



Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 05:54 pm GMT

PDB ID : 7ARB
EMDB ID : EMD-11878
Title : Cryo-EM structure of Arabidopsis thaliana Complex-I (complete composition)
Authors : Klusch, N.; Kuelbrandt, W.; Yildiz, O.
Deposited on : 2020-10-23
Resolution : 3.41 Å(reported)

This is a Full wwPDB EM Validation 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:

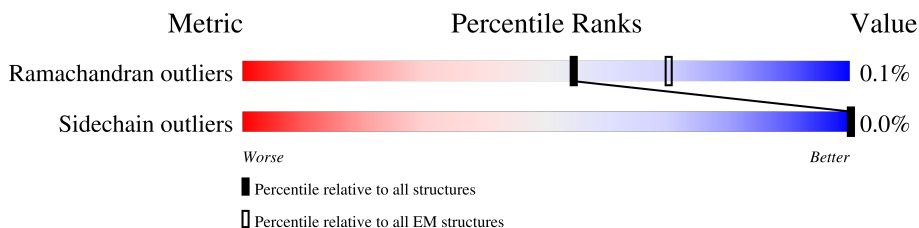
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 3.41 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.



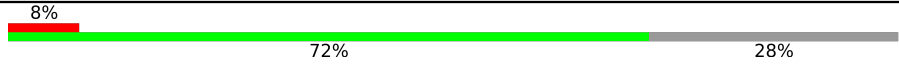
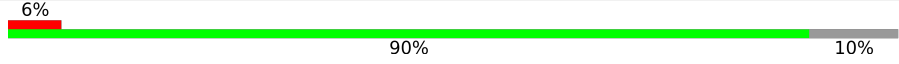
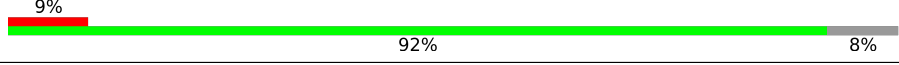
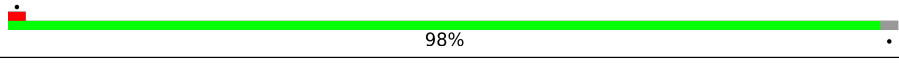
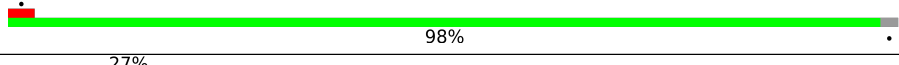
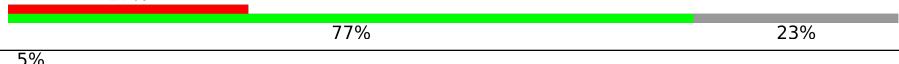
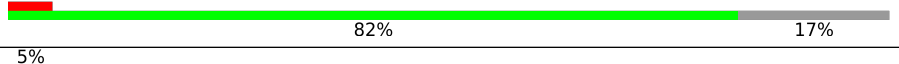

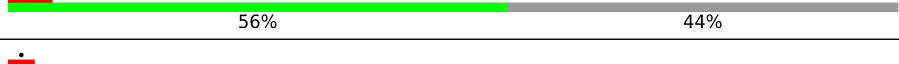
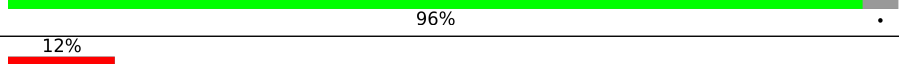

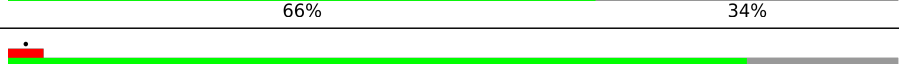
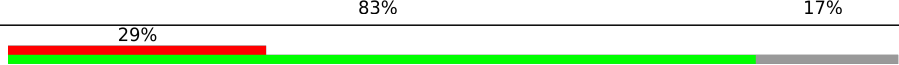
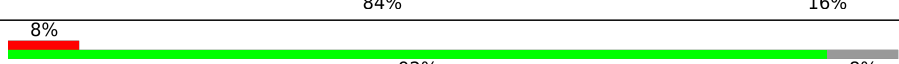
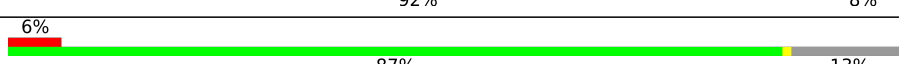
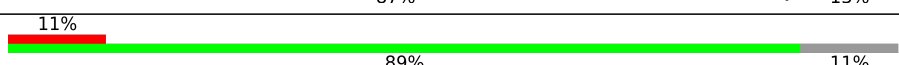
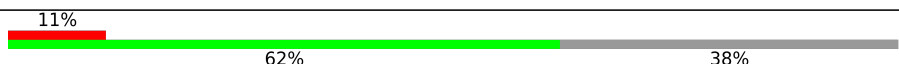
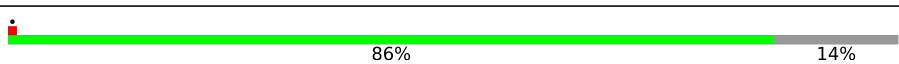
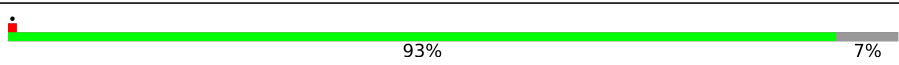

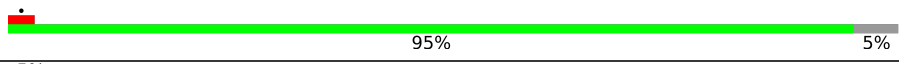
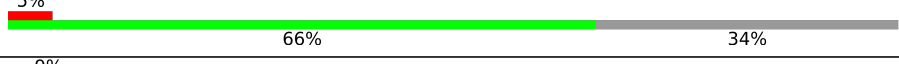
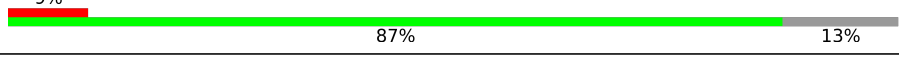


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	
2	B	218	
3	C	190	
4	D	394	
5	E	255	
6	F	486	
7	G	748	
8	H	325	
9	I	222	



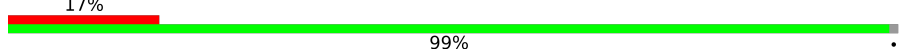
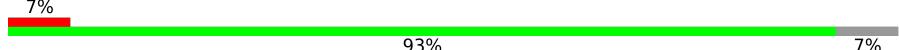

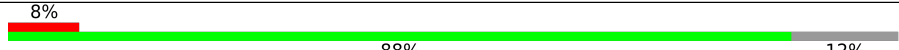
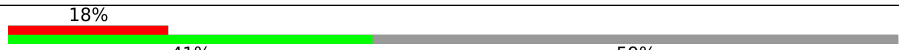

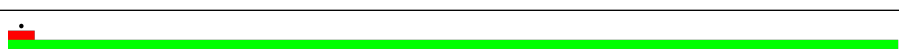
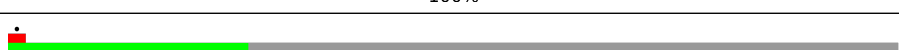
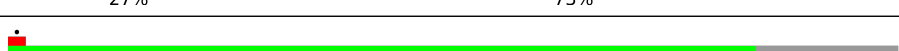

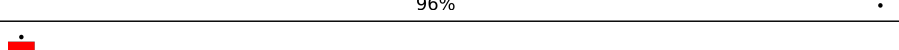
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Mol	Chain	Length	Quality of chain
10	J	205	 8% 72% 28%
11	K	100	 6% 90% 10%
12	L	669	 9% 92% 8%
13	M	495	 98%
14	N	499	 98%
15	O	159	 27% 77% 23%
16	P	402	 5% 82% 17%
17	Q	154	 5% 77% 23%
18	R	110	 5% 56% 44%
19	S	97	 96%
20	T	122	 12% 69% 31%
21	U	126	 62% 66% 34%
22	V	169	 83% 17%
23	W	133	 29% 84% 16%
24	X	106	 8% 92% 8%
25	Z	143	 6% 87% 13%
26	a	65	 11% 89% 11%
27	b	65	 11% 62% 38%
28	c	88	 86% 14%
29	d	81	 93% 7%
30	e	83	 78% 22%
31	f	106	 95% 5%
32	g	114	 5% 66% 34%
33	i	98	 9% 87% 13%
34	j	69	 74% 26%

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Mol	Chain	Length	Quality of chain
35	k	72	 65% 35%
36	l	125	 53% 47%
37	m	71	 99%
38	n	117	 93% 7%
39	o	103	 78% 22%
40	p	106	 88% 12%
41	q	159	 41% 59%
42	r	131	 92%
43	u	30	 100%
44	v	113	 27% 73%
45	x	256	 84% 16%
46	y	278	 96%
47	z	275	 85% 15%

2 Entry composition i

There are 61 unique types of molecules in this entry. The entry contains 61765 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 dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	165	1349	849	229	261	10	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	615	4807	3191	748	832	36	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 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

- Molecule 15 is a protein called AT3G07480.1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	112	Total	C	N	O	S	0	0
			904	578	161	162	3		

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

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

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

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

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

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

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

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

- Molecule 28 is a protein called Transmembrane protein.

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

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

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

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

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

- Molecule 31 is a protein called At4g16450.

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

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

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

- Molecule 33 is a protein called P1.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	l	66	502	328	80	93	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	m	70	577	370	107	98	2	0	0

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

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

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

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

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

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

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

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

- Molecule 42 is a protein called Furry.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	r	10	Total	C	N	O	0	0
			89	56	18	15		

- Molecule 43 is a protein called unknown.

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

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

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

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

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

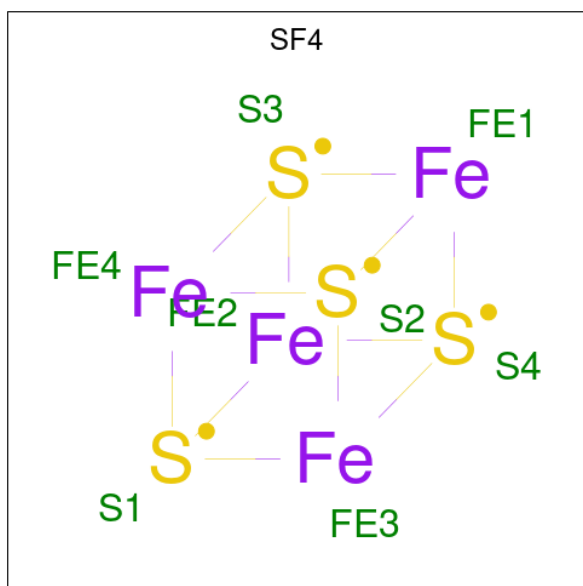
- Molecule 46 is a protein called Gamma carbonic anhydrase 2, mitochondrial.

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

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

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

- Molecule 48 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



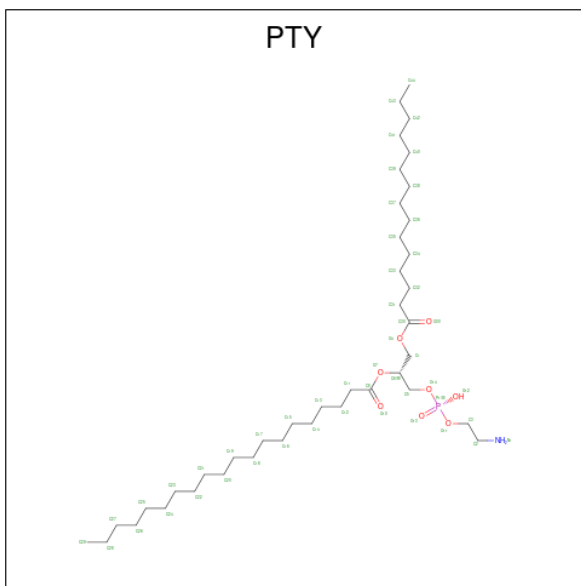
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
48	B	1	8	4	4	0
48	F	1	8	4	4	0
48	G	1	16	8	8	0
48	G	1	16	8	8	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
48	I	1	16	8	8	0
48	I	1	16	8	8	0

- Molecule 49 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



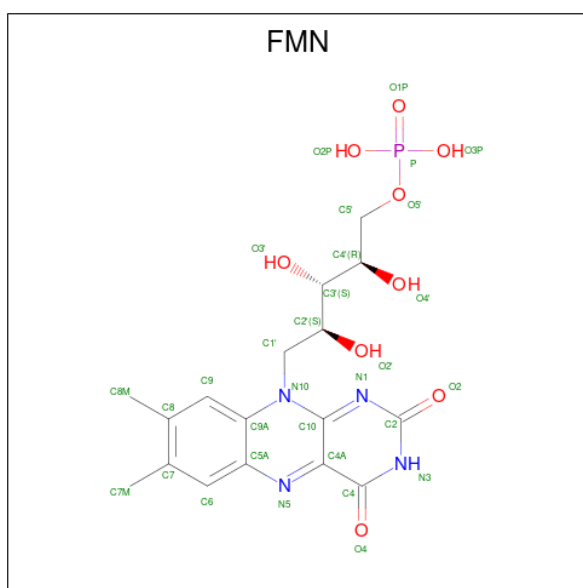
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	D	1	50	40	1	8	1	0
49	M	1	50	40	1	8	1	0
49	N	1	50	40	1	8	1	0

- Molecule 50 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



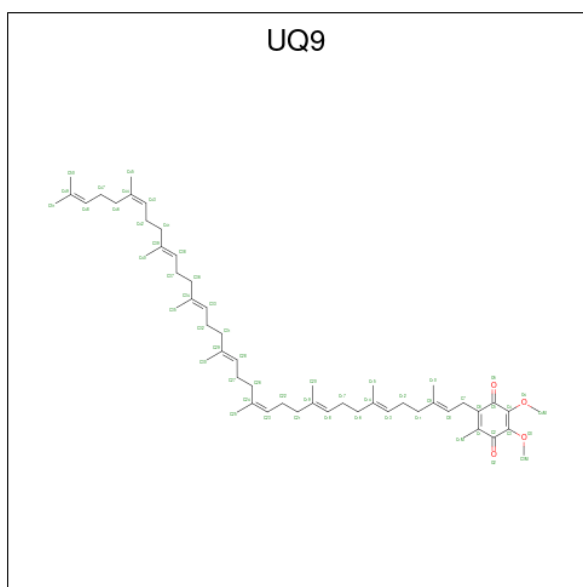
Mol	Chain	Residues	Atoms			AltConf
50	E	1	Total	Fe	S	0
			4	2	2	
50	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 51 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



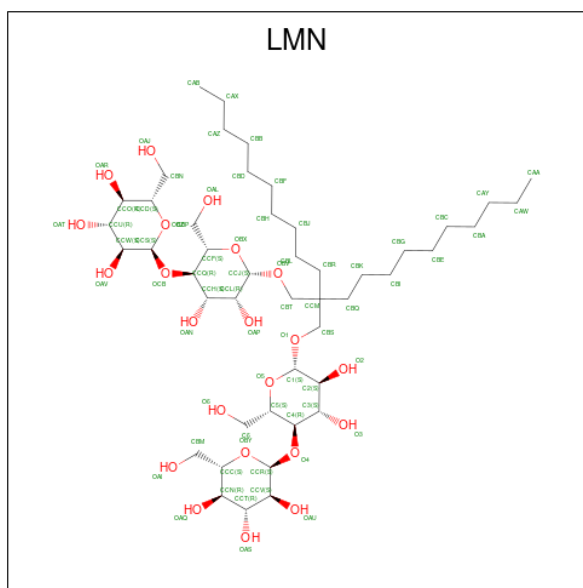
Mol	Chain	Residues	Atoms					AltConf
51	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 52 is Ubiquinone-9 (three-letter code: UQ9) (formula: C₅₄H₈₂O₄).



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

- Molecule 53 is Lauryl Maltose Neopentyl Glycol (three-letter code: LMN) (formula: $C_{47}H_{88}O_{22}$).

