



Full wwPDB EM Validation Report ⓘ

Jan 20, 2024 – 07:39 am GMT

PDB ID : 8CA3
EMDB ID : EMD-16516
Title : Cryo-EM structure NDUFS4 knockout complex I from *Mus musculus* heart (Class 2).
Authors : Yin, Z.; Bridges, H.R.; Agip, A.N.A.; Hirst, J.
Deposited on : 2023-01-24
Resolution : 3.20 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:

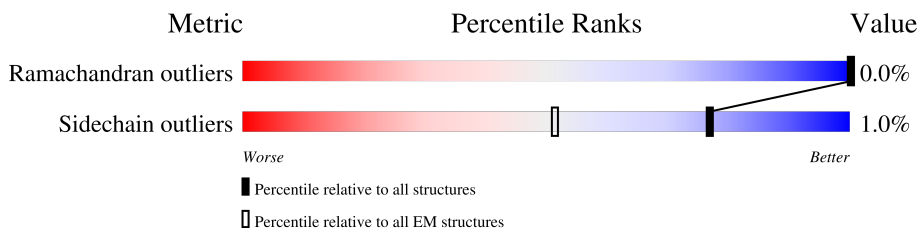
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 3.20 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	115	99%
2	B	224	69% 30%
3	C	263	78% 21%
4	D	463	92% 7%
5	E	245	14% 85% 14%
6	F	464	10% 91% 8%
7	G	727	23% 94% 5%
8	H	318	99%
9	I	212	83% 16%




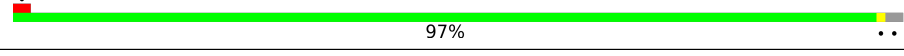
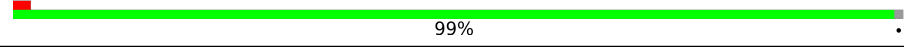

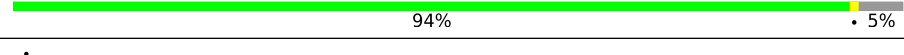

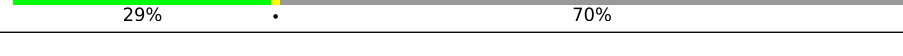
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Mol	Chain	Length	Quality of chain
10	J	172	97%
11	K	98	98%
12	L	607	99%
13	M	459	98%
14	N	345	100%
15	O	355	90%
16	P	377	85%
17	R	116	46%
18	S	99	82%
19	T	156	47%
19	U	156	54%
20	V	116	97%
21	W	131	83%
22	X	172	98%
23	Y	143	96%
24	Z	144	98%
25	a	70	97%
26	b	84	94%
27	c	76	63%
28	d	120	100%
29	e	106	98%
30	f	57	91%
31	g	151	66%
32	h	189	73%
33	i	127	72%

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Mol	Chain	Length	Quality of chain
34	j	105	
35	k	104	
36	l	186	
37	m	129	
38	n	179	
39	o	137	
40	p	176	
41	r	113	
42	s	104	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
46	FMN	F	502	-	X	-	-

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 63712 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	115	933	633	133	160	7	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	156	1247	796	223	214	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	207	1721	1111	296	311	3	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	430	3463	2215	595	629	24	0	0

- 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	210	1639	1043	275	310	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	428	3300	2080	589	609	22	0	0

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	688	5248	3294	910	1003	41	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	318	2540	1706	384	428	22	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	178	1431	898	245	276	12	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	171	1300	874	185	226	15	0	0

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	98	737	477	112	137	11	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	606	4800	3182	746	827	45	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	459	3632	2408	567	617	40	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	344	2696	1791	416	452	37	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	320	2607	1674	431	492	10	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	325	2626	1702	456	461	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	R	55	413	258	74	78	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	S	82	594	374	108	110	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	T	76	611	392	90	124	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	U	86	692	446	102	139	5	0	0

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	V	112	915	596	152	164	3	0	0

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W	109	935	598	175	156	6	0	0

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	X	171	1396	889	250	247	10	0	0

- Molecule 23 is a protein called MCG5603.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Y	140	1037	662	175	192	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Z	141	1167	750	207	202	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	a	68	556	360	99	93	4	0	0

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	b	80	628	414	99	111	4	0	0

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	c	48	398	261	69	67	1	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	d	120	996	651	171	165	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	e	105	877	555	162	152	8	0	0

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	f	53	456	295	82	77	2	0	0

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	g	101	850	549	136	161	4	0	0

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	h	138	1162	762	194	203	3	0	0

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	i	94	787	515	134	135	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	j	62	537	355	88	93	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	k	75	609	404	103	100	2	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	154	1294	834	215	234	11	0	0

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	m	126	1050	676	189	185	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	n	177	1534	981	275	267	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	o	113	979	617	184	170	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	p	168	1424	896	256	264	8	0	0

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	r	61	487	311	87	86	3	0	0

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

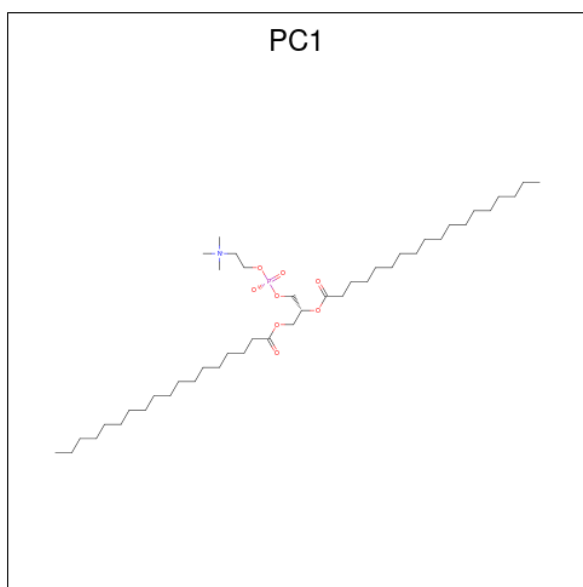
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	s	31	269	174	45	50	0	0

