,29,29	1.18	4 (14%)	32,36,36	1.22	2 (6%)
22	UQ9	H	401	-	35,35,58	2.51	12 (34%)	42,45,73	1.86	12 (28%)

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
28	PGT	y	302	-	-	22/45/45/55	-
26	PC7	v	201	-	-	23/55/55/55	-
30	T7X	z	302	-	-	29/56/80/80	0/1/1/1
23	PTY	N	501	-	-	26/53/53/53	-
23	PTY	H	402	-	-	19/53/53/53	-
24	LMN	M	501	-	-	34/50/130/130	0/4/4/4
29	PSF	z	301	-	-	12/35/35/35	-
22	UQ9	H	401	-	-	8/30/54/81	0/1/1/1

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	H	401	UQ9	C6-C1	9.90	1.53	1.35
24	M	501	LMN	O5-C1	4.69	1.53	1.41
22	H	401	UQ9	C4-C3	4.32	1.53	1.36
24	M	501	LMN	CBS-CCM	4.16	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M	501	LMN	CBT-CCM	4.07	1.62	1.53

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	H	401	UQ9	C7-C6-C5	4.75	124.20	118.48
30	z	302	T7X	O16-C10-C12	4.26	120.69	111.50
23	N	501	PTY	O7-C8-C11	4.17	120.49	111.50
28	y	302	PGT	O2-C31-C32	4.08	120.29	111.50