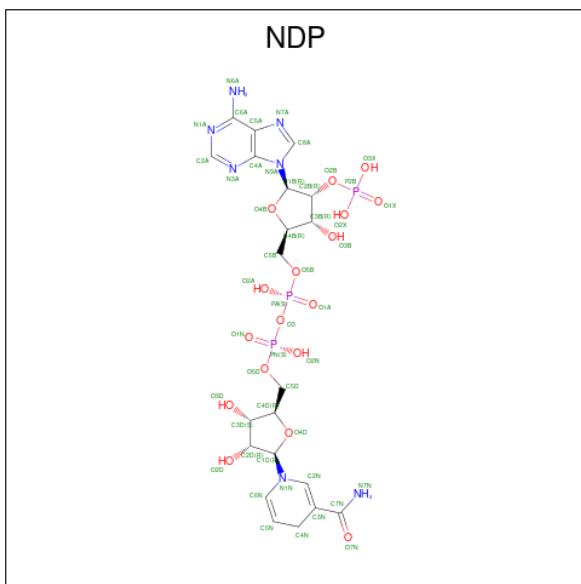


Mol	Chain	Residues	Atoms		AltConf
53	M	1	Total	C O	0
			69	47 22	

- Molecule 54 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 55 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

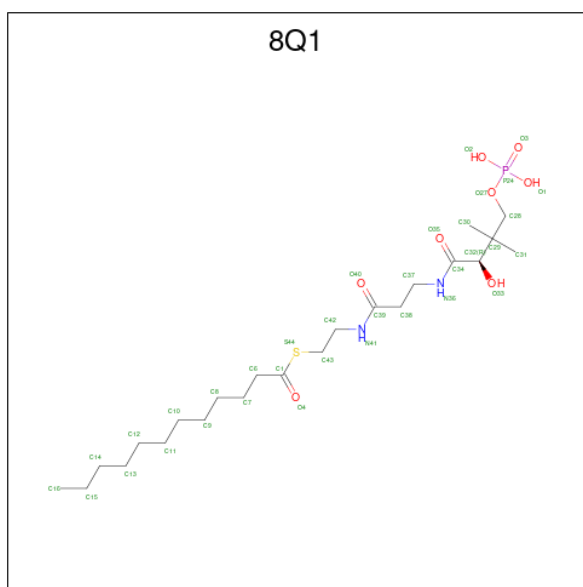


Mol	Chain	Residues	Atoms	AltConf
55	P	1	Total C N O P 48 21 7 17 3	0

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

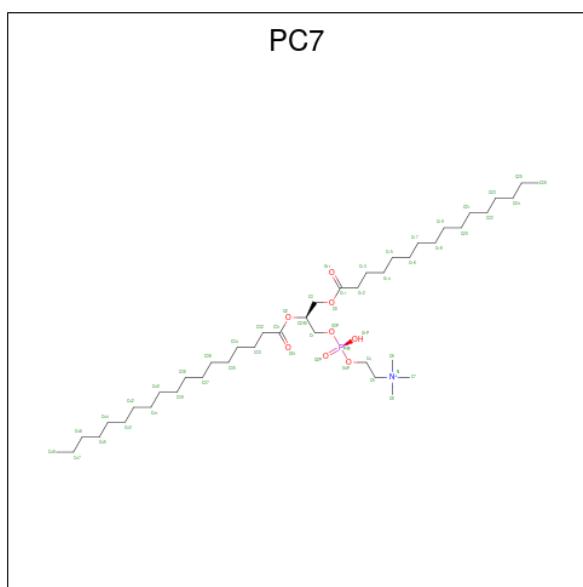
Mol	Chain	Residues	Atoms	AltConf
56	R	1	Total Zn 1 1	0
56	y	1	Total Zn 1 1	0

- Molecule 57 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).



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

- Molecule 58 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).



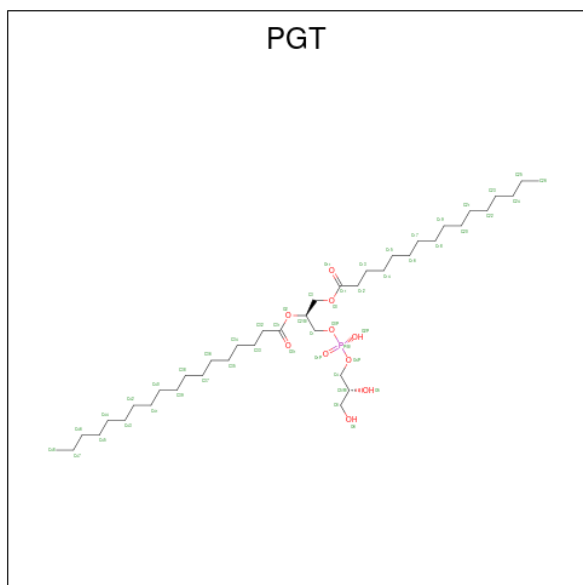
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
58	c	1	52	42	1	8	1	0

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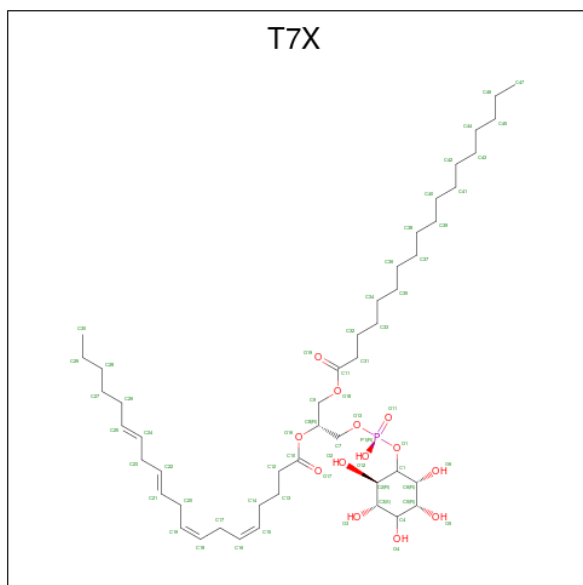
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	v	1	52	42	1	8	1	0

- Molecule 59 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: C₄₀H₇₉O₁₀P).



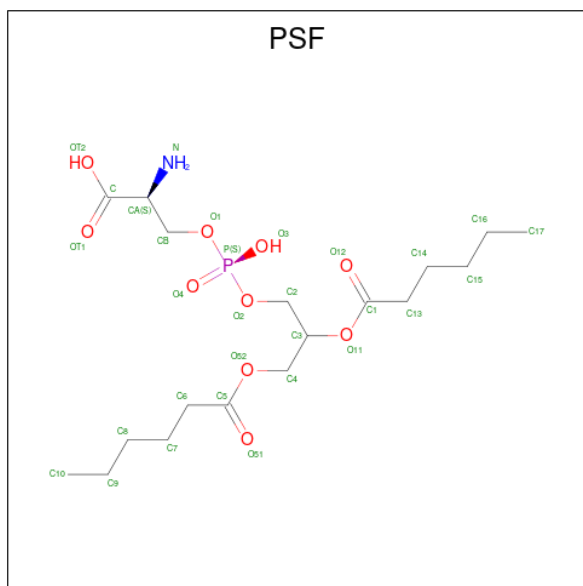
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
59	f	1	41	30	10	1	0

- Molecule 60 is Phosphatidylinositol (three-letter code: T7X) (formula: C₄₇H₈₃O₁₃P).



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

- Molecule 61 is 1,2-DICAPROYL-SN-PHOSPHATIDYL-L-SERINE (three-letter code: PSF) (formula: $C_{18}H_{34}NO_{10}P$).

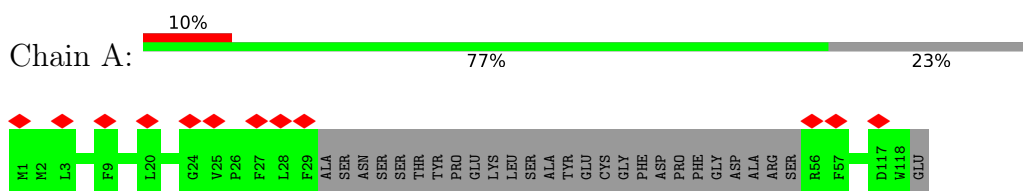


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
61	z	1	30	18	1	10	1	0

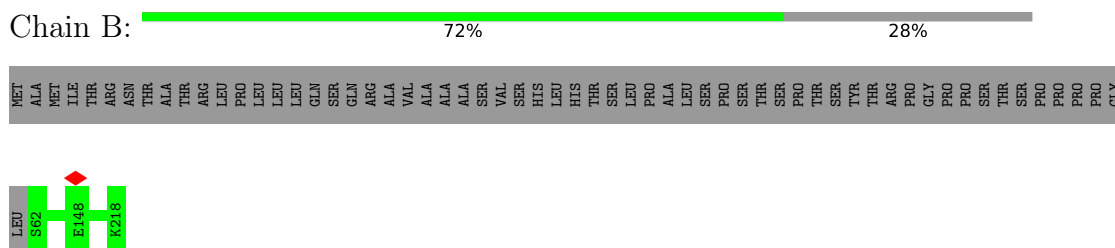
3 Residue-property plots [i](#)

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 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.

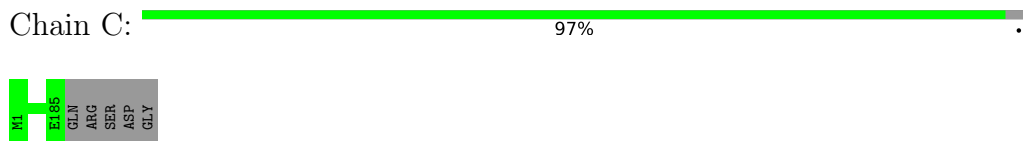
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



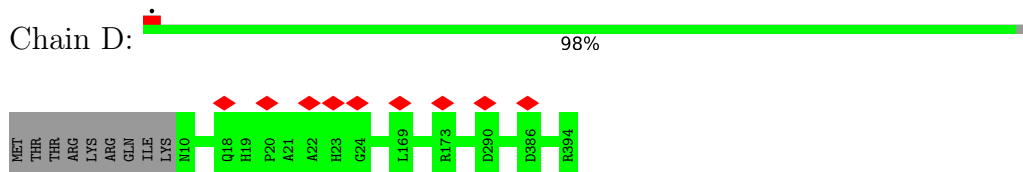
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



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

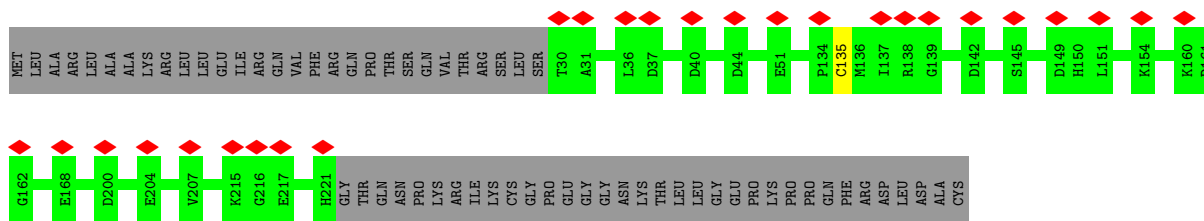


- Molecule 4: NADH dehydrogenase subunit 7

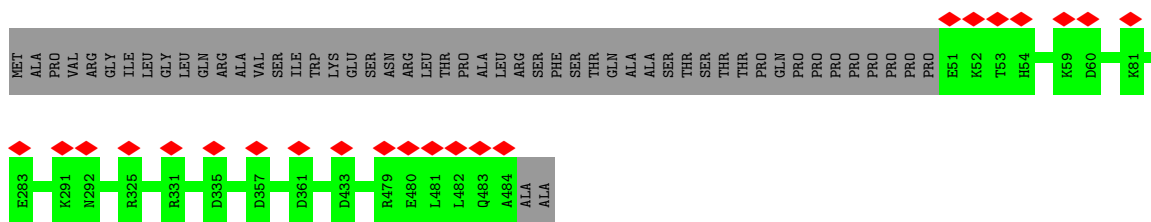
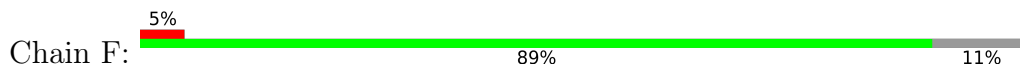


- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

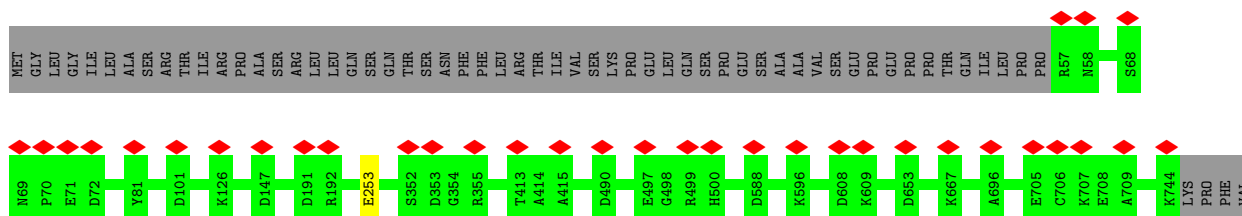




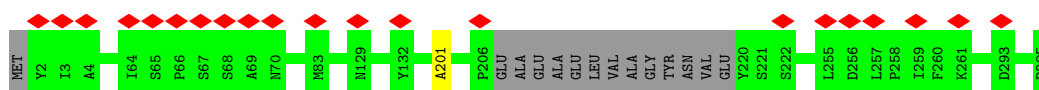
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



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



- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



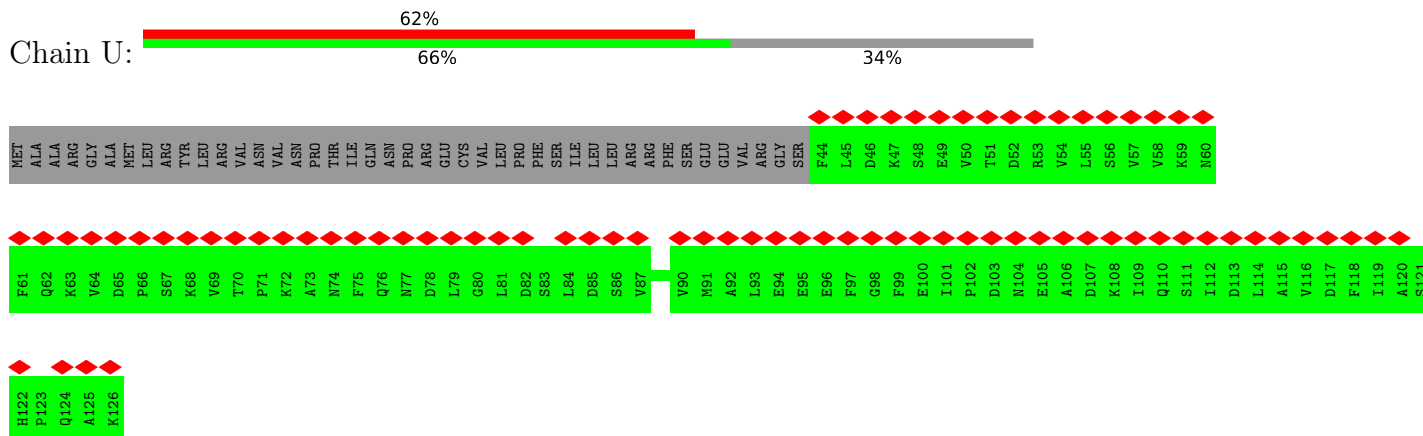
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8-A, mitochondrial



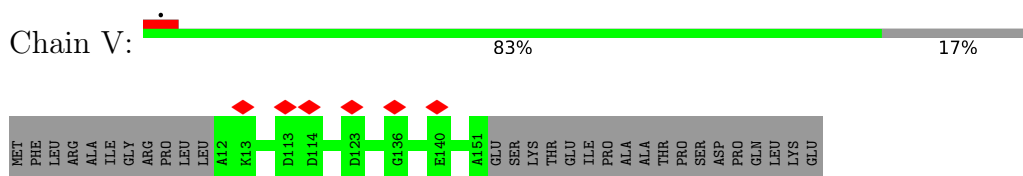
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



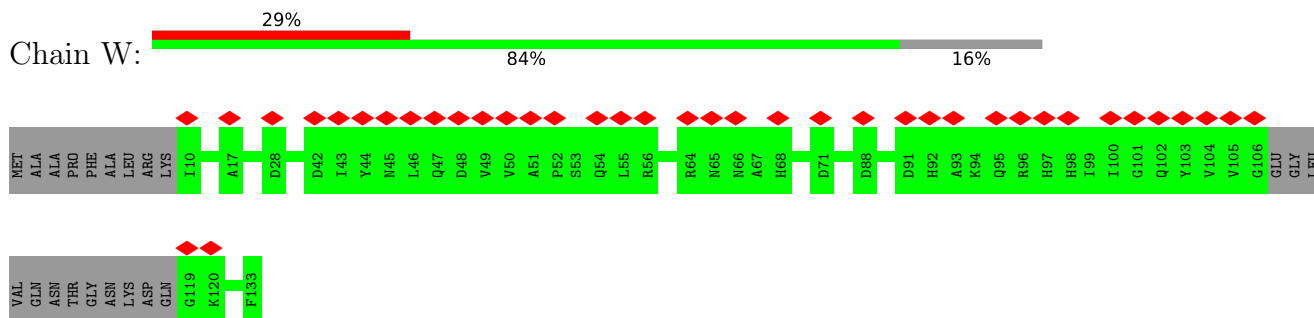
- Molecule 21: Acyl carrier protein 2, mitochondrial



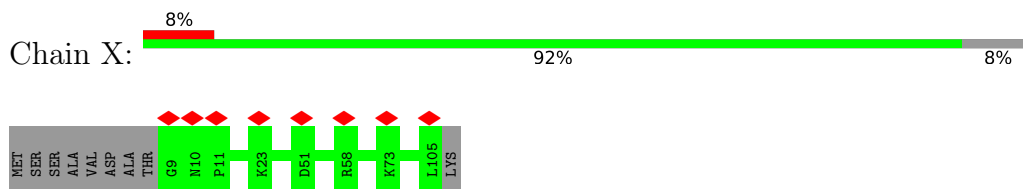
- Molecule 22: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial



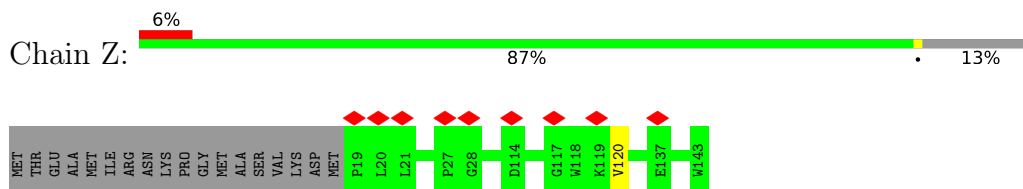
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



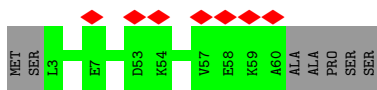
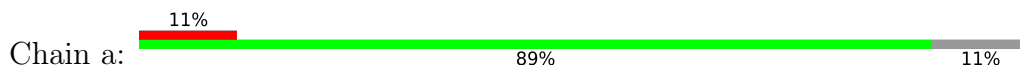
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B