- Molecule 43 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



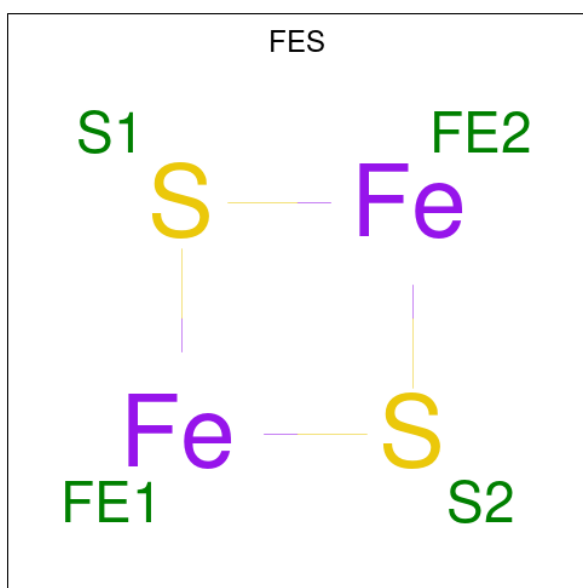
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
43	B	1	8	4	4	0
43	F	1	8	4	4	0
43	G	1	8	4	4	0
43	G	1	8	4	4	0
43	I	1	8	4	4	0
43	I	1	8	4	4	0

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



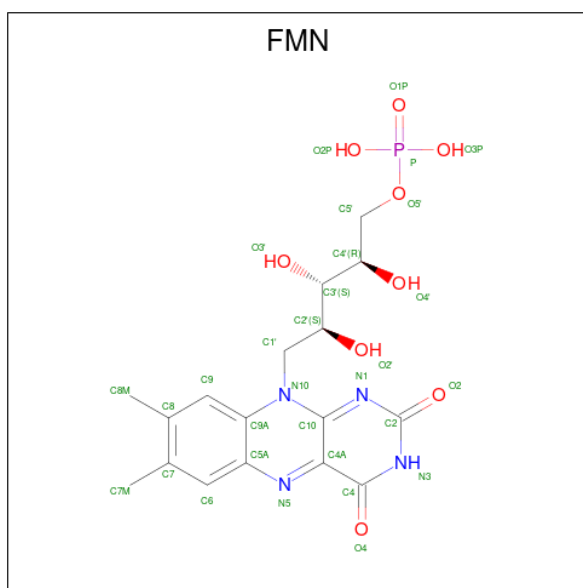
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
44	B	1	41	31	1	8	1	0
44	H	1	42	32	1	8	1	0

- Molecule 45 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



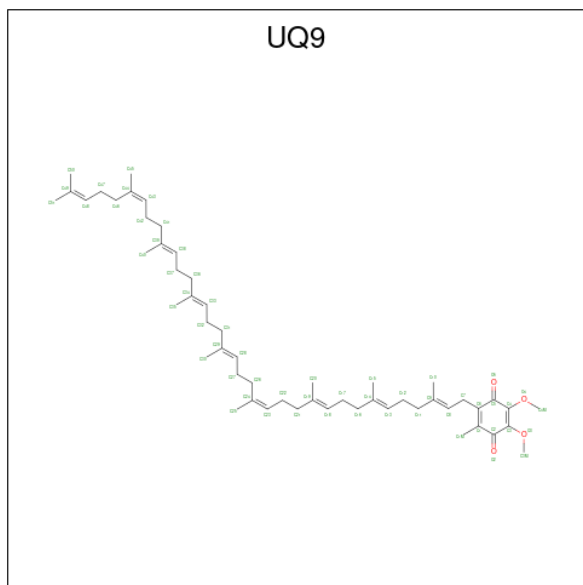
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	E	1	4	2	2	0
45	G	1	4	2	2	0

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



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

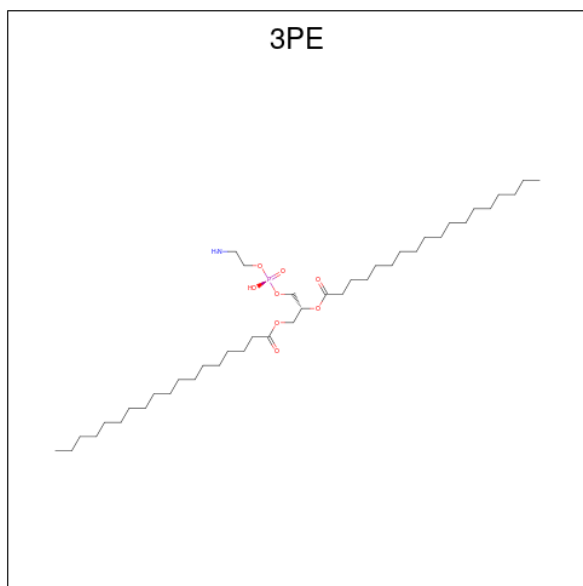
- Molecule 47 is Ubiquinone-9 (three-letter code: UQ9) (formula: $C_{54}H_{82}O_4$).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
47	H	1	45	45	0

- Molecule 48 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE)

(formula: $C_{41}H_{82}NO_8P$).



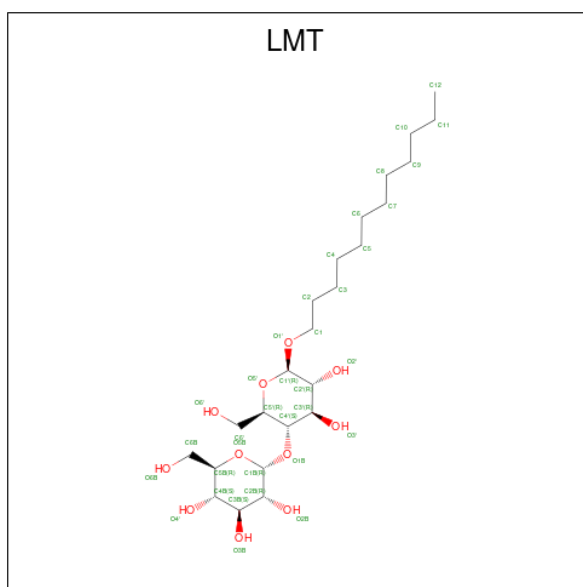
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	H	1	Total 51	41	1	8	1	0
48	J	1	Total 33	23	1	8	1	0
48	L	1	Total 49	39	1	8	1	0
48	L	1	Total 42	32	1	8	1	0
48	Y	1	Total 41	31	1	8	1	0
48	Z	1	Total 44	34	1	8	1	0
48	i	1	Total 42	32	1	8	1	0