23	H	402	PTY	O7-C8-C11	4.07	120.27	111.50

There are no chirality outliers.

5 of 173 torsion outliers are listed below:

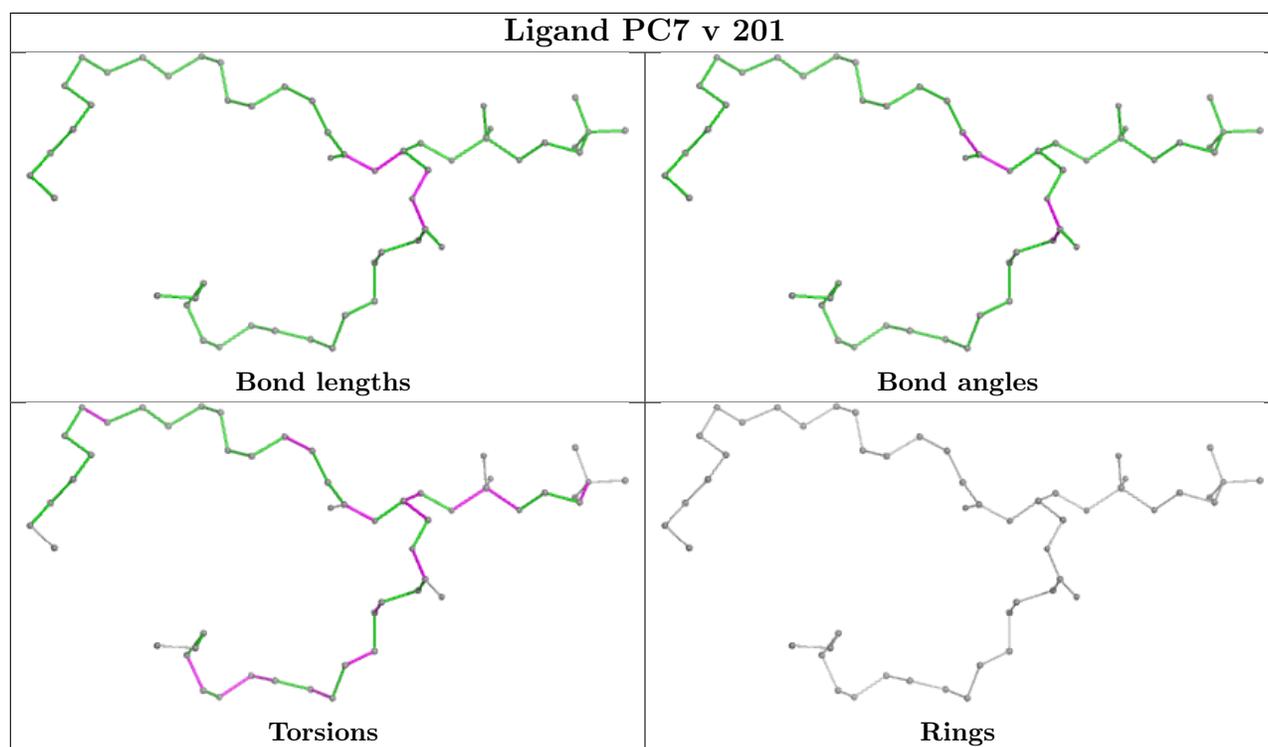
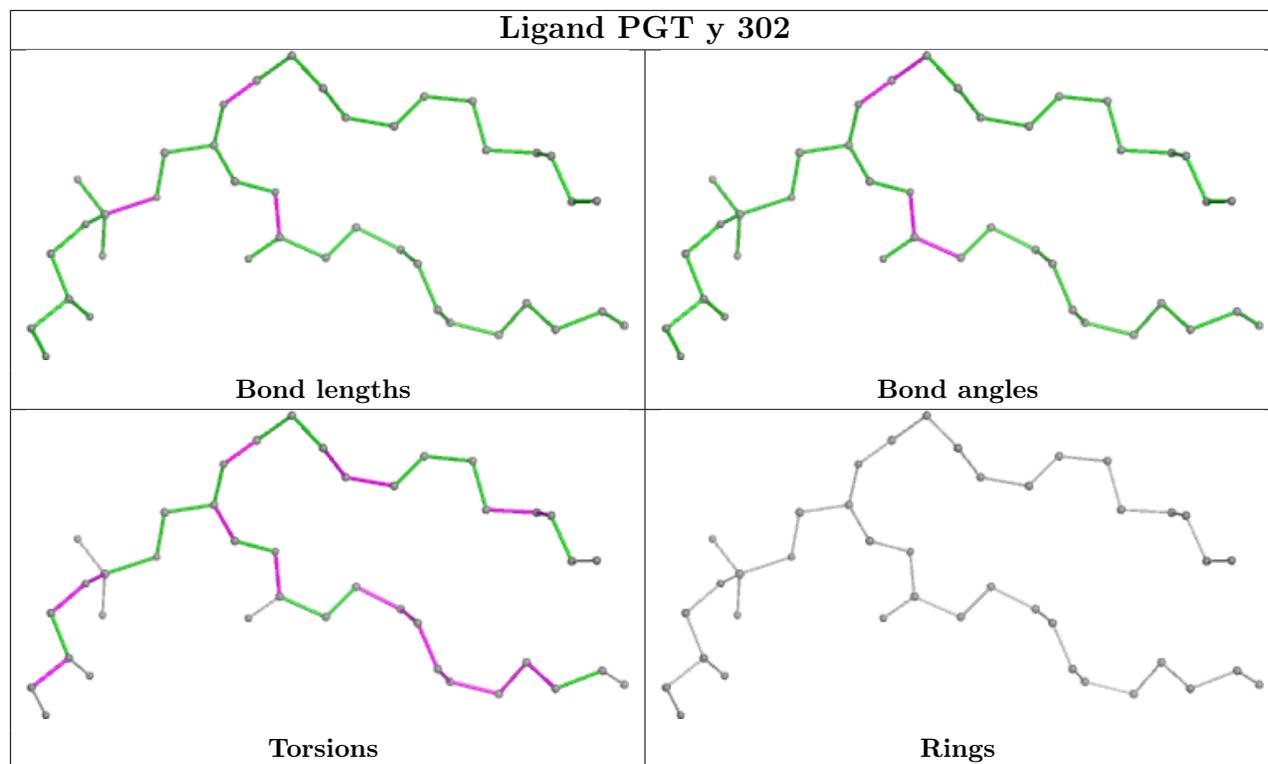
Mol	Chain	Res	Type	Atoms
22	H	401	UQ9	C9-C11-C12-C13
22	H	401	UQ9	C1-C6-C7-C8
22	H	401	UQ9	C5-C6-C7-C8
23	H	402	PTY	C5-O14-P1-O13
23	N	501	PTY	C5-C6-O7-C8

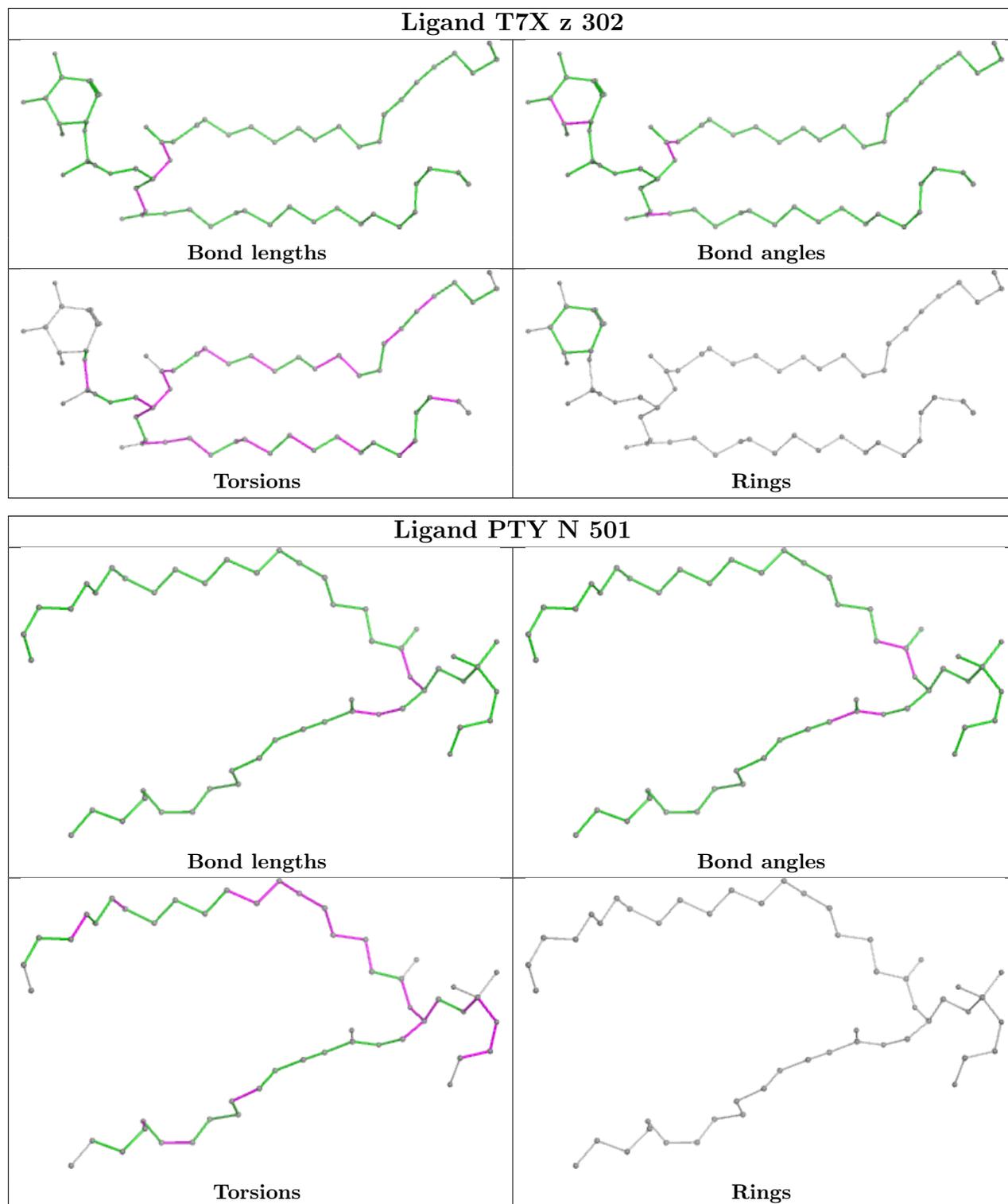
There are no ring outliers.