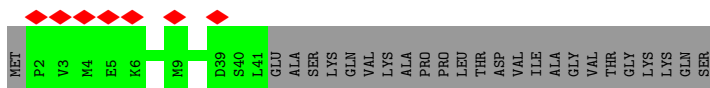
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A



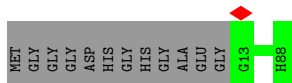
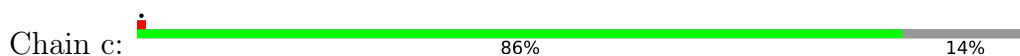
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



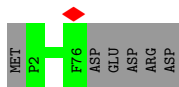
- Molecule 27: At2g46540/F11C10.23



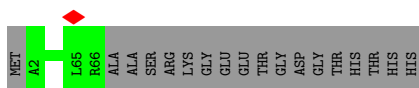
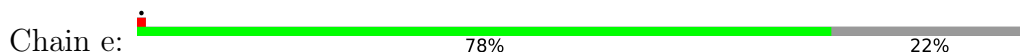
- Molecule 28: Transmembrane protein



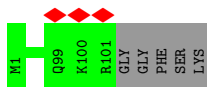
- Molecule 29: Excitatory amino acid transporter



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

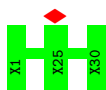


- Molecule 31: At4g16450

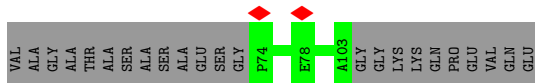
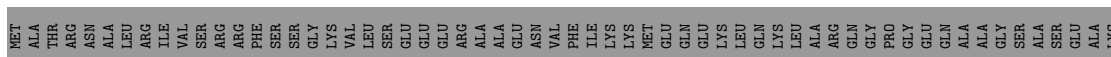


- Molecule 32: ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein

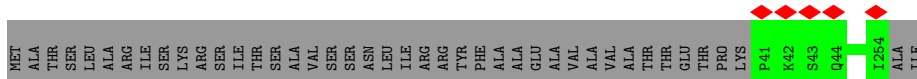
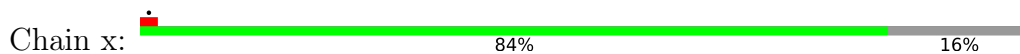




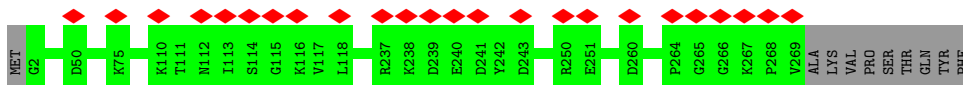
- Molecule 44: Uncharacterized protein At2g27730, mitochondrial



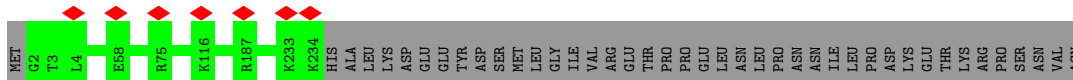
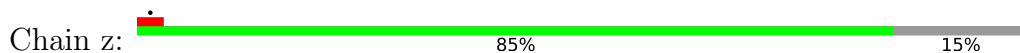
- Molecule 45: Gamma carbonic anhydrase-like 2, mitochondrial



- Molecule 46: Gamma carbonic anhydrase 2, mitochondrial



- Molecule 47: Gamma carbonic anhydrase 1, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	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
Maximum map value	0.083	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	502.2, 502.2, 502.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.42	0/1096
2	B	0.30	0/1279	0.51	0/1734
3	C	0.28	0/1629	0.51	0/2207
4	D	0.29	0/3147	0.51	0/4256
5	E	0.27	0/1535	0.48	0/2084
6	F	0.27	0/3441	0.50	0/4641
7	G	0.27	0/5347	0.49	0/7242
8	H	0.30	0/2510	0.49	0/3416
9	I	0.28	0/1378	0.51	0/1862
10	J	0.28	0/1187	0.46	0/1617
11	K	0.28	0/717	0.48	0/969
12	L	0.27	0/4938	0.47	0/6706
13	M	0.27	0/3995	0.44	0/5428
14	N	0.28	0/3924	0.47	0/5327
15	O	0.24	0/971	0.49	0/1314
16	P	0.27	0/2617	0.49	0/3544
17	Q	0.27	0/966	0.45	0/1305
18	R	0.27	0/493	0.44	0/668
19	S	0.27	0/739	0.52	0/996
20	T	0.26	0/679	0.50	0/922
21	U	0.24	0/660	0.42	0/892
22	V	0.27	0/1146	0.48	0/1555
23	W	0.26	0/923	0.46	0/1249
24	X	0.25	0/781	0.45	0/1049
25	Z	0.27	0/1027	0.50	0/1392
26	a	0.25	0/481	0.50	0/646
27	b	0.25	0/300	0.44	0/407
28	c	0.25	0/637	0.46	0/860
29	d	0.26	0/605	0.47	0/815
30	e	0.26	0/570	0.49	0/759
31	f	0.27	0/779	0.46	0/1052
32	g	0.24	0/635	0.47	0/863

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	i	0.25	0/757	0.49	0/1019
34	j	0.24	0/433	0.41	0/592
35	k	0.24	0/384	0.50	0/515
36	l	0.26	0/513	0.48	0/696
37	m	0.26	0/592	0.49	0/793
38	n	0.25	0/938	0.50	0/1273
39	o	0.25	0/666	0.47	0/886
40	p	0.28	0/799	0.48	0/1074
41	q	0.24	0/553	0.48	0/750
42	r	0.23	0/89	0.59	0/118
44	v	0.24	0/230	0.39	0/311
45	x	0.28	0/1700	0.50	0/2320
46	y	0.27	0/2066	0.48	0/2800
47	z	0.27	0/1804	0.49	0/2441
All	All	0.27	0/62367	0.48	0/84461

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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	B	155/218 (71%)	147 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	183/190 (96%)	179 (98%)	4 (2%)	0	100	100
4	D	383/394 (97%)	368 (96%)	15 (4%)	0	100	100
5	E	190/255 (74%)	182 (96%)	8 (4%)	0	100	100
6	F	432/486 (89%)	421 (98%)	11 (2%)	0	100	100
7	G	686/748 (92%)	654 (95%)	31 (4%)	1 (0%)	51	83
8	H	307/325 (94%)	289 (94%)	17 (6%)	1 (0%)	41	74
9	I	163/222 (73%)	161 (99%)	2 (1%)	0	100	100
10	J	143/205 (70%)	136 (95%)	7 (5%)	0	100	100
11	K	88/100 (88%)	84 (96%)	4 (4%)	0	100	100
12	L	613/669 (92%)	582 (95%)	31 (5%)	0	100	100
13	M	483/495 (98%)	474 (98%)	8 (2%)	1 (0%)	47	80
14	N	486/499 (97%)	474 (98%)	12 (2%)	0	100	100
15	O	120/159 (76%)	115 (96%)	5 (4%)	0	100	100
16	P	330/402 (82%)	318 (96%)	12 (4%)	0	100	100
17	Q	117/154 (76%)	111 (95%)	6 (5%)	0	100	100
18	R	60/110 (54%)	57 (95%)	3 (5%)	0	100	100
19	S	91/97 (94%)	81 (89%)	10 (11%)	0	100	100
20	T	82/122 (67%)	77 (94%)	5 (6%)	0	100	100
21	U	81/126 (64%)	75 (93%)	6 (7%)	0	100	100
22	V	138/169 (82%)	135 (98%)	3 (2%)	0	100	100
23	W	108/133 (81%)	101 (94%)	7 (6%)	0	100	100
24	X	95/106 (90%)	92 (97%)	3 (3%)	0	100	100
25	Z	123/143 (86%)	118 (96%)	4 (3%)	1 (1%)	19	56
26	a	56/65 (86%)	56 (100%)	0	0	100	100
27	b	38/65 (58%)	38 (100%)	0	0	100	100
28	c	74/88 (84%)	74 (100%)	0	0	100	100
29	d	73/81 (90%)	71 (97%)	2 (3%)	0	100	100
30	e	63/83 (76%)	63 (100%)	0	0	100	100
31	f	99/106 (93%)	96 (97%)	3 (3%)	0	100	100
32	g	73/114 (64%)	71 (97%)	2 (3%)	0	100	100
33	i	83/98 (85%)	80 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	j	49/69 (71%)	44 (90%)	5 (10%)	0	100	100
35	k	45/72 (62%)	42 (93%)	3 (7%)	0	100	100
36	l	62/125 (50%)	57 (92%)	5 (8%)	0	100	100
37	m	68/71 (96%)	63 (93%)	5 (7%)	0	100	100
38	n	107/117 (92%)	105 (98%)	2 (2%)	0	100	100
39	o	78/103 (76%)	76 (97%)	2 (3%)	0	100	100
40	p	91/106 (86%)	87 (96%)	4 (4%)	0	100	100
41	q	63/159 (40%)	56 (89%)	7 (11%)	0	100	100
42	r	8/131 (6%)	7 (88%)	1 (12%)	0	100	100
44	v	28/113 (25%)	27 (96%)	1 (4%)	0	100	100
45	x	212/256 (83%)	206 (97%)	6 (3%)	0	100	100
46	y	266/278 (96%)	255 (96%)	11 (4%)	0	100	100
47	z	231/275 (84%)	227 (98%)	4 (2%)	0	100	100
All	All	7612/9221 (83%)	7318 (96%)	290 (4%)	4 (0%)	54	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	201	ALA
7	G	253	GLU
13	M	231	VAL
25	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	B	132/184 (72%)	132 (100%)	0	100	100
3	C	175/179 (98%)	175 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	331/340 (97%)	331 (100%)	0	100	100
5	E	166/220 (76%)	165 (99%)	1 (1%)	86	94
6	F	353/396 (89%)	353 (100%)	0	100	100
7	G	571/625 (91%)	571 (100%)	0	100	100
8	H	262/272 (96%)	262 (100%)	0	100	100
9	I	147/195 (75%)	147 (100%)	0	100	100
10	J	131/186 (70%)	131 (100%)	0	100	100
11	K	78/86 (91%)	78 (100%)	0	100	100
12	L	518/568 (91%)	518 (100%)	0	100	100
13	M	426/434 (98%)	426 (100%)	0	100	100
14	N	406/416 (98%)	406 (100%)	0	100	100
15	O	107/141 (76%)	107 (100%)	0	100	100
16	P	273/334 (82%)	272 (100%)	1 (0%)	91	96
17	Q	100/128 (78%)	100 (100%)	0	100	100
18	R	55/97 (57%)	55 (100%)	0	100	100
19	S	82/85 (96%)	82 (100%)	0	100	100
20	T	79/112 (70%)	79 (100%)	0	100	100
21	U	75/113 (66%)	75 (100%)	0	100	100
22	V	123/148 (83%)	123 (100%)	0	100	100
23	W	98/114 (86%)	98 (100%)	0	100	100
24	X	87/94 (93%)	87 (100%)	0	100	100
25	Z	100/115 (87%)	100 (100%)	0	100	100
26	a	48/53 (91%)	48 (100%)	0	100	100
27	b	33/53 (62%)	33 (100%)	0	100	100
28	c	66/71 (93%)	66 (100%)	0	100	100
29	d	60/66 (91%)	60 (100%)	0	100	100
30	e	60/73 (82%)	60 (100%)	0	100	100
31	f	81/84 (96%)	81 (100%)	0	100	100
32	g	65/96 (68%)	65 (100%)	0	100	100
33	i	77/90 (86%)	77 (100%)	0	100	100
34	j	42/51 (82%)	42 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	k	38/60 (63%)	38 (100%)	0	100	100
36	l	53/97 (55%)	53 (100%)	0	100	100
37	m	58/59 (98%)	58 (100%)	0	100	100
38	n	92/99 (93%)	92 (100%)	0	100	100
39	o	70/87 (80%)	70 (100%)	0	100	100
40	p	83/93 (89%)	83 (100%)	0	100	100
41	q	54/133 (41%)	54 (100%)	0	100	100
42	r	10/118 (8%)	10 (100%)	0	100	100
44	v	23/84 (27%)	23 (100%)	0	100	100
45	x	183/216 (85%)	183 (100%)	0	100	100
46	y	223/232 (96%)	223 (100%)	0	100	100
47	z	188/228 (82%)	188 (100%)	0	100	100
All	All	6565/7831 (84%)	6563 (100%)	2 (0%)	100	100

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

Mol	Chain	Res	Type
5	E	135	CYS
16	P	343	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
6	F	304	HIS
7	G	320	ASN
7	G	638	GLN
10	J	136	ASN
12	L	567	GLN
14	N	53	ASN
16	P	361	GLN
26	a	26	GLN
32	g	95	GLN
36	l	99	ASN
39	o	85	GLN
45	x	116	ASN
46	y	107	HIS
47	z	47	ASN

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Mol	Chain	Res	Type
47	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 3 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	SF4	I	500	9	0,12,12	-	-	-	-	-
49	PTY	M	501	-	49,49,49	0.88	4 (8%)	52,54,54	1.10	2 (3%)
48	SF4	G	802	7	0,12,12	-	-	-	-	-
58	PC7	v	201	-	51,51,51	0.96	4 (7%)	57,59,59	1.04	2 (3%)
52	UQ9	H	500	-	35,35,58	2.49	13 (37%)	42,45,73	1.94	12 (28%)
59	PGT	f	201	-	40,40,50	1.16	3 (7%)	43,46,56	1.11	2 (4%)
50	FES	E	500	5	0,4,4	-	-	-	-	-
49	PTY	N	501	-	49,49,49	0.86	4 (8%)	52,54,54	1.11	2 (3%)
57	8Q1	W	200	-	31,34,34	1.71	6 (19%)	40,43,43	1.56	4 (10%)
61	PSF	z	301	-	28,29,29	1.18	4 (14%)	32,36,36	1.22	2 (6%)
48	SF4	F	501	6	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	LMN	M	502	-	72,72,72	1.65	14 (19%)	96,98,98	1.02	3 (3%)
49	PTY	D	401	-	49,49,49	0.87	4 (8%)	52,54,54	1.10	2 (3%)
58	PC7	c	101	-	51,51,51	0.97	4 (7%)	57,59,59	1.03	2 (3%)
48	SF4	G	803	7	0,12,12	-	-	-	-	-
57	8Q1	n	200	-	31,34,34	1.68	5 (16%)	40,43,43	1.56	4 (10%)
51	FMN	F	500	-	33,33,33	1.09	2 (6%)	48,50,50	1.22	8 (16%)
55	NDP	P	500	-	45,52,52	2.26	5 (11%)	53,80,80	1.74	11 (20%)
48	SF4	B	500	2	0,12,12	-	-	-	-	-
48	SF4	I	501	9	0,12,12	-	-	-	-	-
60	T7X	f	202	-	61,61,61	0.84	4 (6%)	71,73,73	1.06	2 (2%)
50	FES	G	801	7	0,4,4	-	-	-	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	SF4	I	500	9	-	-	0/6/5/5
49	PTY	M	501	-	-	25/53/53/53	-
48	SF4	G	802	7	-	-	0/6/5/5
58	PC7	v	201	-	-	20/55/55/55	-
52	UQ9	H	500	-	-	7/30/54/81	0/1/1/1
59	PGT	f	201	-	-	22/45/45/55	-
50	FES	E	500	5	-	-	0/1/1/1
49	PTY	N	501	-	-	23/53/53/53	-
57	8Q1	W	200	-	-	25/41/41/41	-
61	PSF	z	301	-	-	12/35/35/35	-
48	SF4	F	501	6	-	-	0/6/5/5
53	LMN	M	502	-	-	38/50/130/130	0/4/4/4
49	PTY	D	401	-	-	19/53/53/53	-
58	PC7	c	101	-	-	29/55/55/55	-
48	SF4	G	803	7	-	-	0/6/5/5
57	8Q1	n	200	-	-	19/41/41/41	-
51	FMN	F	500	-	-	8/18/18/18	0/3/3/3
55	NDP	P	500	-	-	8/30/77/77	0/5/5/5
48	SF4	B	500	2	-	-	0/6/5/5
48	SF4	I	501	9	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	T7X	f	202	-	-	29/56/80/80	0/1/1/1
50	FES	G	801	7	-	-	0/1/1/1