- Molecule 49 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



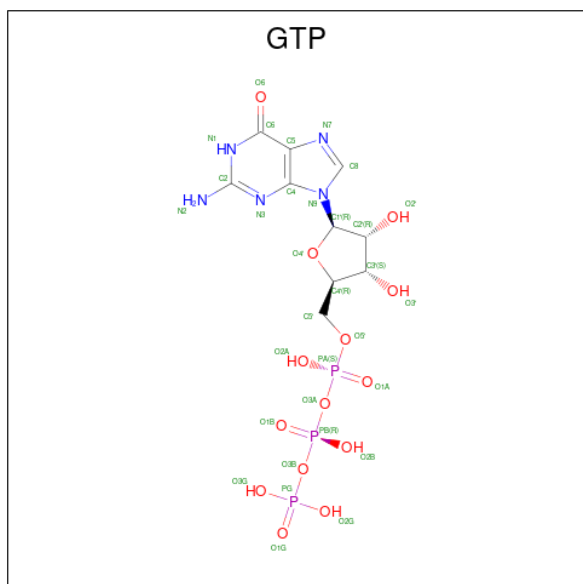
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
49	L	1	74	55	17	2	0
49	M	1	59	41	16	2	0
49	N	1	65	46	17	2	0
49	N	1	63	44	17	2	0
49	d	1	67	48	17	2	0
49	h	1	70	51	17	2	0

- Molecule 50 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



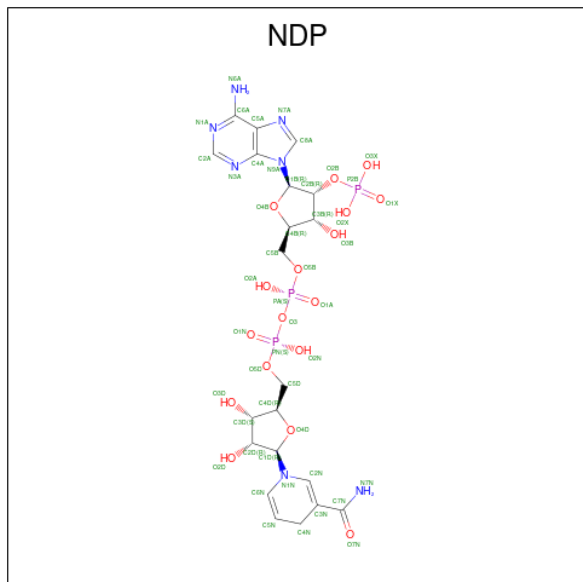
Mol	Chain	Residues	Atoms			AltConf
50	L	1	Total	C	O	0
			35	24	11	
50	L	1	Total	C	O	0
			35	24	11	

- Molecule 51 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
51	O	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

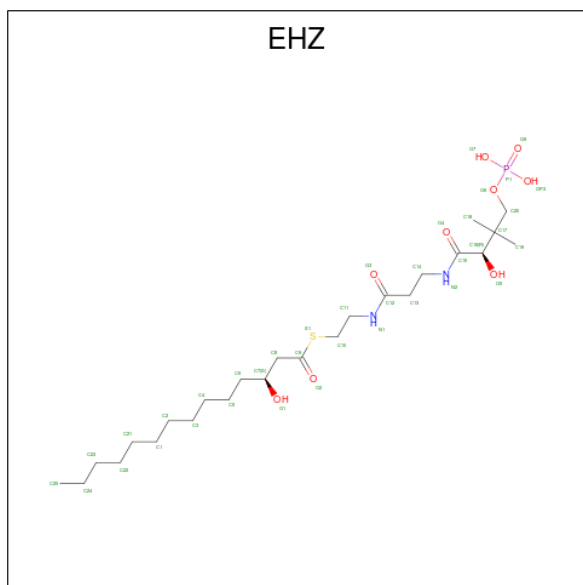


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
52	P	1	48	21	7	17	3	0

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
53	R	1	1	1	0

- Molecule 54 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonoxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).

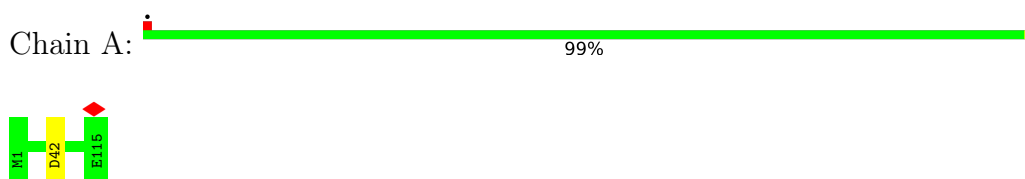


Mol	Chain	Residues	Atoms					AltConf		
			Total	C	N	O	P		S	
54	T	1	Total	37	25	2	8	1	1	0
54	U	1	Total	37	25	2	8	1	1	0

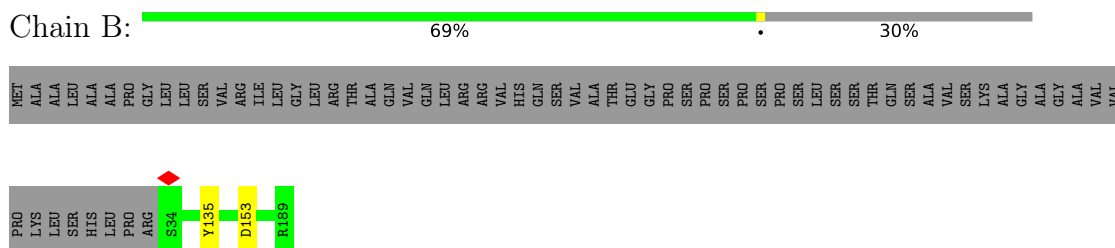
3 Residue-property plots [i](#)

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.