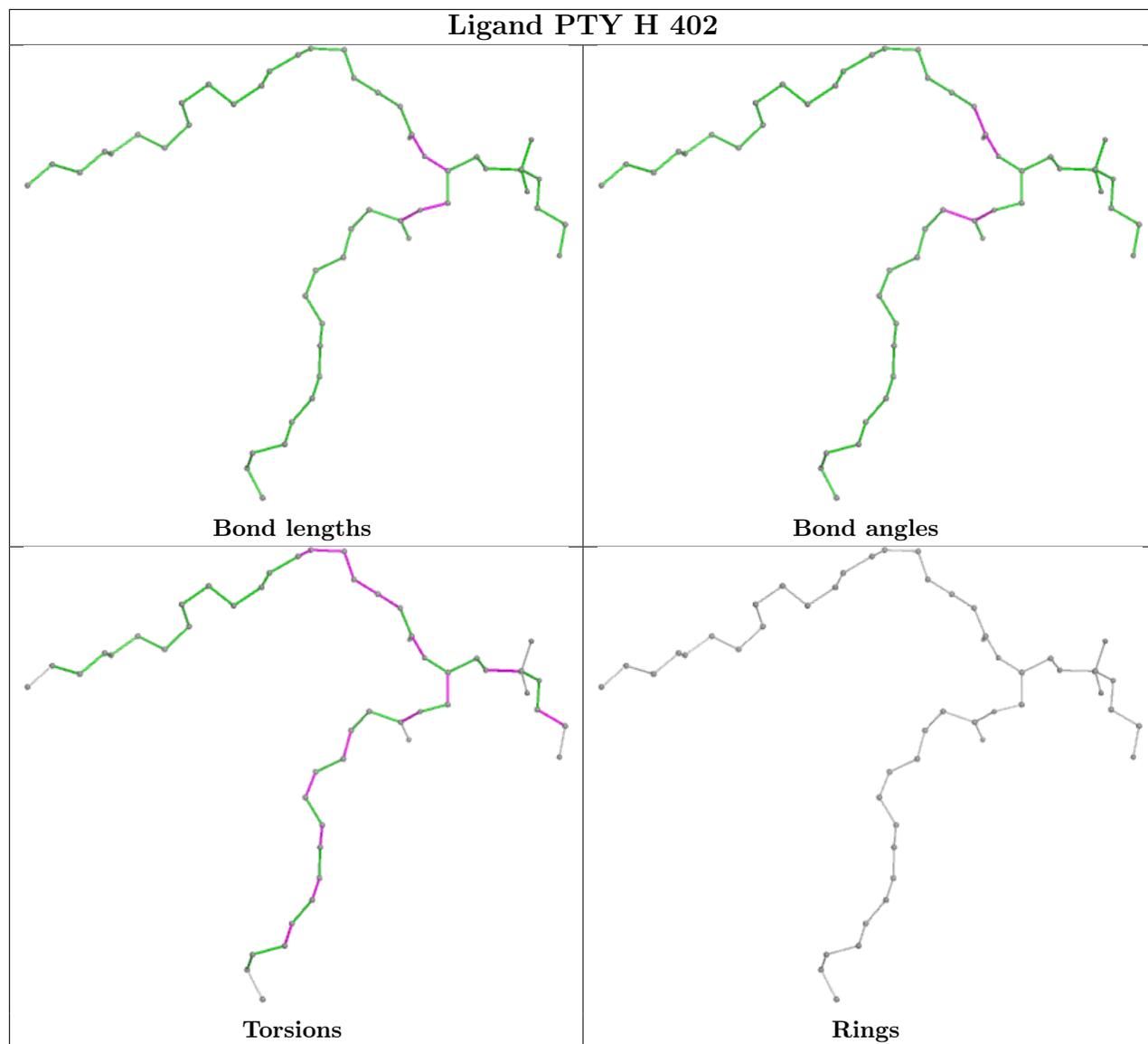
4 monomers are involved in 12 short contacts:

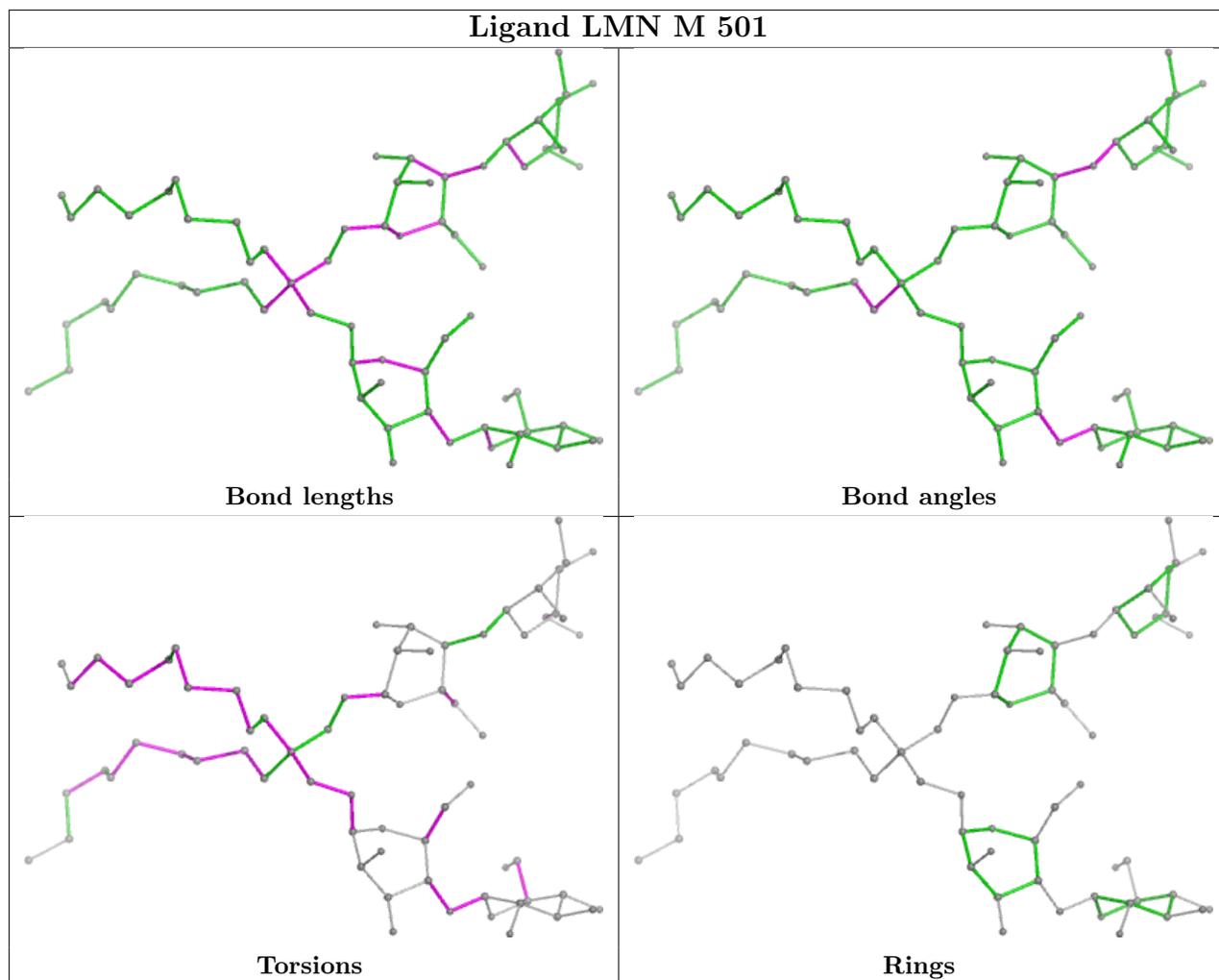