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	P	500	NDP	P2B-O2B	12.70	1.83	1.59
52	H	500	UQ9	C6-C1	9.77	1.53	1.35
57	W	200	8Q1	C34-N36	5.54	1.45	1.33
57	n	200	8Q1	C34-N36	5.45	1.45	1.33
57	W	200	8Q1	C39-N41	5.37	1.45	1.33
57	n	200	8Q1	C39-N41	5.30	1.45	1.33
53	M	502	LMN	O5-C1	4.71	1.53	1.41
52	H	500	UQ9	C4-C3	4.32	1.53	1.36
53	M	502	LMN	CBS-CCM	4.17	1.63	1.53
53	M	502	LMN	CBT-CCM	4.05	1.62	1.53
52	H	500	UQ9	C7-C8	3.88	1.56	1.50
55	P	500	NDP	PN-O5D	3.87	1.75	1.59
51	F	500	FMN	C4A-N5	3.77	1.38	1.30
53	M	502	LMN	CBR-CCM	3.66	1.61	1.54
53	M	502	LMN	O1-C1	-3.61	1.34	1.40
55	P	500	NDP	O2B-C2B	-3.05	1.33	1.44
59	f	201	PGT	O3-C11	2.94	1.41	1.33
59	f	201	PGT	O2-C31	2.93	1.42	1.34
53	M	502	LMN	OBY-CCR	2.85	1.49	1.41
53	M	502	LMN	OBZ-CCS	2.82	1.49	1.41
53	M	502	LMN	O4-C4	2.77	1.51	1.43
52	H	500	UQ9	C7-C6	2.77	1.56	1.51
58	c	101	PC7	O2-C2	-2.70	1.39	1.46
53	M	502	LMN	OBX-CCF	2.63	1.50	1.44
58	v	201	PC7	O2-C2	-2.60	1.40	1.46
49	M	501	PTY	O7-C6	-2.60	1.40	1.46
61	z	301	PSF	O11-C3	-2.58	1.40	1.46
52	H	500	UQ9	C11-C9	2.58	1.56	1.51
49	D	401	PTY	O7-C6	-2.54	1.40	1.46
52	H	500	UQ9	C16-C14	2.47	1.56	1.51
52	H	500	UQ9	C6-C5	2.46	1.53	1.46
52	H	500	UQ9	C21-C19	2.43	1.56	1.51
57	W	200	8Q1	C1-S44	2.41	1.82	1.76
49	M	501	PTY	O4-C30	2.40	1.40	1.33
58	v	201	PC7	O3-C11	2.39	1.40	1.33
57	n	200	8Q1	C1-S44	2.39	1.81	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	M	502	LMN	OBX-CCJ	2.37	1.47	1.41
52	H	500	UQ9	C26-C24	2.36	1.56	1.51
49	N	501	PTY	O4-C30	2.36	1.40	1.33
51	F	500	FMN	C10-N1	2.36	1.38	1.33
60	f	202	T7X	O18-C11	2.36	1.40	1.33
60	f	202	T7X	O16-C10	2.35	1.40	1.34
61	z	301	PSF	O52-C5	2.34	1.40	1.33
58	c	101	PC7	O3-C11	2.34	1.40	1.33
57	W	200	8Q1	O40-C39	-2.32	1.18	1.23
49	D	401	PTY	O4-C30	2.31	1.40	1.33
52	H	500	UQ9	O4-C4M	-2.31	1.39	1.45
57	n	200	8Q1	O35-C34	-2.28	1.18	1.23
53	M	502	LMN	C3-C4	-2.26	1.46	1.52
49	N	501	PTY	O7-C8	2.25	1.40	1.34
58	c	101	PC7	O3-C3	-2.23	1.40	1.45
49	D	401	PTY	O4-C1	-2.23	1.40	1.45
57	W	200	8Q1	O35-C34	-2.23	1.19	1.23
57	n	200	8Q1	O40-C39	-2.22	1.18	1.23
49	N	501	PTY	O7-C6	-2.20	1.41	1.46
49	M	501	PTY	O4-C1	-2.19	1.40	1.45
61	z	301	PSF	O52-C4	-2.18	1.40	1.45
49	N	501	PTY	O4-C1	-2.17	1.40	1.45
59	f	201	PGT	P-O3P	2.17	1.68	1.59
55	P	500	NDP	C2A-N1A	2.17	1.37	1.33
58	v	201	PC7	O3-C3	-2.16	1.40	1.45
60	f	202	T7X	O16-C8	-2.15	1.41	1.46
60	f	202	T7X	O18-C9	-2.14	1.40	1.45
49	M	501	PTY	O7-C8	2.12	1.40	1.34
49	D	401	PTY	O7-C8	2.11	1.40	1.34
52	H	500	UQ9	O2-C2	-2.11	1.18	1.23
52	H	500	UQ9	O5-C5	-2.10	1.18	1.23
53	M	502	LMN	O5-C5	2.09	1.49	1.44
58	v	201	PC7	O2-C31	2.09	1.40	1.34
55	P	500	NDP	O5D-C5D	-2.08	1.36	1.44
53	M	502	LMN	OCB-CCQ	2.07	1.49	1.43
57	W	200	8Q1	C6-C1	2.06	1.53	1.50
61	z	301	PSF	O11-C1	2.06	1.40	1.34
53	M	502	LMN	CBQ-CCM	2.04	1.58	1.54
58	c	101	PC7	O2-C31	2.04	1.40	1.34
52	H	500	UQ9	C17-C18	2.01	1.57	1.50

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	P	500	NDP	PN-O3-PA	-7.01	108.78	132.83
57	n	200	8Q1	C6-C1-S44	5.65	120.03	113.46
57	W	200	8Q1	C6-C1-S44	5.61	119.98	113.46
52	H	500	UQ9	C7-C6-C5	5.45	125.03	118.48
60	f	202	T7X	O16-C10-C12	4.30	120.76	111.50
52	H	500	UQ9	C7-C8-C9	-4.16	119.87	126.79
59	f	201	PGT	O2-C31-C32	4.11	120.36	111.50
49	N	501	PTY	O7-C8-C11	4.11	120.35	111.50
49	M	501	PTY	O7-C8-C11	4.10	120.34	111.50
53	M	502	LMN	CCR-O4-C4	-4.07	107.90	117.96
61	z	301	PSF	O11-C1-C13	4.01	120.14	111.50
49	D	401	PTY	O7-C8-C11	3.94	119.99	111.50
58	v	201	PC7	O2-C31-C32	3.90	119.92	111.50
58	c	101	PC7	O2-C31-C32	3.80	119.69	111.50
57	W	200	8Q1	O4-C1-C6	-3.64	119.69	123.99
52	H	500	UQ9	C12-C13-C14	-3.60	119.00	127.66
57	n	200	8Q1	O4-C1-C6	-3.46	119.90	123.99
55	P	500	NDP	O2B-P2B-O1X	-3.33	96.55	109.39
52	H	500	UQ9	C17-C18-C19	-3.24	119.85	127.66
51	F	500	FMN	C4-N3-C2	-3.24	119.66	125.64
52	H	500	UQ9	C1M-C1-C6	-3.21	119.17	124.40
52	H	500	UQ9	C27-C26-C24	-3.20	109.39	114.62
55	P	500	NDP	PA-O5B-C5B	-3.08	103.60	121.68
52	H	500	UQ9	C22-C23-C24	-3.00	120.44	127.66
55	P	500	NDP	PN-O5D-C5D	-2.90	104.65	121.68
57	W	200	8Q1	C43-S44-C1	2.81	110.62	101.87
51	F	500	FMN	C4A-C4-N3	2.79	120.27	113.19
60	f	202	T7X	O18-C11-C31	2.72	120.45	111.91
49	N	501	PTY	O4-C30-C31	2.71	120.40	111.91
49	M	501	PTY	O4-C30-C31	2.68	120.31	111.91
51	F	500	FMN	O4-C4-C4A	-2.66	119.55	126.60
52	H	500	UQ9	C25-C24-C26	2.64	119.71	115.27
52	H	500	UQ9	C20-C19-C21	2.63	119.70	115.27
52	H	500	UQ9	C15-C14-C16	2.62	119.67	115.27
49	D	401	PTY	O4-C30-C31	2.61	120.11	111.91
52	H	500	UQ9	C10-C9-C11	2.61	119.66	115.27
58	v	201	PC7	O3-C11-C12	2.54	119.89	111.91
55	P	500	NDP	O3X-P2B-O2X	2.54	117.35	107.64
58	c	101	PC7	O3-C11-C12	2.54	119.86	111.91
57	W	200	8Q1	C38-C39-N41	2.52	120.66	116.42
52	H	500	UQ9	C6-C1-C2	2.50	121.16	119.18
61	z	301	PSF	O52-C5-C6	2.50	119.77	111.91
51	F	500	FMN	C4A-C10-N10	2.48	120.10	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	P	500	NDP	O5D-PN-O1N	-2.47	99.41	109.07
55	P	500	NDP	O4B-C4B-C3B	2.47	110.00	105.11
57	n	200	8Q1	C43-S44-C1	2.45	109.51	101.87
59	f	201	PGT	O3-C11-C12	2.38	119.36	111.91
55	P	500	NDP	C2A-N1A-C6A	-2.37	114.70	118.75
55	P	500	NDP	O2N-PN-O1N	2.35	123.86	112.24
57	n	200	8Q1	C38-C39-N41	2.34	120.36	116.42
53	M	502	LMN	CCS-OCB-CCQ	-2.31	112.24	117.96
55	P	500	NDP	C5B-C4B-C3B	-2.25	106.75	115.18
51	F	500	FMN	C4A-C10-N1	-2.23	119.56	124.73
51	F	500	FMN	C10-C4A-N5	-2.14	120.31	124.86
51	F	500	FMN	C9A-C5A-N5	-2.11	120.14	122.43
53	M	502	LMN	CBK-CBQ-CCM	-2.06	110.54	117.16
51	F	500	FMN	C5A-C9A-N10	2.04	120.06	117.95
55	P	500	NDP	C3N-C2N-N1N	-2.03	120.20	123.10

There are no chirality outliers.

All (284) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
49	D	401	PTY	N1-C2-C3-O11
49	D	401	PTY	C5-O14-P1-O13
49	M	501	PTY	N1-C2-C3-O11
49	M	501	PTY	O10-C8-O7-C6
49	M	501	PTY	C11-C8-O7-C6
49	N	501	PTY	C2-C3-O11-P1
49	N	501	PTY	C11-C8-O7-C6
49	N	501	PTY	C3-O11-P1-O12
51	F	500	FMN	N10-C1'-C2'-O2'
51	F	500	FMN	N10-C1'-C2'-C3'
51	F	500	FMN	C1'-C2'-C3'-O3'
51	F	500	FMN	C1'-C2'-C3'-C4'
52	H	500	UQ9	C9-C11-C12-C13
52	H	500	UQ9	C1-C6-C7-C8
52	H	500	UQ9	C5-C6-C7-C8
53	M	502	LMN	O1-CBS-CCM-CBR
53	M	502	LMN	CCM-CBT-OBV-CCJ
53	M	502	LMN	OBV-CBT-CCM-CBQ
53	M	502	LMN	OBV-CBT-CCM-CBR
53	M	502	LMN	OBX-CCJ-OBV-CBT
53	M	502	LMN	CCL-CCJ-OBV-CBT
55	P	500	NDP	C5B-O5B-PA-O2A

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Mol	Chain	Res	Type	Atoms
55	P	500	NDP	O4B-C4B-C5B-O5B
55	P	500	NDP	C3B-C4B-C5B-O5B
55	P	500	NDP	O4D-C4D-C5D-O5D
57	W	200	8Q1	O4-C1-C6-C7
57	W	200	8Q1	O4-C1-S44-C43
57	W	200	8Q1	C6-C1-S44-C43
57	W	200	8Q1	O27-C28-C29-C30
57	W	200	8Q1	O27-C28-C29-C31
57	W	200	8Q1	O27-C28-C29-C32
57	W	200	8Q1	C28-C29-C32-C34
57	W	200	8Q1	C31-C29-C32-C34
57	W	200	8Q1	C29-C32-C34-O35
57	W	200	8Q1	O33-C32-C34-N36
57	W	200	8Q1	N41-C42-C43-S44
57	W	200	8Q1	C28-O27-P24-O3
57	W	200	8Q1	C28-O27-P24-O2
57	W	200	8Q1	C28-O27-P24-O1
57	n	200	8Q1	O4-C1-S44-C43
57	n	200	8Q1	C6-C1-S44-C43
57	n	200	8Q1	C28-C29-C32-C34
57	n	200	8Q1	C28-C29-C32-O33
57	n	200	8Q1	C30-C29-C32-C34
57	n	200	8Q1	C30-C29-C32-O33
57	n	200	8Q1	C31-C29-C32-C34
57	n	200	8Q1	C31-C29-C32-O33
57	n	200	8Q1	C28-O27-P24-O3
57	n	200	8Q1	C28-O27-P24-O2
57	n	200	8Q1	C28-O27-P24-O1
58	c	101	PC7	C1-O3P-P-O1P
58	c	101	PC7	C4-O4P-P-O1P
58	v	201	PC7	C32-C31-O2-C2
58	v	201	PC7	O2-C2-C3-O3
58	v	201	PC7	C1-O3P-P-O4P
59	f	201	PGT	C4-O4P-P-O1P
60	f	202	T7X	C12-C10-O16-C8
61	z	301	PSF	C2-O2-P-O3
61	z	301	PSF	C13-C1-O11-C3
61	z	301	PSF	N-CA-CB-O1
61	z	301	PSF	C-CA-CB-O1
58	v	201	PC7	C12-C11-O3-C3
49	M	501	PTY	O30-C30-O4-C1
58	v	201	PC7	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
49	N	501	PTY	O10-C8-O7-C6
58	v	201	PC7	O31-C31-O2-C2
60	f	202	T7X	O17-C10-O16-C8
49	M	501	PTY	C31-C30-O4-C1
57	n	200	8Q1	C38-C39-N41-C42
52	H	500	UQ9	C15-C14-C16-C17
58	c	101	PC7	O11-C11-O3-C3
53	M	502	LMN	OAI-CBM-CCC-OBY
61	z	301	PSF	O12-C1-O11-C3
60	f	202	T7X	C31-C11-O18-C9
53	M	502	LMN	CCF-CCQ-OCB-CCS
59	f	201	PGT	C14-C15-C16-C17
55	P	500	NDP	C3D-C4D-C5D-O5D
58	c	101	PC7	C12-C11-O3-C3
53	M	502	LMN	OAI-CBM-CCC-CCN
53	M	502	LMN	OAL-CBP-CCF-CCQ
51	F	500	FMN	O2'-C2'-C3'-C4'
60	f	202	T7X	O19-C11-O18-C9
53	M	502	LMN	O5-C1-O1-CBS
57	n	200	8Q1	O40-C39-N41-C42
53	M	502	LMN	OBV-CBT-CCM-CBS
53	M	502	LMN	C4-C5-C6-O6
52	H	500	UQ9	C24-C26-C27-C28
53	M	502	LMN	OBZ-CCS-OCB-CCQ
53	M	502	LMN	CCW-CCS-OCB-CCQ
52	H	500	UQ9	C13-C14-C16-C17
53	M	502	LMN	OAL-CBP-CCF-OBX
49	M	501	PTY	C30-C31-C32-C33
60	f	202	T7X	C11-C31-C32-C33
49	D	401	PTY	C8-C11-C12-C13
49	N	501	PTY	C3-O11-P1-O14
58	c	101	PC7	C1-O3P-P-O4P
58	c	101	PC7	C4-O4P-P-O3P
58	v	201	PC7	C4-O4P-P-O3P
59	f	201	PGT	C4-O4P-P-O3P
61	z	301	PSF	C2-O2-P-O1
53	M	502	LMN	O5-C5-C6-O6
51	F	500	FMN	O2'-C2'-C3'-O3'
53	M	502	LMN	CAY-CBA-CBC-CBE
53	M	502	LMN	CBD-CBF-CBH-CBJ
59	f	201	PGT	C38-C39-C40-C41
49	D	401	PTY	C31-C30-O4-C1

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Mol	Chain	Res	Type	Atoms
60	f	202	T7X	C33-C34-C35-C36
53	M	502	LMN	CBE-CBG-CBI-CBK
53	M	502	LMN	CBG-CBI-CBK-CBQ
58	v	201	PC7	C21-C22-C23-C24
53	M	502	LMN	OAJ-CBN-CCD-CCO
60	f	202	T7X	C34-C35-C36-C37
58	c	101	PC7	C20-C21-C22-C23
58	v	201	PC7	C40-C41-C42-C43
59	f	201	PGT	C15-C16-C17-C18
49	N	501	PTY	N1-C2-C3-O11
59	f	201	PGT	C17-C18-C19-C20
53	M	502	LMN	CCH-CCQ-OCB-CCS
53	M	502	LMN	CBB-CBD-CBF-CBH
58	c	101	PC7	C32-C31-O2-C2
58	v	201	PC7	C18-C19-C20-C21
58	v	201	PC7	C12-C13-C14-C15
58	c	101	PC7	O31-C31-O2-C2
53	M	502	LMN	CBC-CBE-CBG-CBI
59	f	201	PGT	C32-C31-O2-C2
59	f	201	PGT	C16-C17-C18-C19
49	D	401	PTY	O30-C30-O4-C1
60	f	202	T7X	C1-O1-P1-O13
60	f	202	T7X	C36-C37-C38-C39
59	f	201	PGT	C18-C19-C20-C21
58	c	101	PC7	C36-C37-C38-C39
58	c	101	PC7	C15-C16-C17-C18
59	f	201	PGT	C33-C34-C35-C36
49	D	401	PTY	C39-C40-C41-C42
59	f	201	PGT	C13-C14-C15-C16
60	f	202	T7X	C12-C13-C14-C15
61	z	301	PSF	OT1-C-CA-CB
59	f	201	PGT	C37-C38-C39-C40
59	f	201	PGT	O31-C31-O2-C2
49	M	501	PTY	C31-C32-C33-C34
60	f	202	T7X	C38-C39-C40-C41
49	M	501	PTY	C3-O11-P1-O14
58	c	101	PC7	C11-C12-C13-C14
49	N	501	PTY	C8-C11-C12-C13
58	c	101	PC7	C31-C32-C33-C34
49	N	501	PTY	C12-C13-C14-C15
49	D	401	PTY	O4-C1-C6-C5
49	N	501	PTY	O4-C1-C6-C5