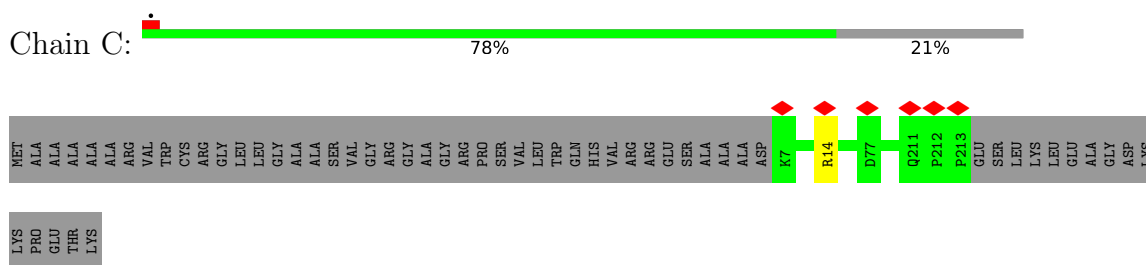
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



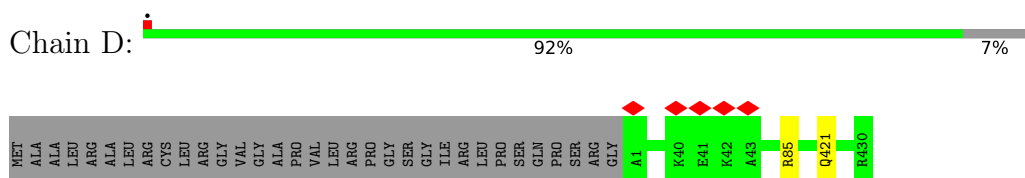
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



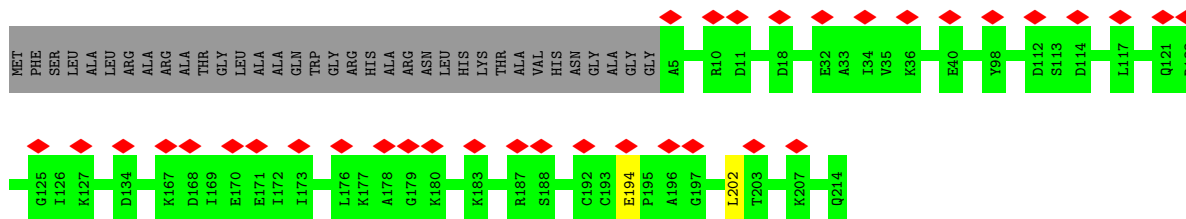
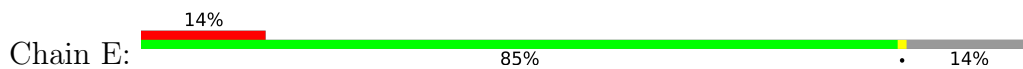
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



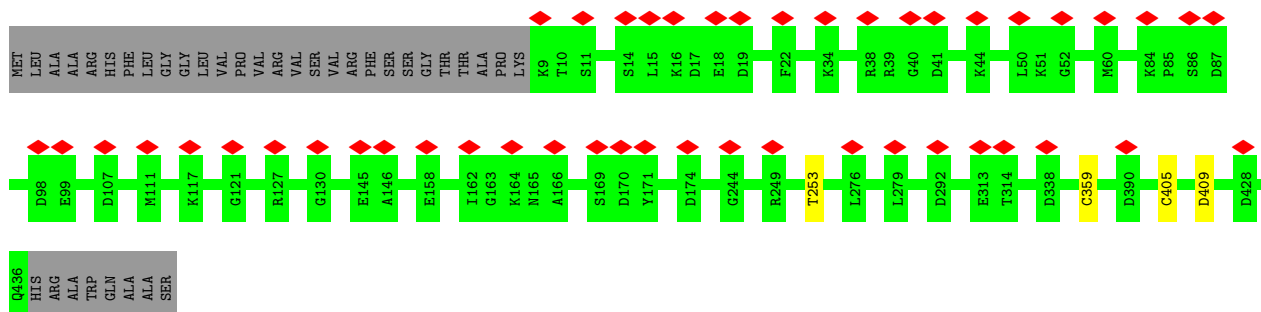
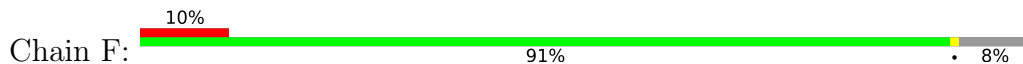
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



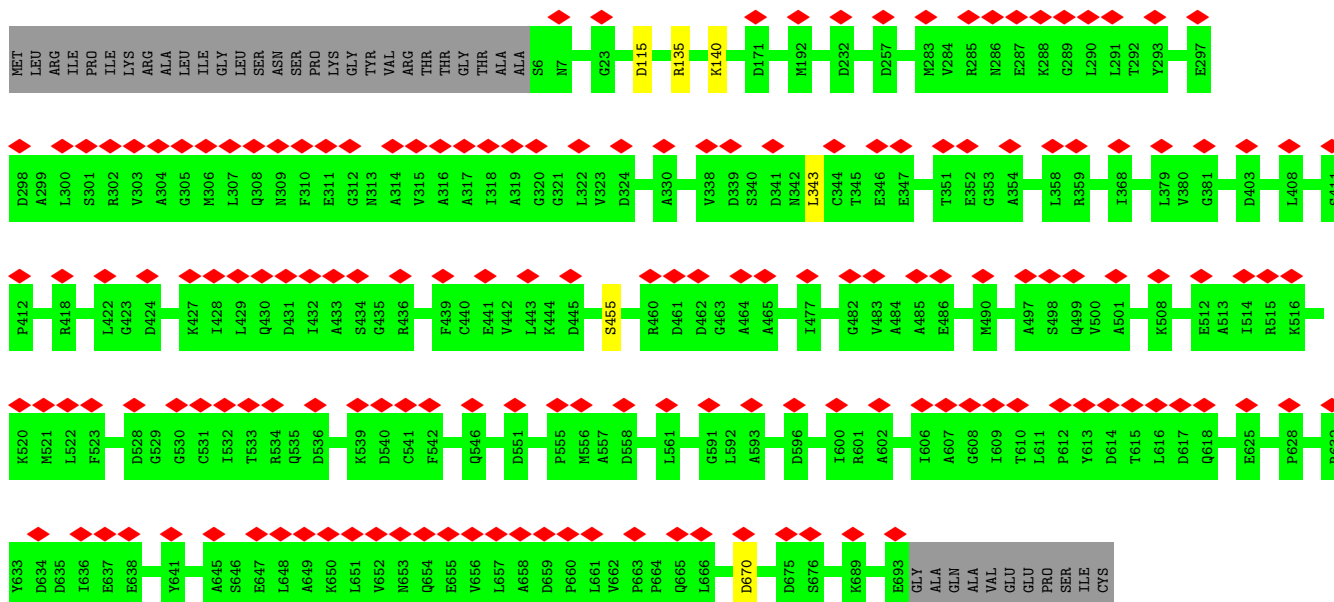
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