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	N	501	PTY	5	0
23	H	402	PTY	4	0
24	M	501	LMN	1	0
22	H	401	UQ9	2	0

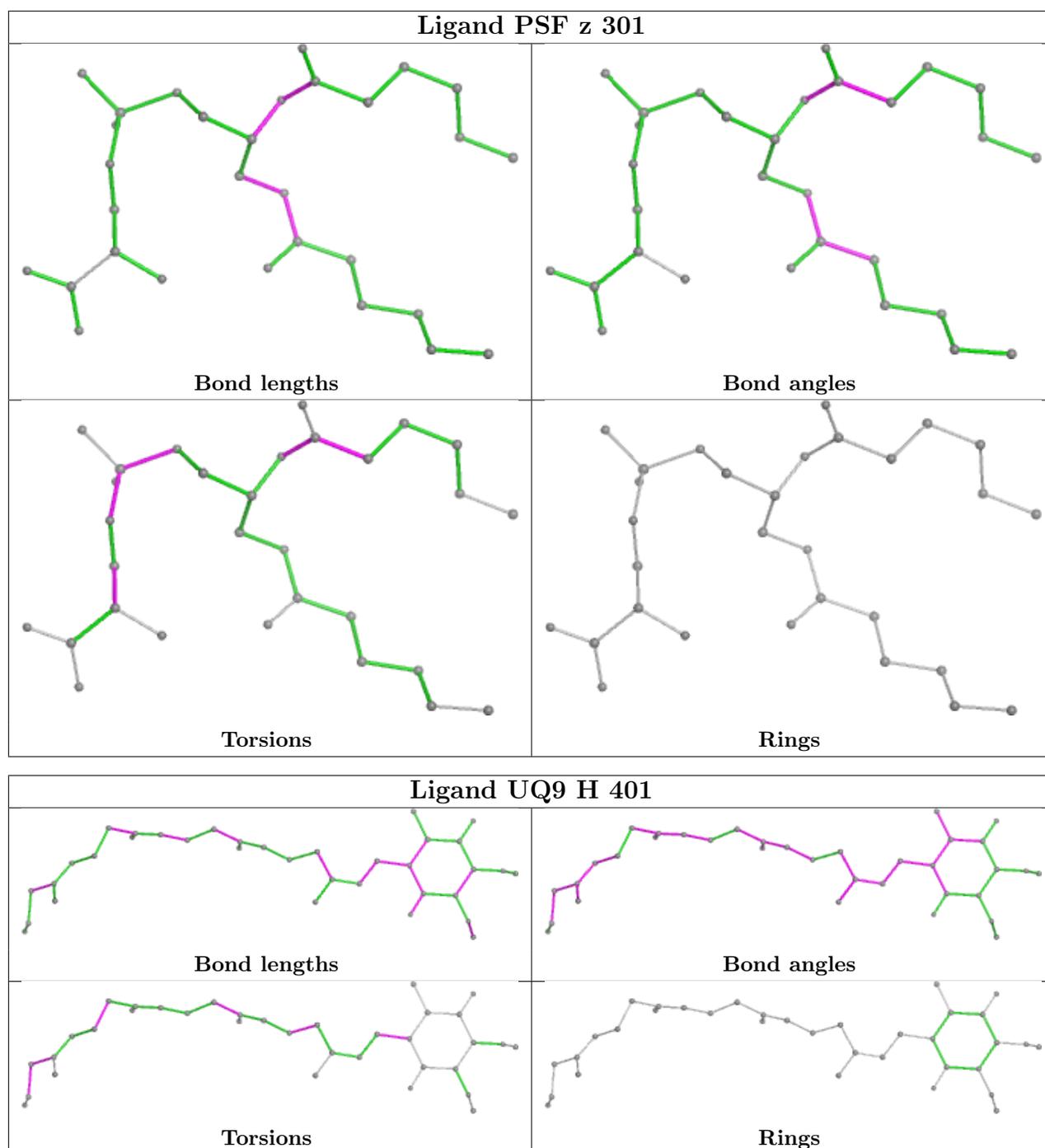
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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