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Mol	Chain	Res	Type	Atoms
59	f	201	PGT	C1-C2-C3-O3
60	f	202	T7X	C7-C8-C9-O18
53	M	502	LMN	CAX-CAZ-CBB-CBD
49	D	401	PTY	C11-C12-C13-C14
60	f	202	T7X	O18-C11-C31-C32
58	c	101	PC7	C38-C39-C40-C41
60	f	202	T7X	C44-C45-C46-C47
52	H	500	UQ9	C19-C21-C22-C23
57	W	200	8Q1	O33-C32-C34-O35
59	f	201	PGT	C32-C33-C34-C35
49	N	501	PTY	C5-C6-O7-C8
51	F	500	FMN	C5'-O5'-P-O1P
49	D	401	PTY	O4-C1-C6-O7
49	N	501	PTY	O4-C1-C6-O7
57	W	200	8Q1	C30-C29-C32-O33
57	W	200	8Q1	C31-C29-C32-O33
58	c	101	PC7	C35-C36-C37-C38
53	M	502	LMN	CBJ-CBL-CBR-CCM
53	M	502	LMN	CAW-CAY-CBA-CBC
58	c	101	PC7	C32-C33-C34-C35
58	c	101	PC7	O3P-C1-C2-C3
49	N	501	PTY	C13-C14-C15-C16
57	n	200	8Q1	N41-C42-C43-S44
49	D	401	PTY	C12-C13-C14-C15
49	N	501	PTY	C37-C38-C39-C40
53	M	502	LMN	CBK-CBQ-CCM-CBR
58	v	201	PC7	C1-C2-C3-O3
49	M	501	PTY	C16-C17-C18-C19
57	W	200	8Q1	C29-C32-C34-N36
60	f	202	T7X	C15-C16-C17-C18
60	f	202	T7X	C19-C20-C21-C22
58	c	101	PC7	O3P-C1-C2-O2
60	f	202	T7X	O13-C7-C8-O16
49	M	501	PTY	C8-C11-C12-C13
49	M	501	PTY	C15-C16-C17-C18
60	f	202	T7X	C31-C32-C33-C34
49	N	501	PTY	C16-C17-C18-C19
57	W	200	8Q1	S44-C1-C6-C7
49	N	501	PTY	C11-C12-C13-C14
49	D	401	PTY	C14-C15-C16-C17
53	M	502	LMN	OAJ-CBN-CCD-OBZ
58	c	101	PC7	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
60	f	202	T7X	C9-C8-O16-C10
58	v	201	PC7	C15-C16-C17-C18
58	v	201	PC7	C14-C15-C16-C17
49	N	501	PTY	C33-C34-C35-C36
53	M	502	LMN	O1-CBS-CCM-CBQ
55	P	500	NDP	C5B-O5B-PA-O3
49	D	401	PTY	C11-C8-O7-C6
61	z	301	PSF	OT2-C-CA-CB
49	D	401	PTY	O10-C8-O7-C6
49	D	401	PTY	C37-C38-C39-C40
53	M	502	LMN	CAA-CAW-CAY-CBA
49	N	501	PTY	C5-O14-P1-O11
49	N	501	PTY	C24-C25-C26-C27
59	f	201	PGT	C5-C4-O4P-P
49	M	501	PTY	C3-O11-P1-O12
49	M	501	PTY	C3-O11-P1-O13
49	N	501	PTY	C3-O11-P1-O13
58	c	101	PC7	C4-O4P-P-O2P
58	v	201	PC7	C4-O4P-P-O1P
61	z	301	PSF	C2-O2-P-O4
58	v	201	PC7	C32-C33-C34-C35
58	v	201	PC7	O3P-C1-C2-C3
60	f	202	T7X	O13-C7-C8-C9
53	M	502	LMN	O1-CBS-CCM-CBT
58	v	201	PC7	O3P-C1-C2-O2
53	M	502	LMN	CBK-CBQ-CCM-CBT
49	M	501	PTY	C25-C26-C27-C28
49	N	501	PTY	C21-C22-C23-C24
57	W	200	8Q1	C28-C29-C32-O33
58	c	101	PC7	O4P-C4-C5-N
59	f	201	PGT	O2-C2-C3-O3
60	f	202	T7X	O16-C8-C9-O18
49	M	501	PTY	C11-C12-C13-C14
49	M	501	PTY	C13-C14-C15-C16
49	M	501	PTY	C18-C19-C20-C21
49	D	401	PTY	C35-C36-C37-C38
57	W	200	8Q1	C11-C10-C9-C8
49	M	501	PTY	C19-C20-C21-C22
49	N	501	PTY	C39-C40-C41-C42
49	D	401	PTY	C13-C14-C15-C16
58	c	101	PC7	C13-C14-C15-C16
53	M	502	LMN	CAZ-CBB-CBD-CBF

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Mol	Chain	Res	Type	Atoms
58	c	101	PC7	C12-C13-C14-C15
60	f	202	T7X	O19-C11-C31-C32
57	n	200	8Q1	C11-C10-C9-C8
57	n	200	8Q1	C13-C14-C15-C16
53	M	502	LMN	CBH-CBJ-CBL-CBR
55	P	500	NDP	O4D-C1D-N1N-C6N
49	D	401	PTY	C33-C34-C35-C36
57	W	200	8Q1	C6-C7-C8-C9
57	n	200	8Q1	O27-C28-C29-C31
49	D	401	PTY	C31-C32-C33-C34
60	f	202	T7X	C18-C19-C20-C21
60	f	202	T7X	C22-C23-C24-C25
55	P	500	NDP	C2D-C1D-N1N-C6N
49	M	501	PTY	C41-C42-C43-C44
49	N	501	PTY	C15-C16-C17-C18
49	M	501	PTY	O4-C1-C6-O7
59	f	201	PGT	O11-C11-O3-C3
53	M	502	LMN	CBK-CBQ-CCM-CBS
59	f	201	PGT	C12-C11-O3-C3
49	M	501	PTY	C36-C37-C38-C39
60	f	202	T7X	C24-C25-C26-C27
59	f	201	PGT	C12-C13-C14-C15
58	c	101	PC7	C19-C20-C21-C22
59	f	201	PGT	C35-C36-C37-C38
57	W	200	8Q1	C12-C13-C14-C15
51	F	500	FMN	C5'-O5'-P-O2P
49	D	401	PTY	C5-O14-P1-O11
57	n	200	8Q1	O27-C28-C29-C30
49	M	501	PTY	C21-C22-C23-C24
49	M	501	PTY	C22-C23-C24-C25
57	n	200	8Q1	C6-C7-C8-C9
60	f	202	T7X	O16-C10-C12-C13
60	f	202	T7X	C13-C14-C15-C16
58	c	101	PC7	O2-C31-C32-C33
57	W	200	8Q1	C30-C29-C32-C34
61	z	301	PSF	O11-C1-C13-C14
58	c	101	PC7	C41-C42-C43-C44
60	f	202	T7X	C41-C42-C43-C44
49	M	501	PTY	C37-C38-C39-C40
58	v	201	PC7	C16-C17-C18-C19
58	c	101	PC7	C17-C18-C19-C20
59	f	201	PGT	C4-C5-C6-O6

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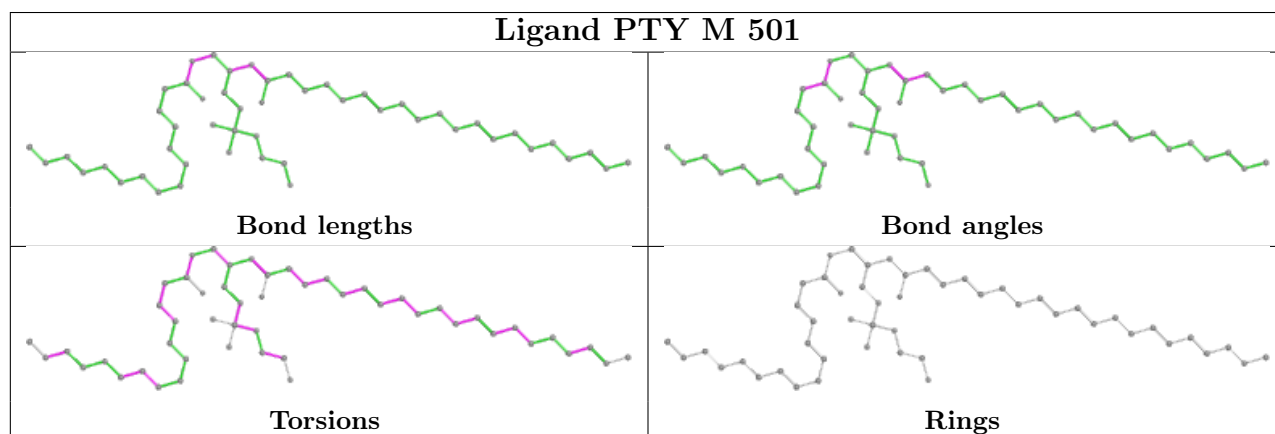
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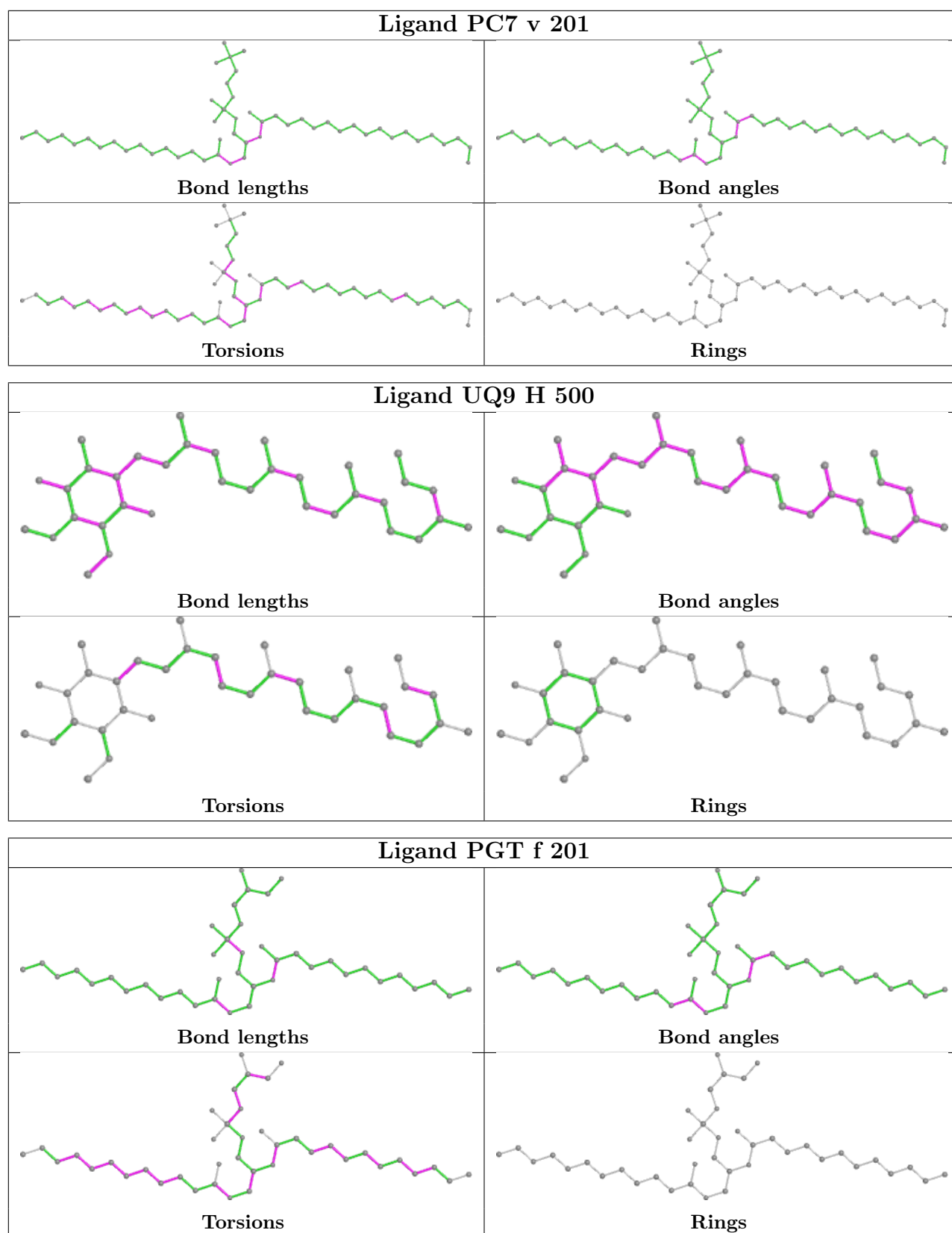
Mol	Chain	Res	Type	Atoms
57	W	200	8Q1	C29-C28-O27-P24
61	z	301	PSF	O12-C1-C13-C14
58	v	201	PC7	C19-C20-C21-C22
60	f	202	T7X	O17-C10-C12-C13
49	M	501	PTY	C5-O14-P1-O13
49	N	501	PTY	C5-O14-P1-O13
61	z	301	PSF	CB-O1-P-O3
58	c	101	PC7	O31-C31-C32-C33
53	M	502	LMN	CBF-CBH-CBJ-CBL
58	c	101	PC7	C21-C22-C23-C24

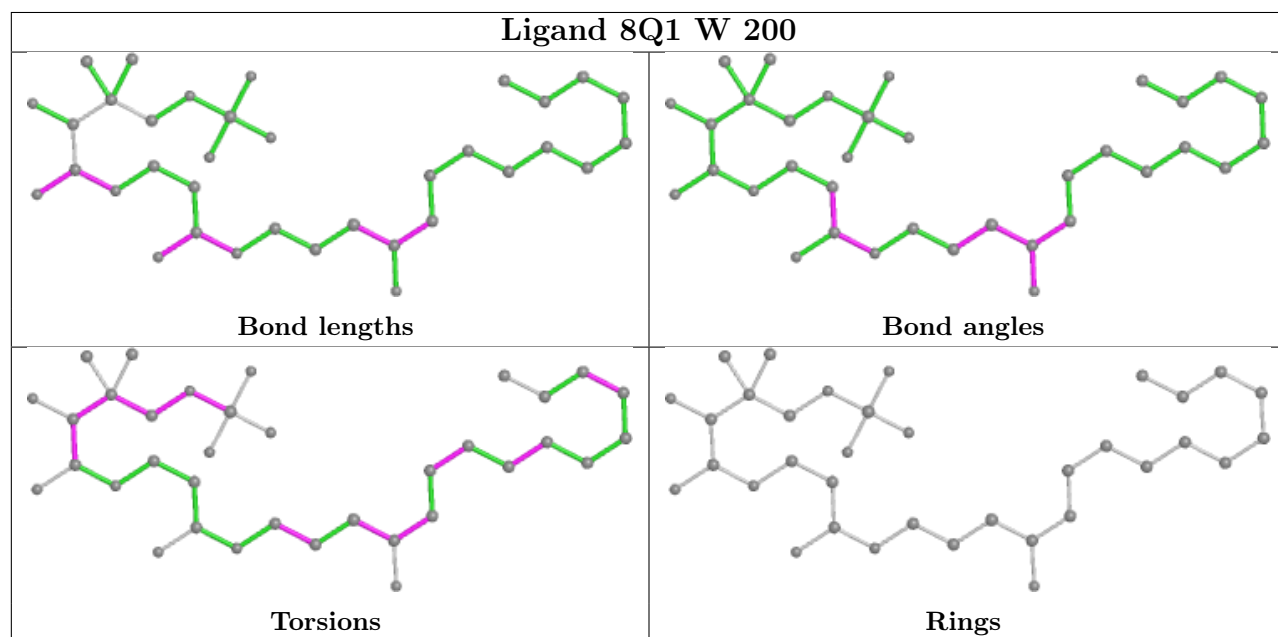
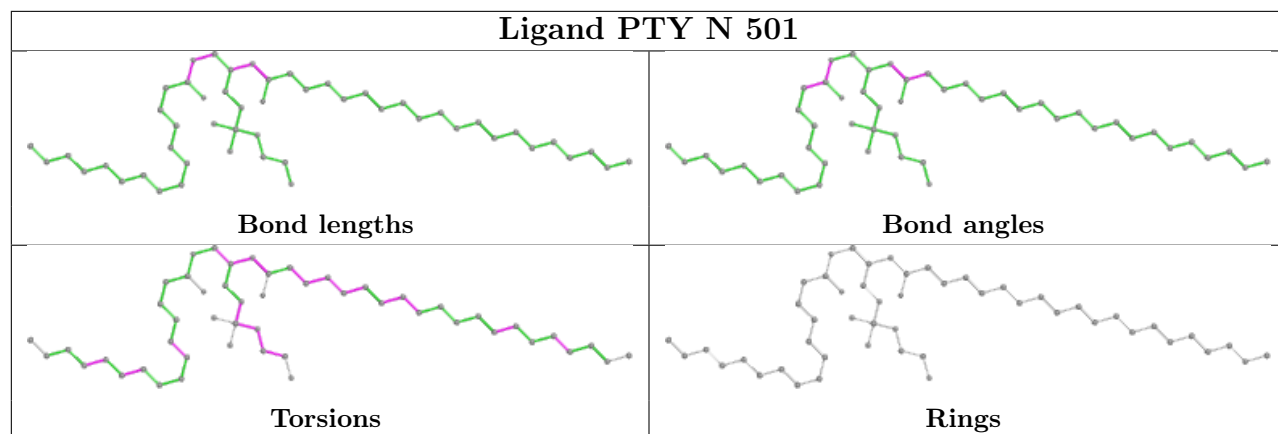
There are no ring outliers.