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

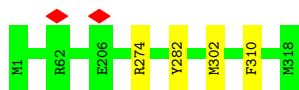


- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

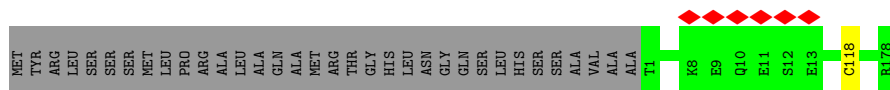
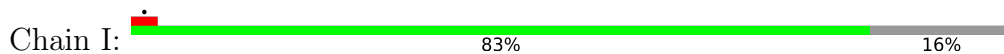


- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

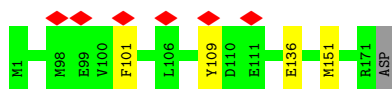




- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



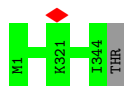
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5




- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

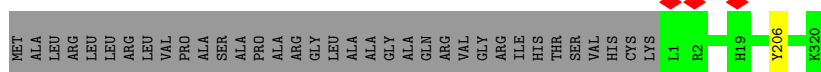


- Molecule 14: NADH-ubiquinone oxidoreductase chain 2




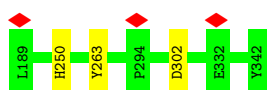
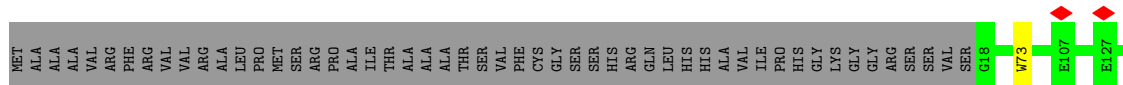
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:  90% 10%



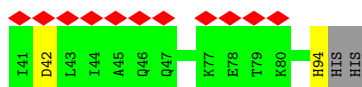
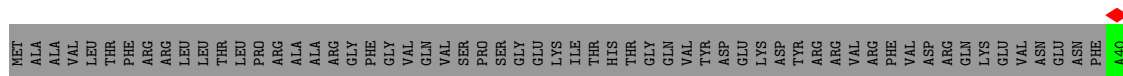
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:  85% 14%




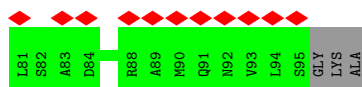
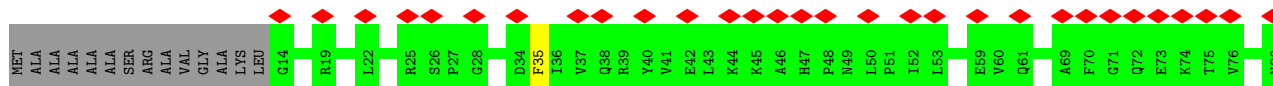
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:  10% 46% 53%



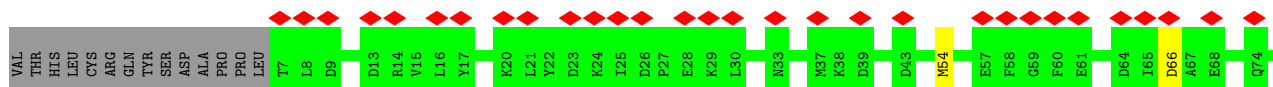
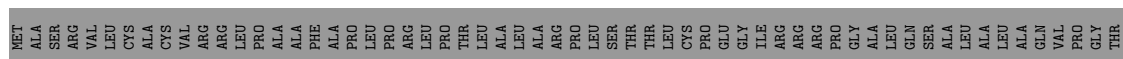
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

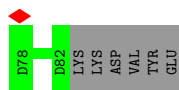
Chain S:  41% 82% 17%



- Molecule 19: Acyl carrier protein, mitochondrial

Chain T:  20% 47% 51%

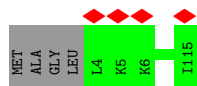




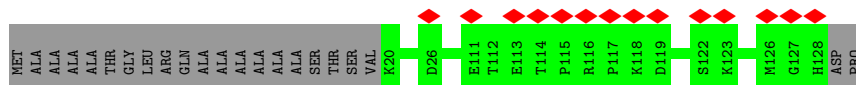
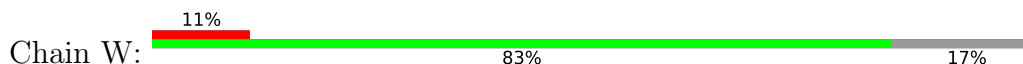
- Molecule 19: Acyl carrier protein, mitochondrial



- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



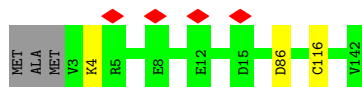
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



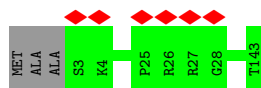
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 23: MCG5603



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



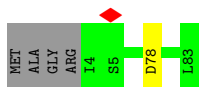
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:  97%



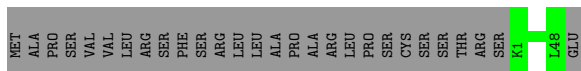
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:  94% 5%



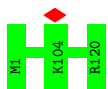
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c:  63% 37%



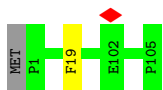
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:  100%

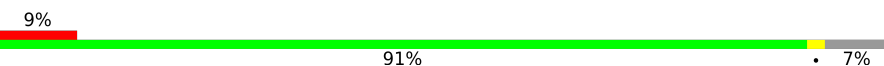


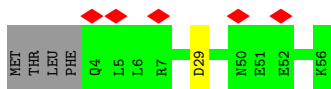
- Molecule 29: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:  98%



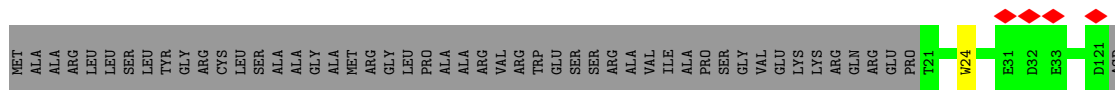
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:  9% 91% 7%