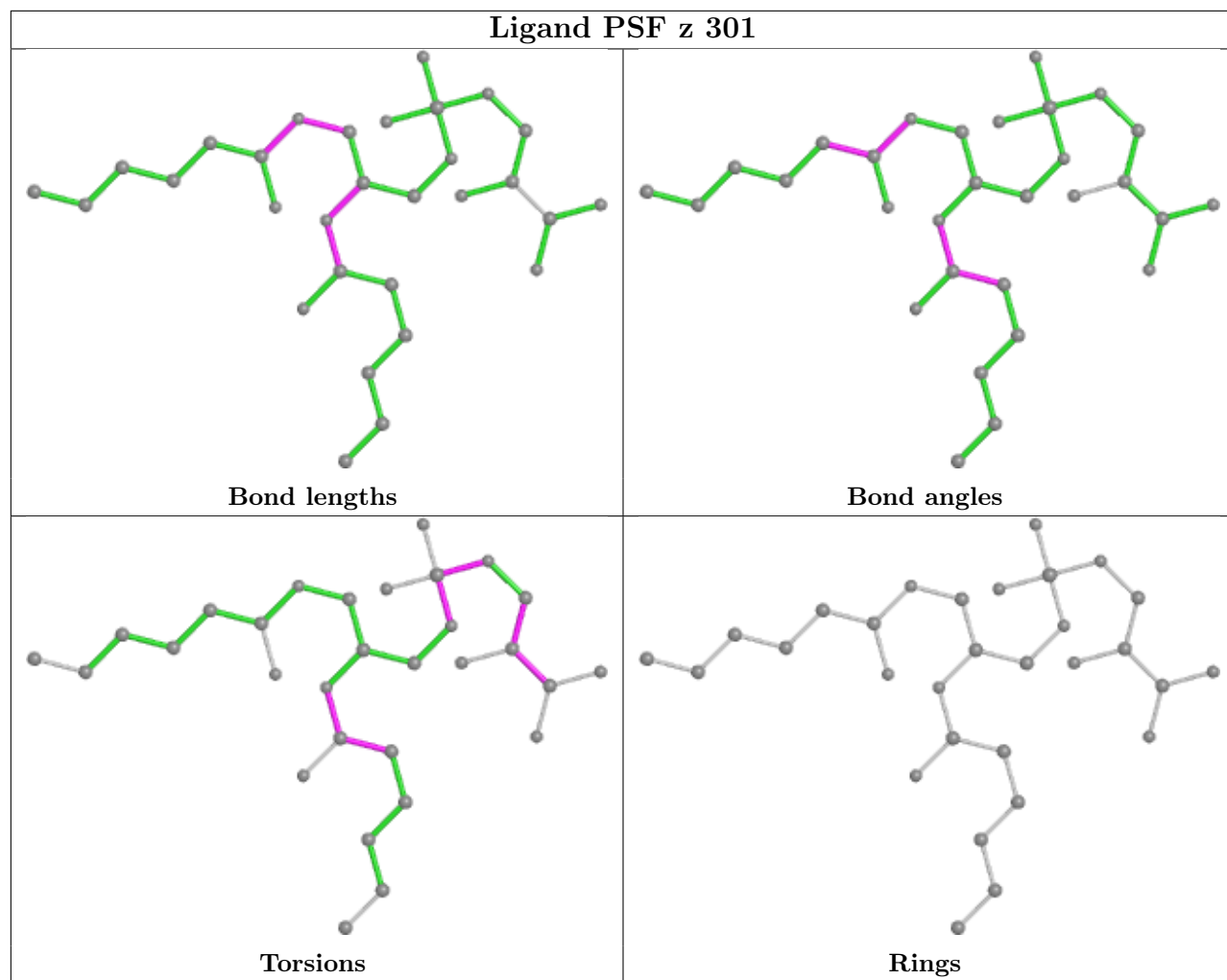
No monomer is involved in short contacts.

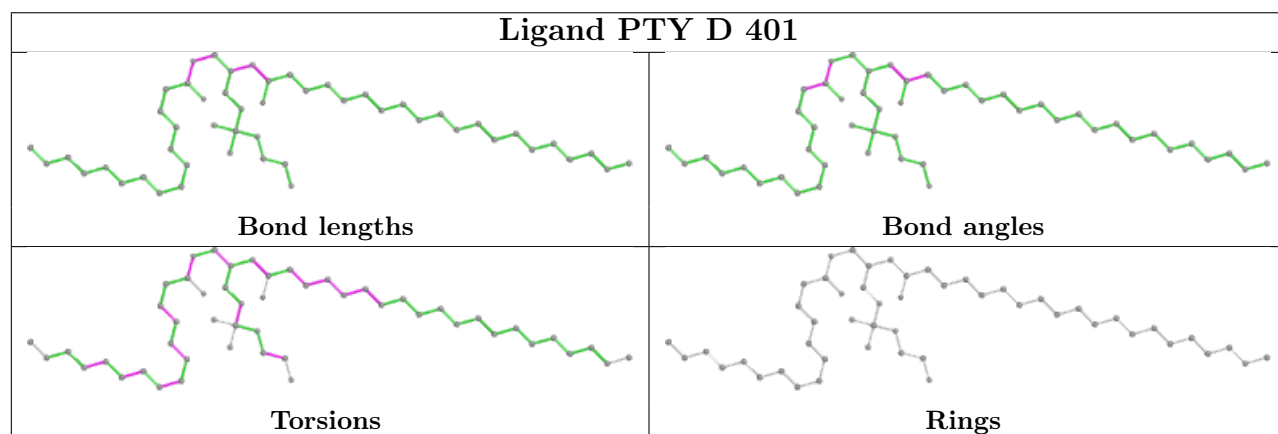
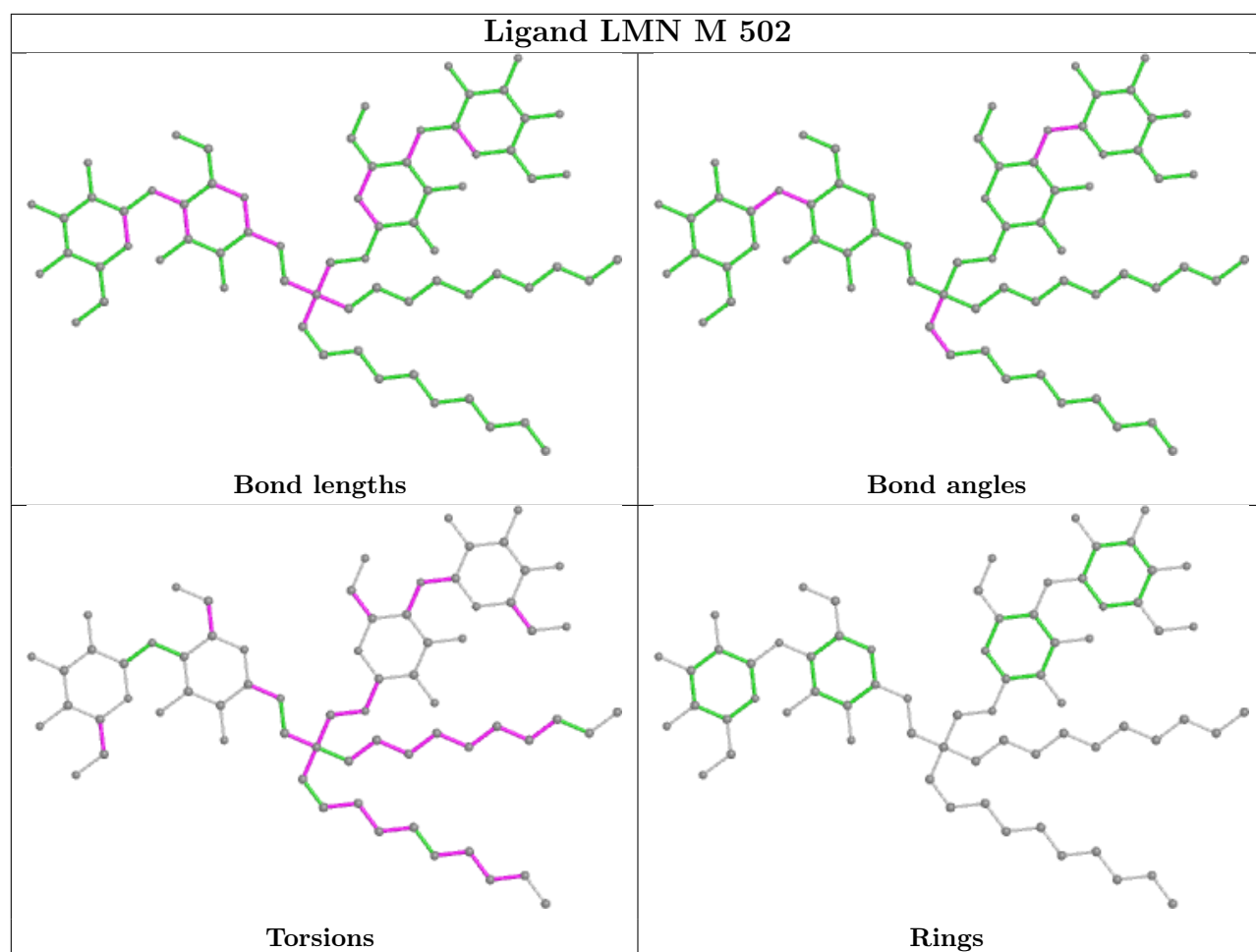
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