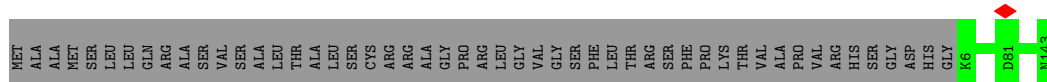


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

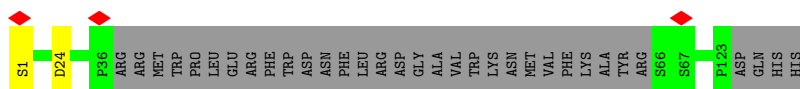
Chain g:  66% 33%



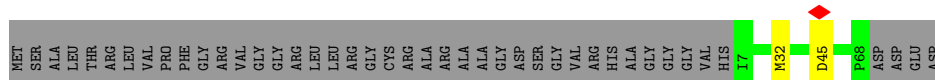
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



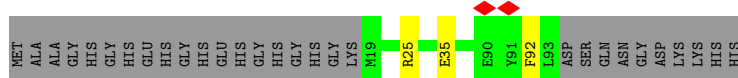
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



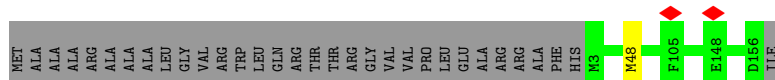
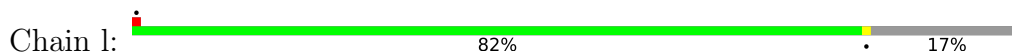
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



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

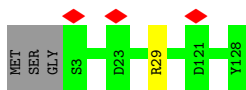


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

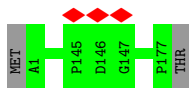


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

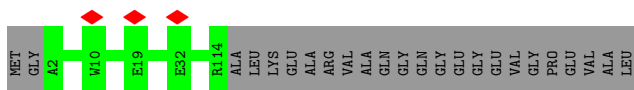
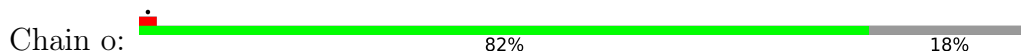




- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



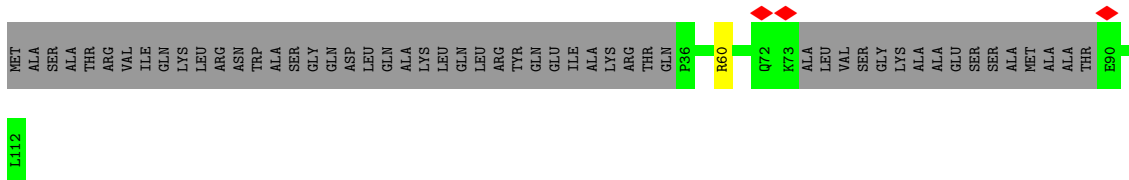
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



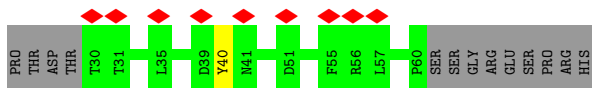
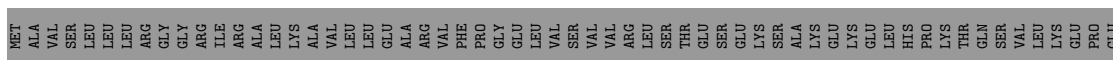
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



- Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 42: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10005	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	13.939	Depositor
Minimum map value	-4.972	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.422	Depositor
Recommended contour level	1.9	Depositor
Map size (Å)	608.4, 608.4, 608.4	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.352, 1.352, 1.352	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, ZN, FMN, 2MR, PC1, UQ9, SAC, FME, GTP, LMT, FES, EHZ, 3PE, CDL, SF4

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	0.27	0/949	0.43	0/1297
2	B	0.33	0/1278	0.55	0/1730
3	C	0.29	0/1771	0.52	0/2412
4	D	0.29	0/3539	0.50	0/4793
5	E	0.26	0/1679	0.48	0/2288
6	F	0.26	0/3374	0.51	0/4557
7	G	0.26	0/5335	0.50	0/7236
8	H	0.29	0/2607	0.45	0/3564
9	I	0.30	0/1461	0.52	0/1974
10	J	0.28	0/1322	0.43	0/1799
11	K	0.26	0/738	0.42	0/1002
12	L	0.27	0/4913	0.43	0/6686
13	M	0.27	0/3709	0.45	0/5052
14	N	0.27	0/2748	0.45	0/3741
15	O	0.29	0/2674	0.46	0/3626
16	P	0.27	0/2697	0.48	0/3658
17	R	0.27	0/420	0.49	0/566
18	S	0.24	0/604	0.49	0/827
19	T	0.25	0/620	0.42	0/836
19	U	0.28	0/704	0.43	0/951
20	V	0.26	0/937	0.40	0/1270
21	W	0.26	0/957	0.51	0/1284
22	X	0.27	0/1434	0.47	0/1937
23	Y	0.26	0/1061	0.46	0/1439
24	Z	0.29	0/1198	0.53	0/1616
25	a	0.29	0/569	0.51	0/766
26	b	0.32	0/651	0.42	0/895
27	c	0.28	0/409	0.45	0/555
28	d	0.30	0/1028	0.47	0/1387
29	e	0.27	0/900	0.49	0/1199
30	f	0.25	0/468	0.51	0/630
31	g	0.30	0/878	0.47	0/1196

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	h	0.29	0/1197	0.47	0/1621
33	i	0.27	0/804	0.50	0/1094
34	j	0.26	0/561	0.43	0/768
35	k	0.27	0/629	0.47	0/851
36	l	0.29	0/1348	0.47	0/1840
37	m	0.29	0/1079	0.54	0/1463
38	n	0.29	0/1589	0.50	0/2152
39	o	0.26	0/1004	0.50	0/1348
40	p	0.28	0/1457	0.50	0/1969
41	r	0.27	0/502	0.46	0/680
42	s	0.26	0/277	0.43	0/377
All	All	0.28	0/64079	0.48	0/86932

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

Mol	Chain	#Chirality outliers	#Planarity outliers
37	m	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
37	m	29	ARG	Sidechain

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	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
2	B	154/224 (69%)	147 (96%)	7 (4%)	0	100	100
3	C	205/263 (78%)	196 (96%)	9 (4%)	0	100	100
4	D	427/463 (92%)	407 (95%)	20 (5%)	0	100	100
5	E	208/245 (85%)	193 (93%)	15 (7%)	0	100	100
6	F	426/464 (92%)	391 (92%)	35 (8%)	0	100	100
7	G	686/727 (94%)	631 (92%)	55 (8%)	0	100	100
8	H	316/318 (99%)	300 (95%)	16 (5%)	0	100	100
9	I	176/212 (83%)	169 (96%)	7 (4%)	0	100	100
10	J	169/172 (98%)	155 (92%)	14 (8%)	0	100	100
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	604/607 (100%)	572 (95%)	30 (5%)	2 (0%)	41	74
13	M	457/459 (100%)	448 (98%)	9 (2%)	0	100	100
14	N	342/345 (99%)	330 (96%)	12 (4%)	0	100	100
15	O	318/355 (90%)	308 (97%)	10 (3%)	0	100	100
16	P	323/377 (86%)	301 (93%)	21 (6%)	1 (0%)	41	74
17	R	53/116 (46%)	52 (98%)	1 (2%)	0	100	100
18	S	80/99 (81%)	75 (94%)	5 (6%)	0	100	100
19	T	74/156 (47%)	70 (95%)	4 (5%)	0	100	100
19	U	84/156 (54%)	81 (96%)	3 (4%)	0	100	100
20	V	110/116 (95%)	108 (98%)	2 (2%)	0	100	100
21	W	107/131 (82%)	101 (94%)	6 (6%)	0	100	100
22	X	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
23	Y	138/143 (96%)	128 (93%)	10 (7%)	0	100	100
24	Z	139/144 (96%)	134 (96%)	5 (4%)	0	100	100
25	a	66/70 (94%)	65 (98%)	1 (2%)	0	100	100
26	b	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
27	c	46/76 (60%)	44 (96%)	2 (4%)	0	100	100
28	d	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
29	e	103/106 (97%)	102 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	f	51/57 (90%)	47 (92%)	4 (8%)	0	100	100
31	g	99/151 (66%)	96 (97%)	3 (3%)	0	100	100
32	h	136/189 (72%)	132 (97%)	4 (3%)	0	100	100
33	i	90/127 (71%)	84 (93%)	6 (7%)	0	100	100
34	j	60/105 (57%)	60 (100%)	0	0	100	100
35	k	73/104 (70%)	72 (99%)	1 (1%)	0	100	100
36	l	152/186 (82%)	147 (97%)	5 (3%)	0	100	100
37	m	124/129 (96%)	119 (96%)	5 (4%)	0	100	100
38	n	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
39	o	111/137 (81%)	107 (96%)	4 (4%)	0	100	100
40	p	166/176 (94%)	158 (95%)	8 (5%)	0	100	100
41	r	57/113 (50%)	55 (96%)	2 (4%)	0	100	100
42	s	29/104 (28%)	28 (97%)	1 (3%)	0	100	100
All	All	7708/8890 (87%)	7332 (95%)	373 (5%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	P	250	HIS
12	L	249	SER
12	L	562	ILE

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	103/103 (100%)	102 (99%)	1 (1%)	76	90
2	B	132/185 (71%)	130 (98%)	2 (2%)	65	85
3	C	189/227 (83%)	188 (100%)	1 (0%)	88	95
4	D	370/394 (94%)	369 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	183/205 (89%)	181 (99%)	2 (1%)	73	88
6	F	343/370 (93%)	339 (99%)	4 (1%)	71	88
7	G	567/610 (93%)	561 (99%)	6 (1%)	73	88
8	H	279/279 (100%)	275 (99%)	4 (1%)	67	86
9	I	152/178 (85%)	151 (99%)	1 (1%)	84	94
10	J	136/137 (99%)	132 (97%)	4 (3%)	42	74
11	K	87/87 (100%)	86 (99%)	1 (1%)	73	88
12	L	548/549 (100%)	546 (100%)	2 (0%)	91	95
13	M	414/414 (100%)	406 (98%)	8 (2%)	57	81
14	N	306/307 (100%)	306 (100%)	0	100	100
15	O	284/309 (92%)	283 (100%)	1 (0%)	91	95
16	P	286/325 (88%)	283 (99%)	3 (1%)	76	90
17	R	43/96 (45%)	41 (95%)	2 (5%)	26	62
18	S	56/80 (70%)	55 (98%)	1 (2%)	59	82
19	T	70/135 (52%)	68 (97%)	2 (3%)	42	74
19	U	79/135 (58%)	77 (98%)	2 (2%)	47	77
20	V	100/102 (98%)	100 (100%)	0	100	100
21	W	103/114 (90%)	103 (100%)	0	100	100
22	X	153/154 (99%)	151 (99%)	2 (1%)	69	87
23	Y	105/107 (98%)	102 (97%)	3 (3%)	42	74
24	Z	122/123 (99%)	122 (100%)	0	100	100
25	a	58/60 (97%)	58 (100%)	0	100	100
26	b	71/73 (97%)	70 (99%)	1 (1%)	67	86
27	c	42/67 (63%)	42 (100%)	0	100	100
28	d	107/107 (100%)	107 (100%)	0	100	100
29	e	93/94 (99%)	92 (99%)	1 (1%)	73	88
30	f	49/53 (92%)	48 (98%)	1 (2%)	55	80
31	g	92/129 (71%)	91 (99%)	1 (1%)	73	88
32	h	123/162 (76%)	123 (100%)	0	100	100
33	i	88/118 (75%)	87 (99%)	1 (1%)	73	88
34	j	58/87 (67%)	56 (97%)	2 (3%)	37	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	k	58/78 (74%)	55 (95%)	3 (5%)	23	59
36	l	139/161 (86%)	138 (99%)	1 (1%)	84	94
37	m	112/114 (98%)	112 (100%)	0	100	100
38	n	162/164 (99%)	162 (100%)	0	100	100
39	o	106/121 (88%)	106 (100%)	0	100	100
40	p	153/158 (97%)	151 (99%)	2 (1%)	69	87
41	r	57/96 (59%)	56 (98%)	1 (2%)	59	82
42	s	31/95 (33%)	30 (97%)	1 (3%)	39	71
All	All	6809/7662 (89%)	6741 (99%)	68 (1%)	77	90