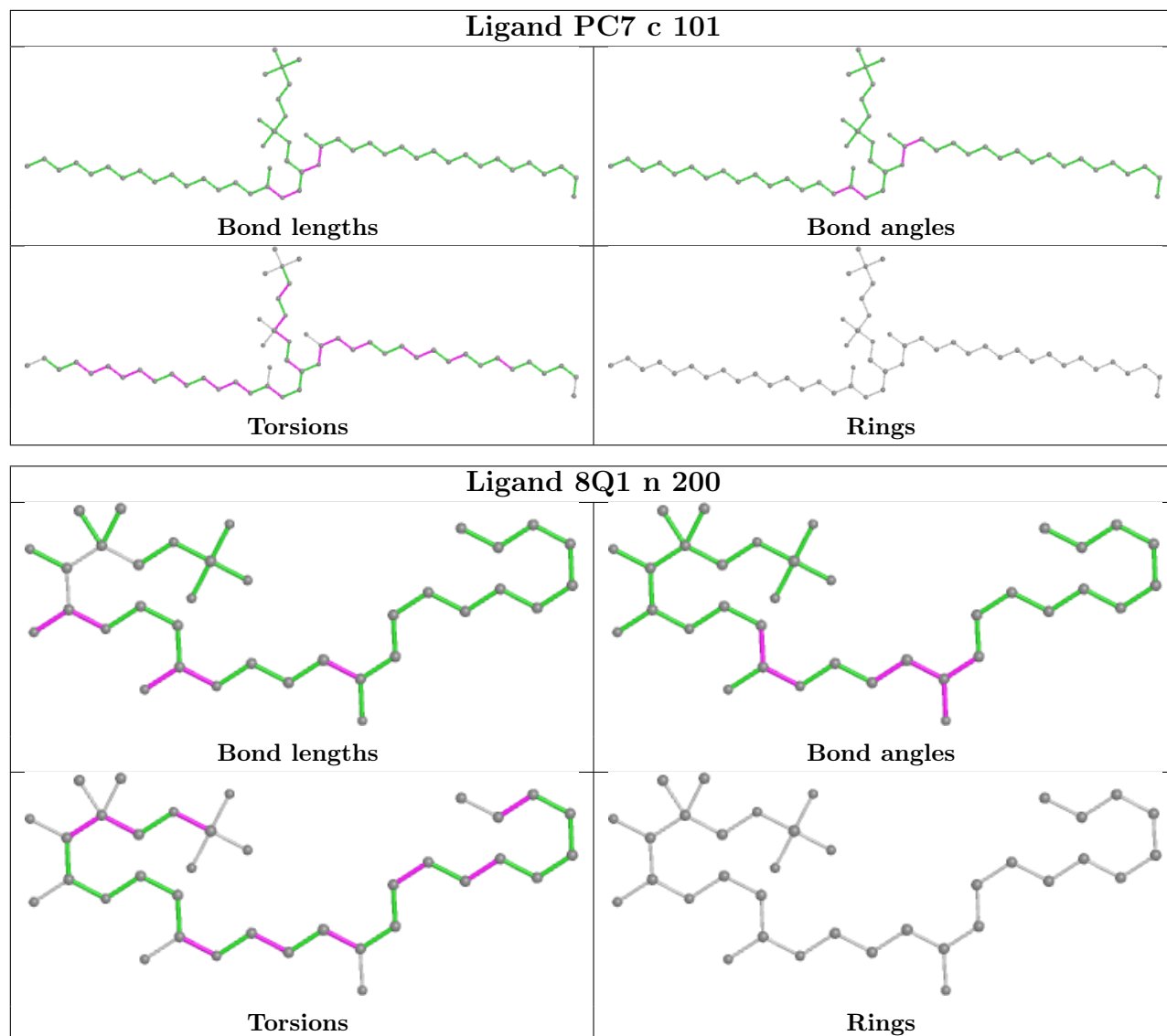


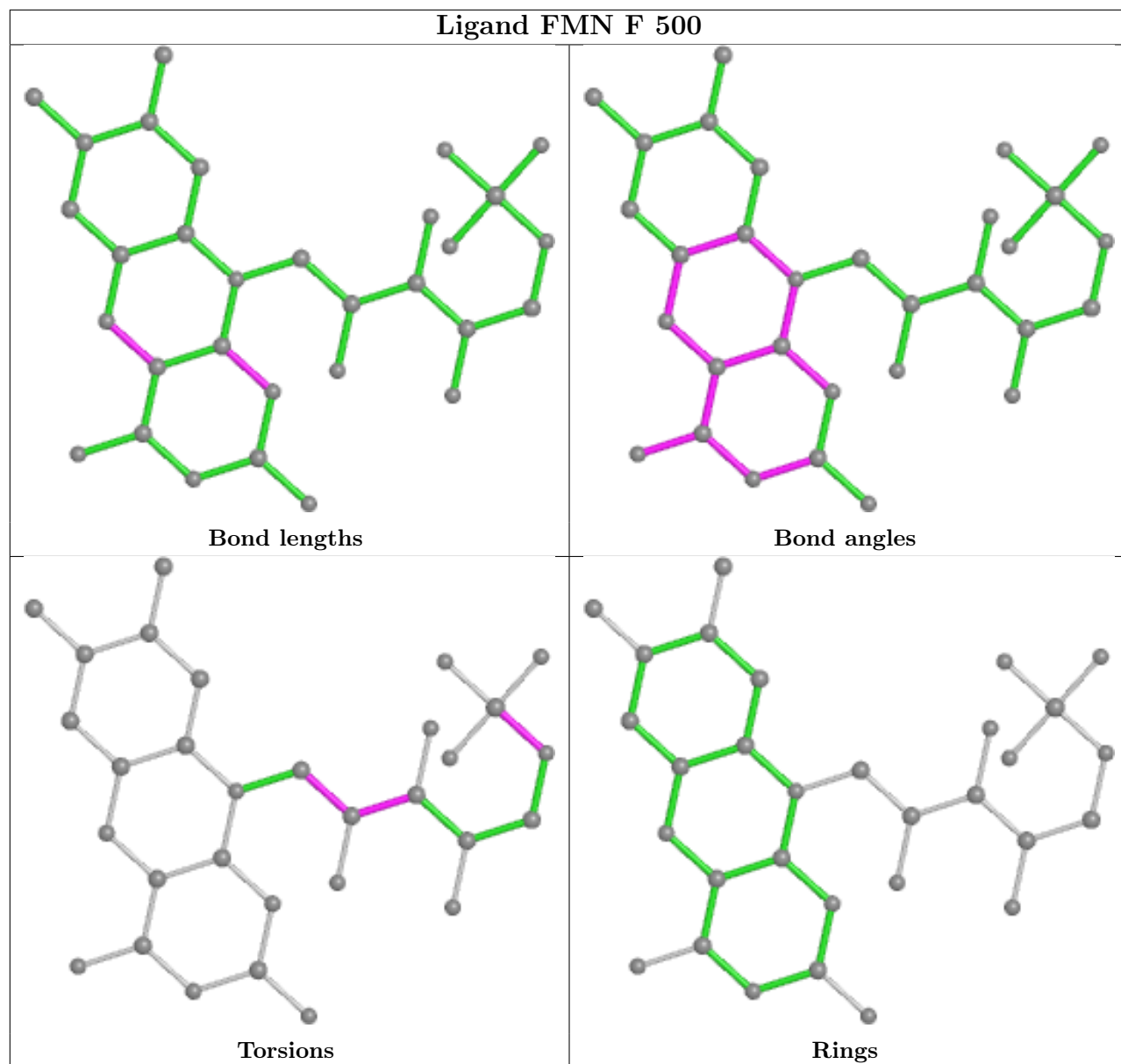


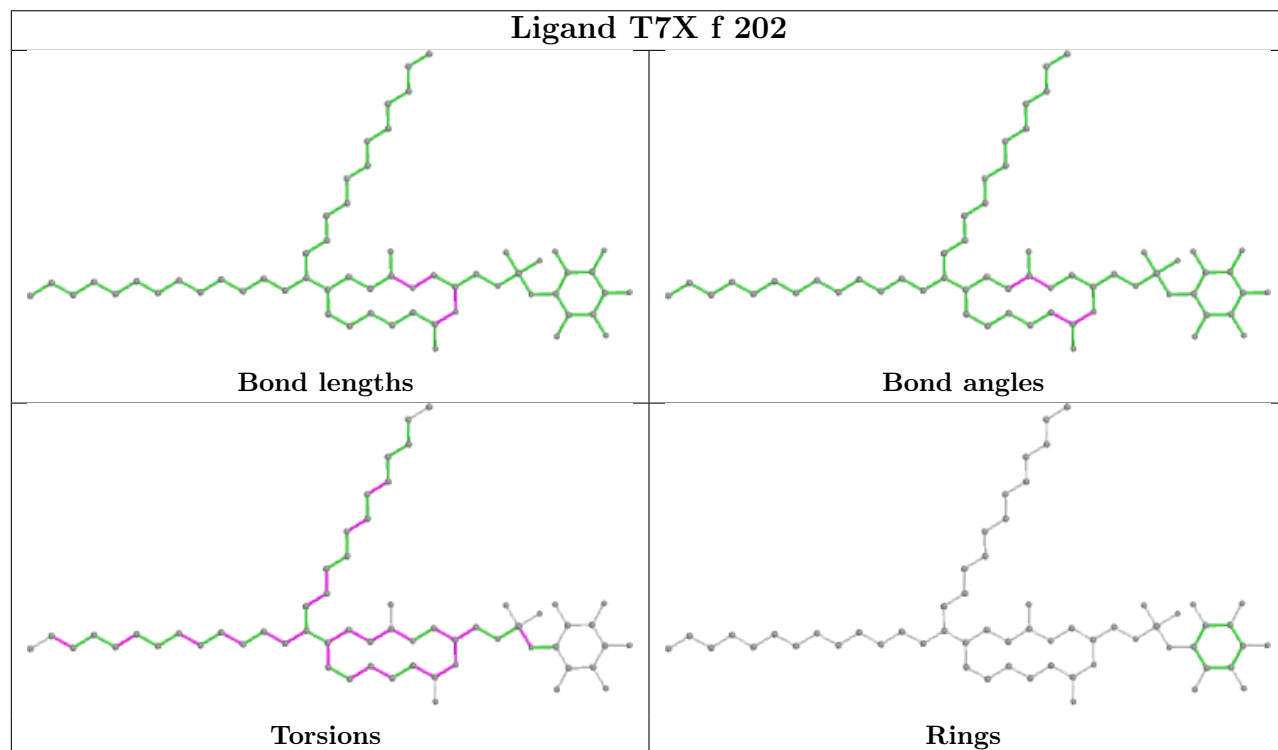
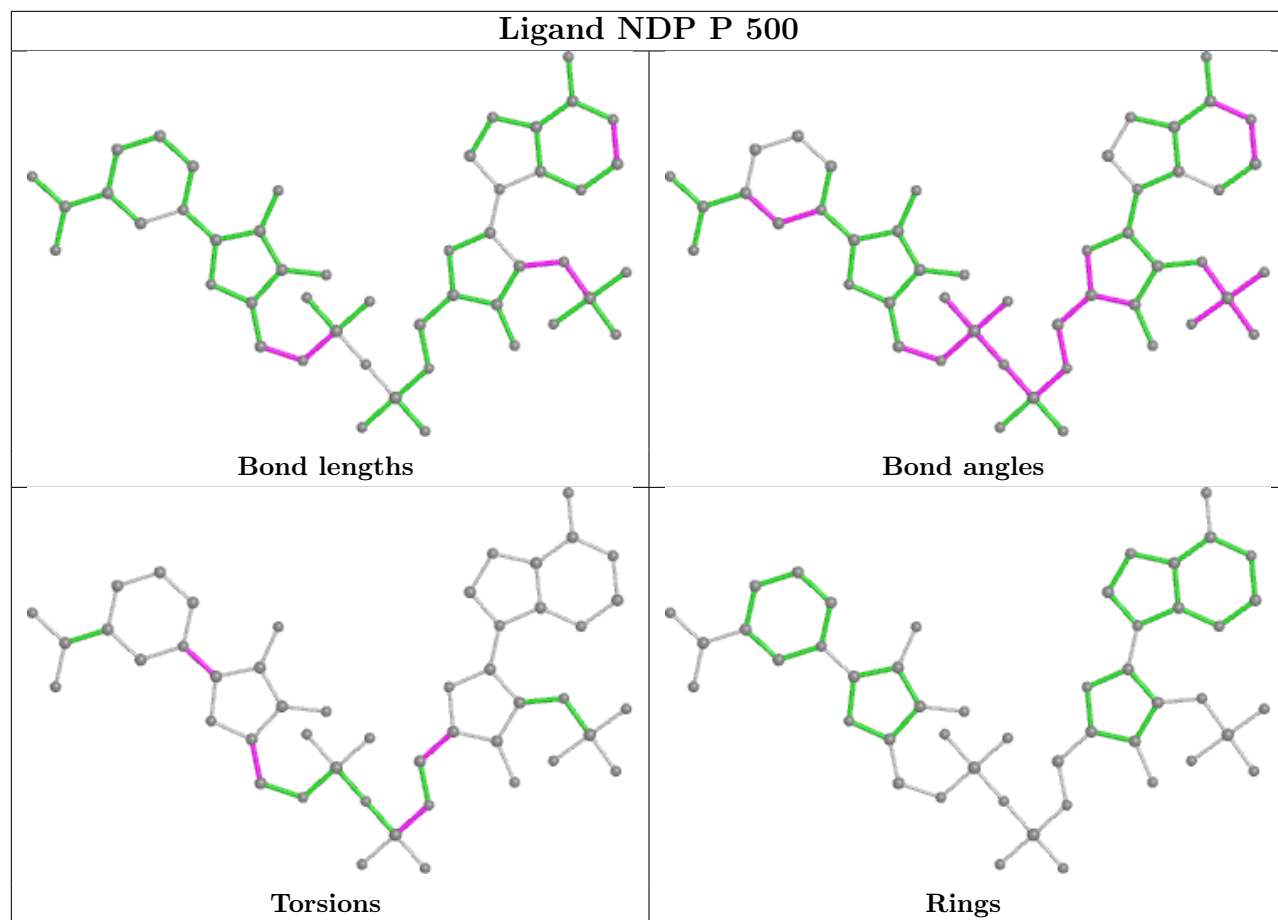












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	270:PRO	C	271:MET	N	3.13

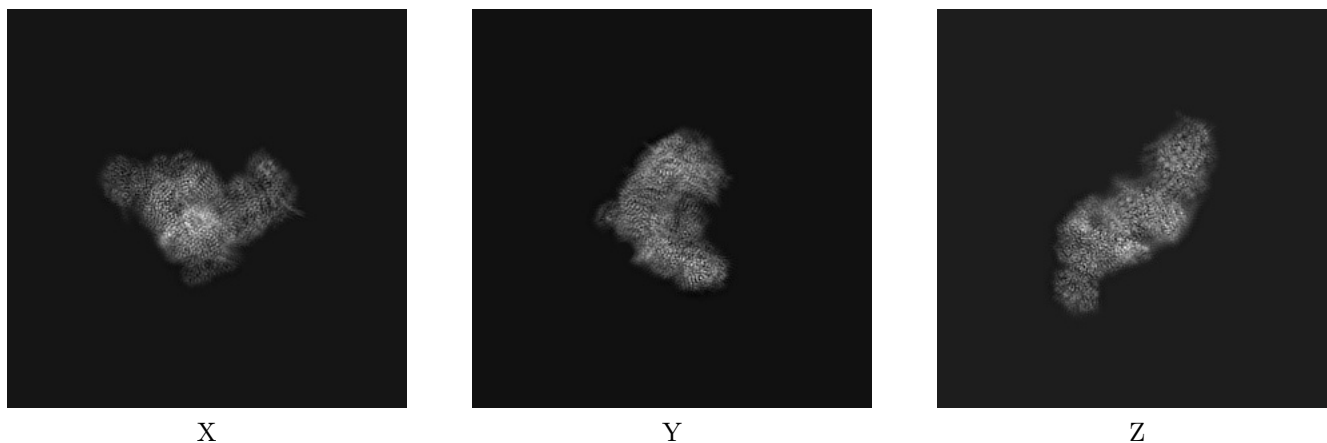
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11878. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

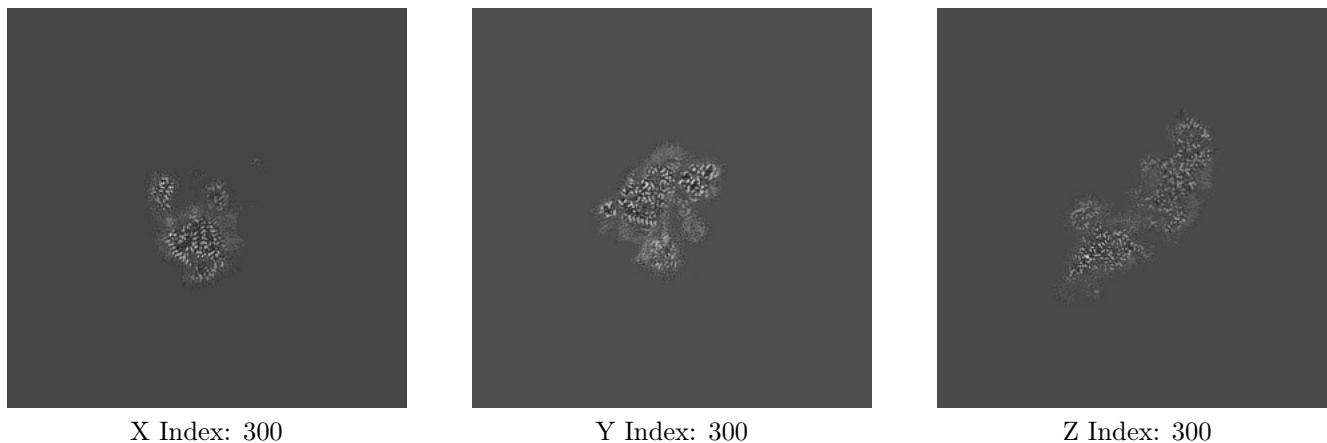
6.1.1 Primary map



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

6.2 Central slices [i](#)

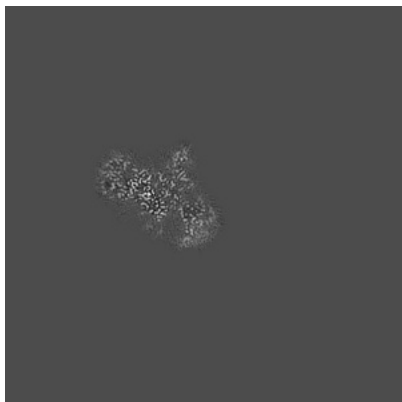
6.2.1 Primary map



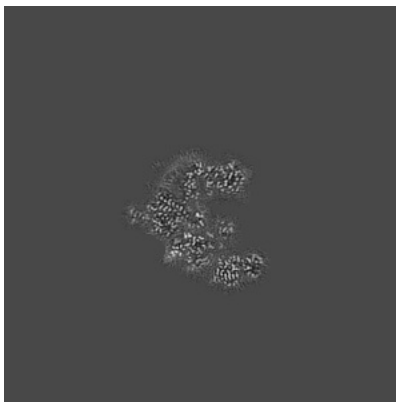
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

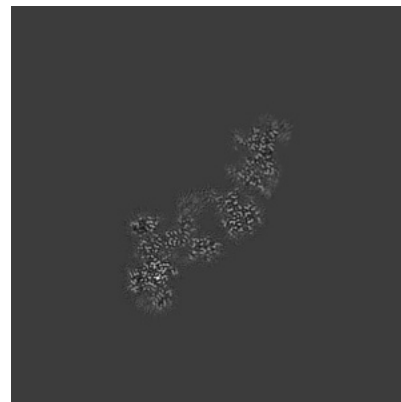
6.3.1 Primary map



X Index: 222



Y Index: 268

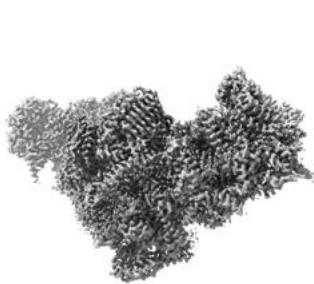


Z Index: 334

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

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.

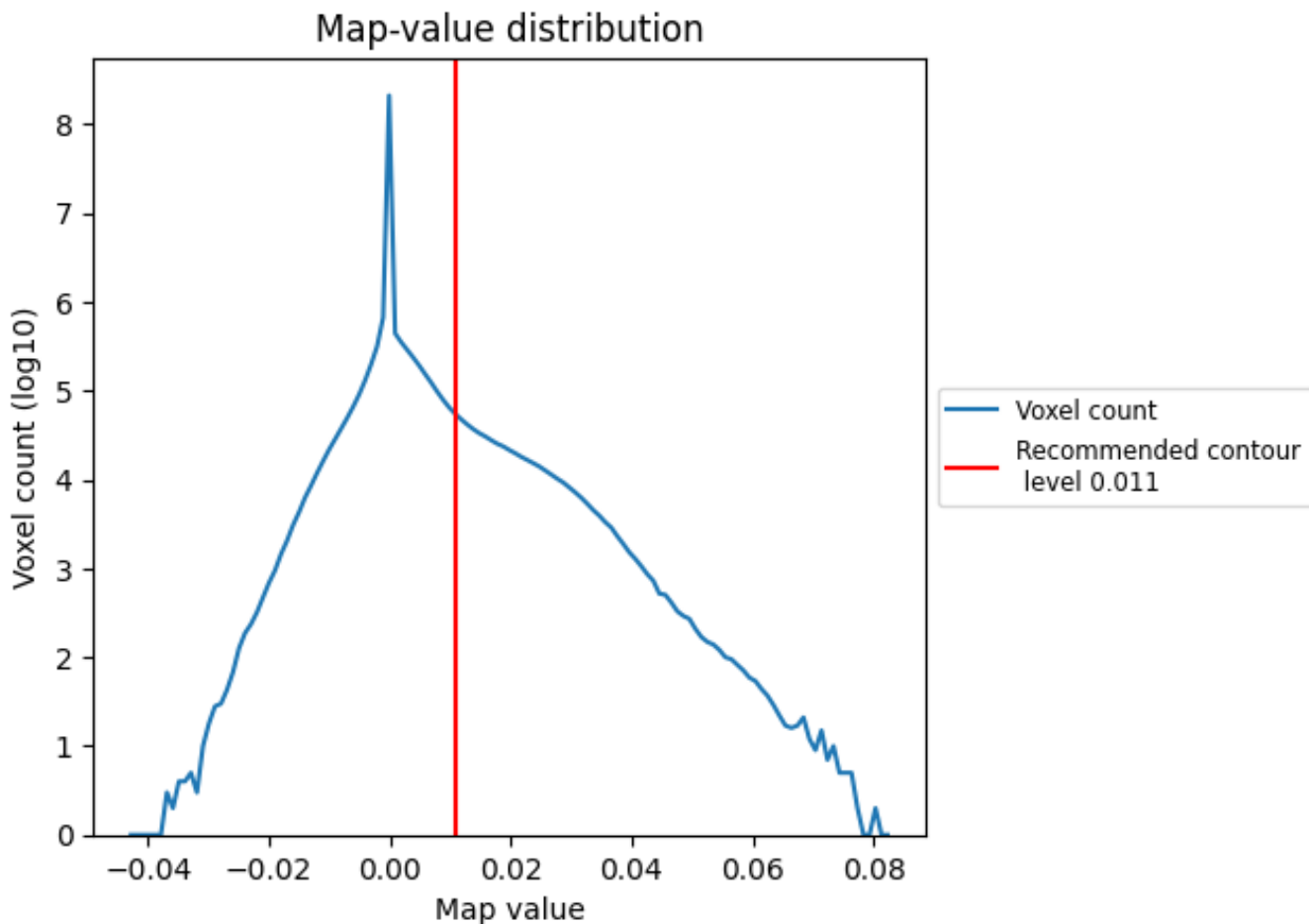
6.5 Mask visualisation

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

7 Map analysis [i](#)

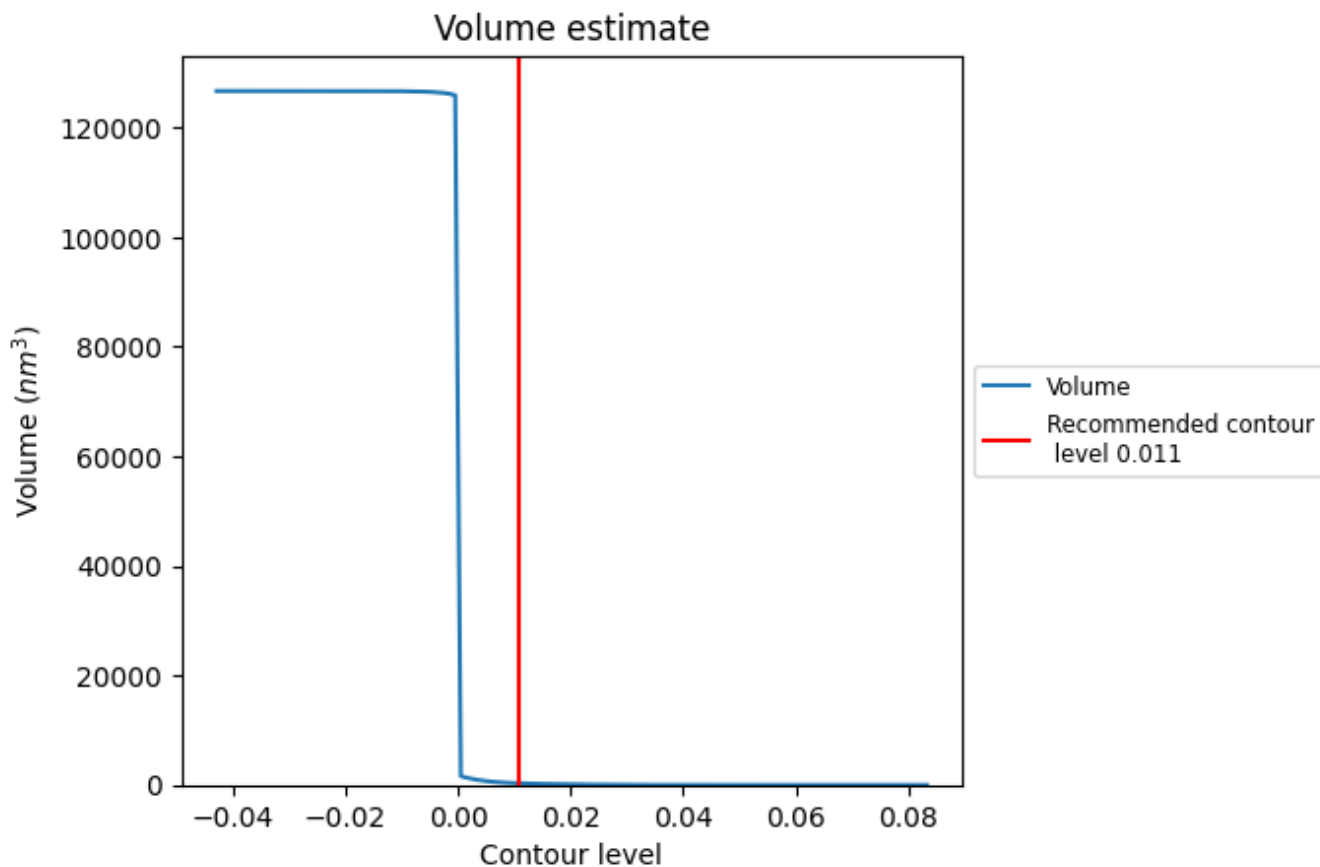
This section contains the results of statistical analysis of the map.

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.

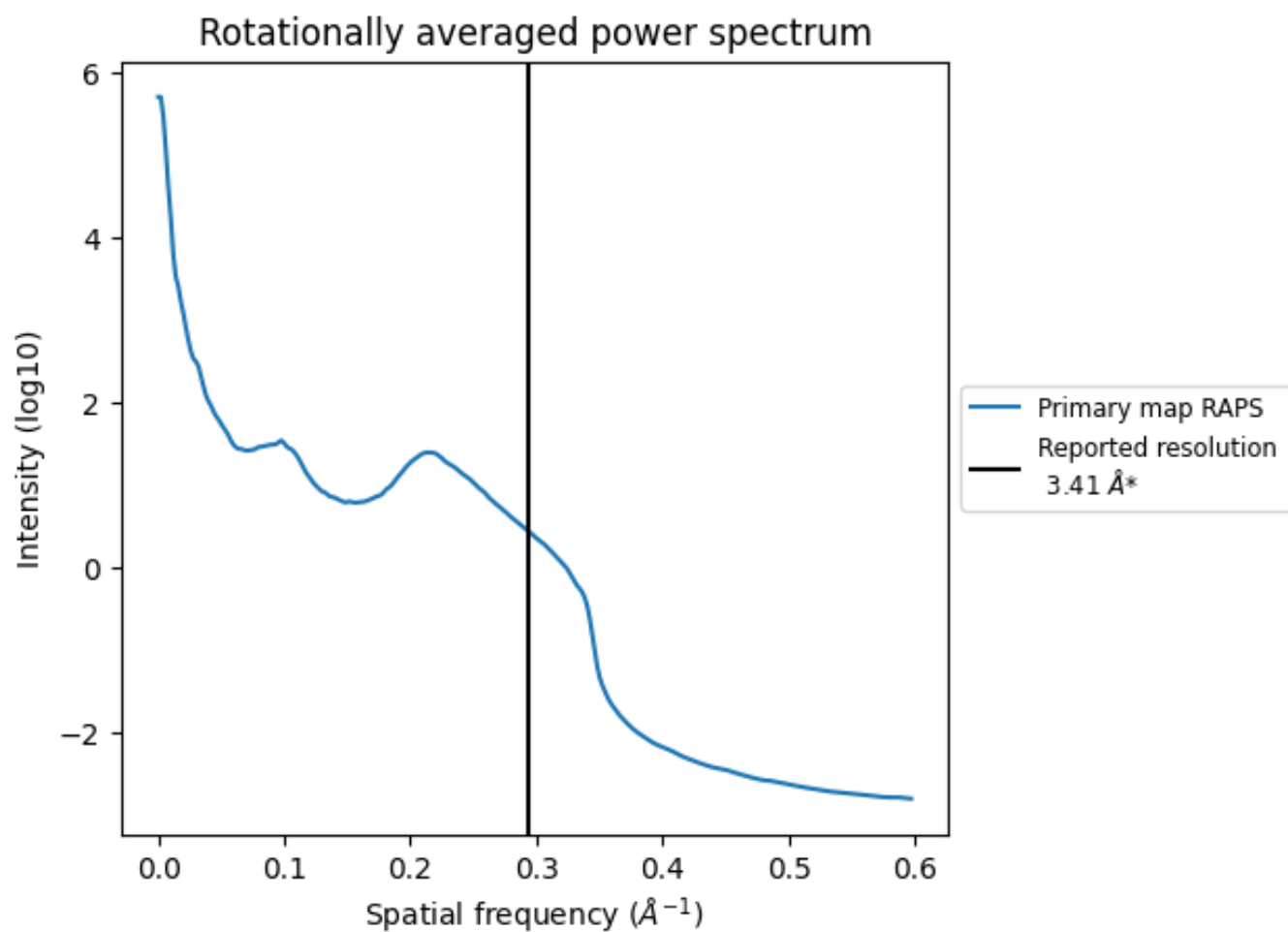
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 303 nm^3 ; this corresponds to an approximate mass of 274 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

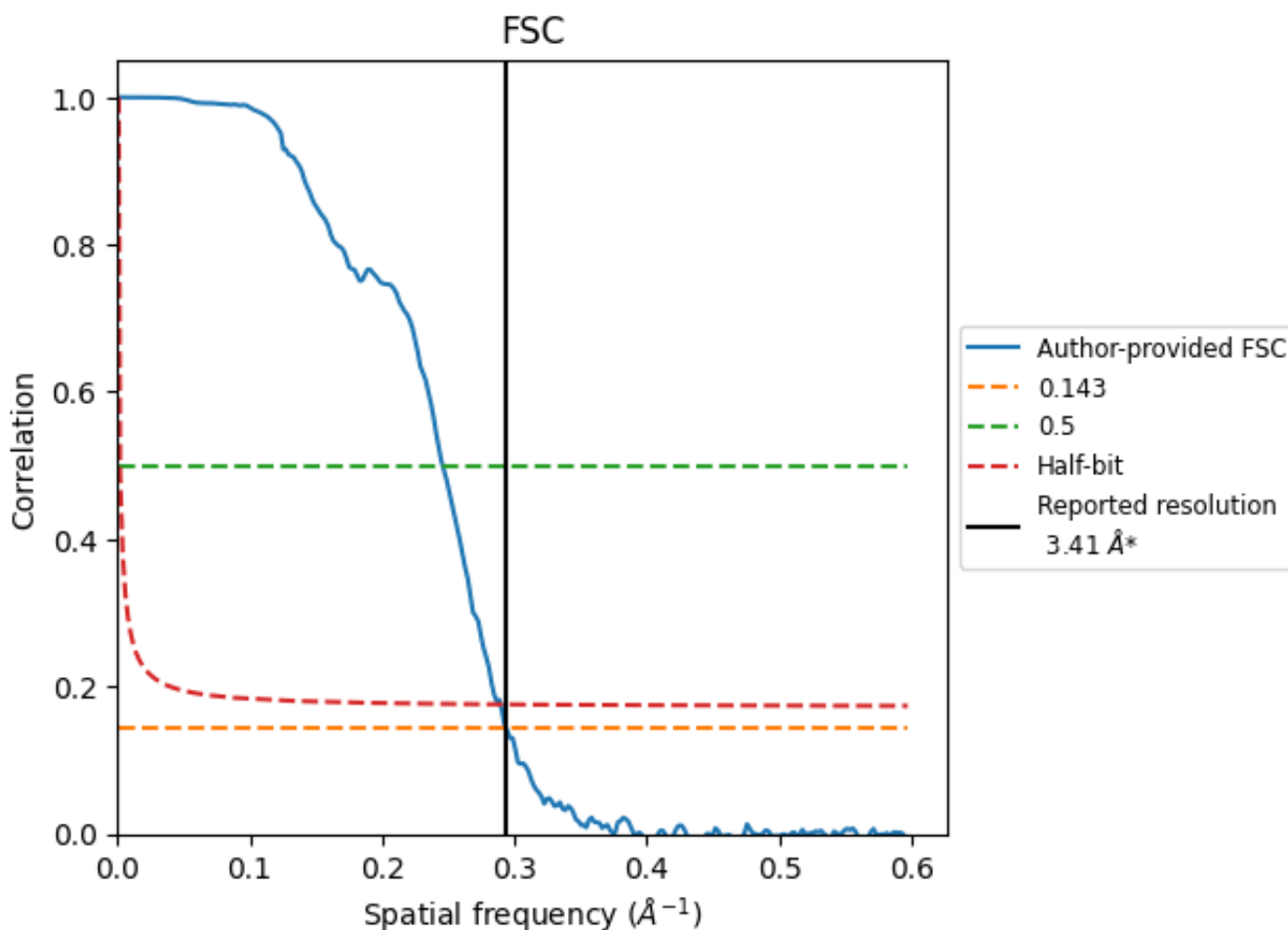


*Reported resolution corresponds to spatial frequency of 0.293\AA^{-1}

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 0.293 Å⁻¹

8.2 Resolution estimates [i](#)

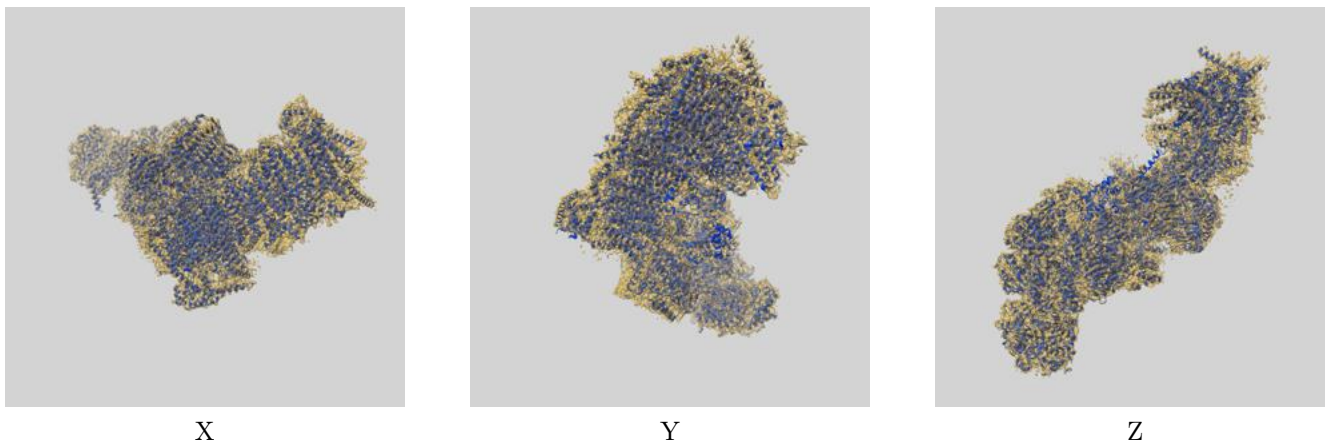
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.41	-	-
Author-provided FSC curve	3.40	4.07	3.45
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

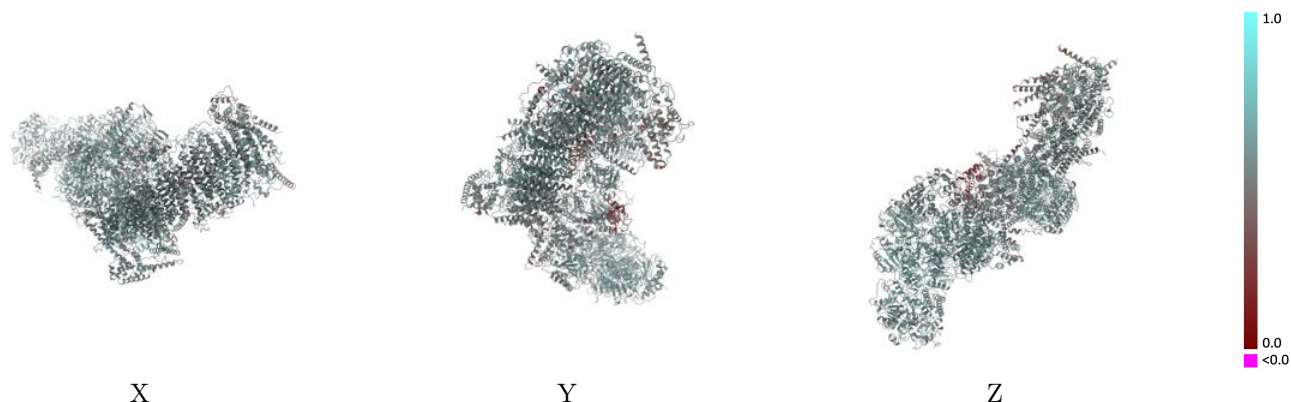
This section contains information regarding the fit between EMDB map EMD-11878 and PDB model 7ARB. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



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

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



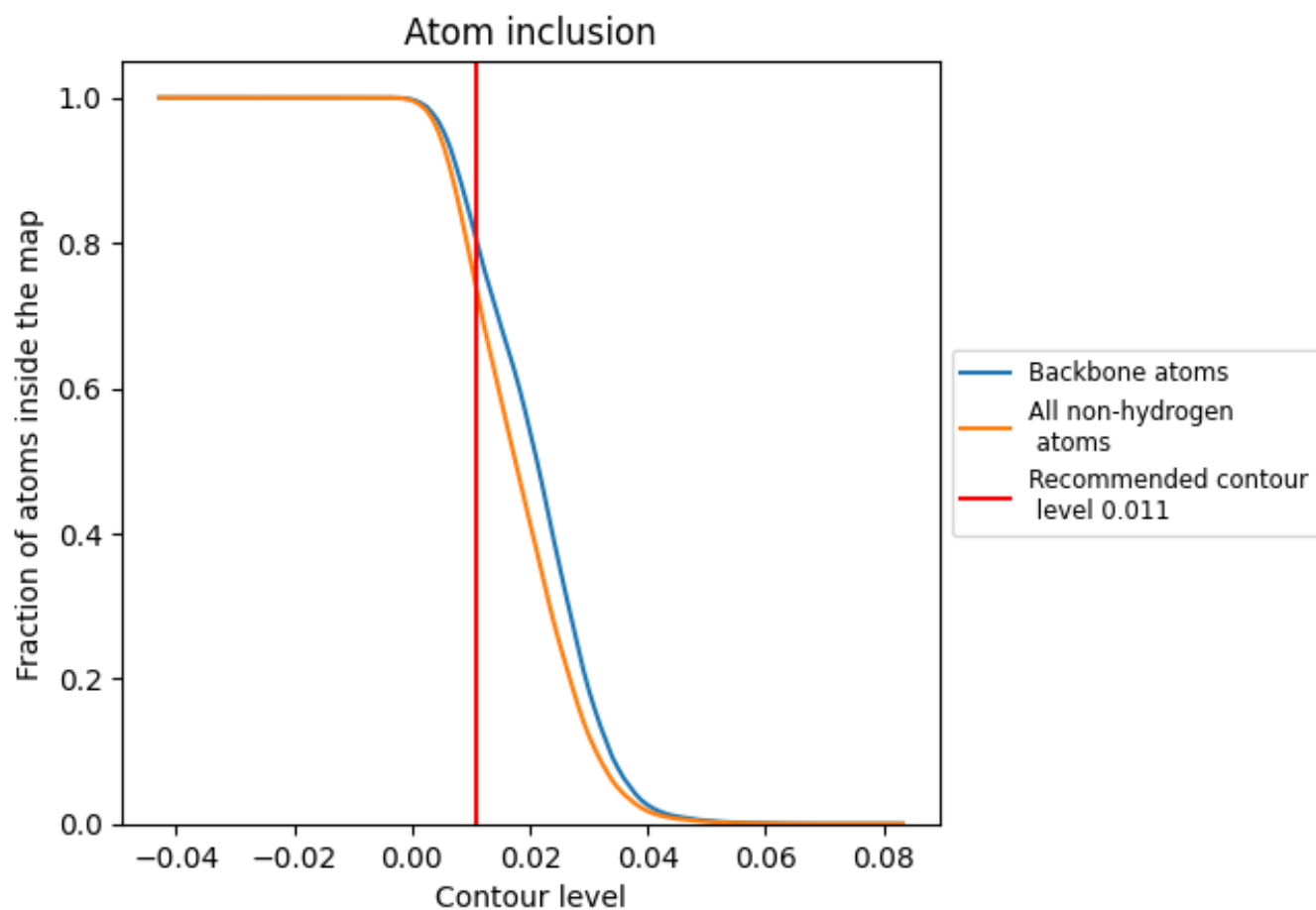
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.011).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 74% 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	 0.7366	 0.5440
A	 0.6966	 0.5420
B	 0.9145	 0.5780
C	 0.8387	 0.5960
D	 0.8459	 0.5850
E	 0.7066	 0.5280
F	 0.7549	 0.5610
G	 0.7964	 0.5810
H	 0.7351	 0.5350
I	 0.8803	 0.5820
J	 0.6906	 0.5410
K	 0.6772	 0.5450
L	 0.7074	 0.5370
M	 0.7454	 0.5480
N	 0.7581	 0.5680
O	 0.4744	 0.5190
P	 0.7479	 0.5180
Q	 0.7549	 0.5930
R	 0.7684	 0.5860
S	 0.7693	 0.5600
T	 0.6218	 0.4570
U	 0.1296	 0.2530
V	 0.7477	 0.5390
W	 0.5240	 0.4890
X	 0.6702	 0.5170
Z	 0.7277	 0.5220
a	 0.7009	 0.5150
b	 0.6598	 0.5300
c	 0.7596	 0.5430
d	 0.7660	 0.5520
e	 0.7929	 0.5590
f	 0.7826	 0.5690
g	 0.7162	 0.5160
i	 0.7257	 0.5190
j	 0.7401	 0.5170



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Chain	Atom inclusion	Q-score
k	 0.7017	 0.5040
l	 0.5850	 0.4970
m	 0.6068	 0.4680
n	 0.6590	 0.4890
o	 0.7434	 0.5130
p	 0.7483	 0.4980
q	 0.4923	 0.4870
r	 0.3810	 0.4860
u	 0.7267	 0.4840
v	 0.6777	 0.5540
x	 0.7898	 0.5640
y	 0.7302	 0.5450
z	 0.7782	 0.5580