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
2	B	135	TYR
2	B	153	ASP
3	C	14	ARG
4	D	421	GLN
5	E	194	GLU
5	E	202	LEU
6	F	253	THR
6	F	359	CYS
6	F	405	CYS
6	F	409	ASP
7	G	115	ASP
7	G	135	ARG
7	G	140	LYS
7	G	343	LEU
7	G	455	SER
7	G	670	ASP
8	H	274	ARG
8	H	282	TYR
8	H	302	MET
8	H	310	PHE
9	I	118	CYS
10	J	101	PHE
10	J	109	TYR
10	J	136	GLU
10	J	151	MET

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Mol	Chain	Res	Type
11	K	5	PHE
12	L	262	ARG
12	L	297	ASP
13	M	122	PHE
13	M	168	GLN
13	M	201	MET
13	M	269	MET
13	M	350	MET
13	M	375	LEU
13	M	406	TYR
13	M	410	MET
15	O	206	TYR
16	P	73	TRP
16	P	263	TYR
16	P	302	ASP
17	R	42	ASP
17	R	94	HIS
18	S	35	PHE
19	T	54	MET
19	T	66	ASP
19	U	12	LYS
19	U	87	TYR
22	X	47	TRP
22	X	87	CYS
23	Y	4	LYS
23	Y	86	ASP
23	Y	116	CYS
26	b	78	ASP
29	e	19	PHE
30	f	29	ASP
31	g	24	TRP
33	i	24	ASP
34	j	32	MET
34	j	45	ASP
35	k	25	ARG
35	k	35	GLU
35	k	92	PHE
36	l	48	MET
40	p	170	ARG
40	p	171	GLN
41	r	60	ARG
42	s	40	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
6	F	148	ASN
7	G	308	GLN
7	G	475	GLN
7	G	665	GLN
8	H	138	GLN
8	H	235	ASN
11	K	7	ASN
11	K	25	HIS
12	L	248	HIS
13	M	51	ASN
13	M	92	GLN
13	M	304	GLN
13	M	427	GLN
14	N	63	GLN
15	O	141	GLN
15	O	288	GLN
16	P	67	GLN
16	P	240	HIS
17	R	94	HIS
22	X	72	GLN
26	b	82	ASN
31	g	84	GLN
31	g	101	ASN
36	l	71	ASN
40	p	171	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](#)

9 non-standard protein/DNA/RNA residues are modelled in this entry.

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
4	2MR	D	85	4	10,12,13	1.83	1 (10%)	5,13,15	2.73	1 (20%)
1	FME	A	1	1	8,9,10	0.94	0	7,9,11	0.79	0
11	FME	K	1	11	8,9,10	0.96	0	7,9,11	1.25	1 (14%)
8	FME	H	1	8	8,9,10	0.91	0	7,9,11	1.23	0
12	FME	L	1	12	8,9,10	0.94	0	7,9,11	0.87	0
14	FME	N	1	14	8,9,10	0.92	0	7,9,11	0.89	0
10	FME	J	1	10	8,9,10	0.95	0	7,9,11	0.94	0
33	SAC	i	1	33	7,8,9	1.01	0	8,9,11	1.55	1 (12%)
13	FME	M	1	13	8,9,10	0.94	0	7,9,11	0.70	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	2MR	D	85	4	-	5/10/13/15	-
1	FME	A	1	1	-	2/7/9/11	-
11	FME	K	1	11	-	2/7/9/11	-
8	FME	H	1	8	-	4/7/9/11	-
12	FME	L	1	12	-	1/7/9/11	-
14	FME	N	1	14	-	1/7/9/11	-
10	FME	J	1	10	-	5/7/9/11	-
33	SAC	i	1	33	-	6/7/8/10	-
13	FME	M	1	13	-	0/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NE	5.13	1.45	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	85	2MR	NE-CZ-NH2	5.77	124.77	119.48
33	i	1	SAC	C2A-C1A-N	2.66	120.60	116.10
11	K	1	FME	C-CA-N	2.64	114.49	109.73

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	85	2MR	N-CA-CB-CG
4	D	85	2MR	C-CA-CB-CG
8	H	1	FME	O1-CN-N-CA
8	H	1	FME	CB-CA-N-CN
10	J	1	FME	O1-CN-N-CA
10	J	1	FME	C-CA-CB-CG
10	J	1	FME	O-C-CA-CB
11	K	1	FME	N-CA-CB-CG
11	K	1	FME	C-CA-CB-CG
33	i	1	SAC	CB-CA-N-C1A
33	i	1	SAC	N-CA-CB-OG
33	i	1	SAC	C-CA-CB-OG
4	D	85	2MR	NE-CD-CG-CB
33	i	1	SAC	C2A-C1A-N-CA
33	i	1	SAC	OAC-C1A-N-CA
4	D	85	2MR	CG-CD-NE-CZ
12	L	1	FME	N-CA-CB-CG
1	A	1	FME	CB-CG-SD-CE
8	H	1	FME	CB-CG-SD-CE
4	D	85	2MR	CA-CB-CG-CD
33	i	1	SAC	C-CA-N-C1A
10	J	1	FME	CB-CA-N-CN
1	A	1	FME	N-CA-CB-CG
14	N	1	FME	CA-CB-CG-SD
8	H	1	FME	C-CA-CB-CG
10	J	1	FME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 1 is monoatomic - leaving 31 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
44	PC1	B	202	-	40,40,53	1.42	6 (15%)	46,48,61	1.07	2 (4%)
48	3PE	Y	401	-	40,40,50	0.95	4 (10%)	43,45,55	1.03	2 (4%)
43	SF4	F	501	6	0,12,12	-	-	-	-	-
48	3PE	i	201	-	41,41,50	0.95	4 (9%)	44,46,55	1.07	2 (4%)
49	CDL	N	402	-	62,62,99	1.12	7 (11%)	68,74,111	1.14	4 (5%)
43	SF4	G	802	7	0,12,12	-	-	-	-	-
43	SF4	G	801	7	0,12,12	-	-	-	-	-
50	LMT	L	704	-	36,36,36	1.15	5 (13%)	47,47,47	1.02	3 (6%)
48	3PE	Z	401	-	43,43,50	0.92	4 (9%)	46,48,55	1.11	2 (4%)
47	UQ9	H	401	-	44,44,58	0.81	0	52,52,73	1.99	16 (30%)
45	FES	E	301	5	0,4,4	-	-	-	-	-
54	EHZ	U	201	19	29,36,37	1.89	5 (17%)	35,44,47	1.68	7 (20%)
49	CDL	N	401	-	64,64,99	1.11	7 (10%)	70,76,111	1.15	4 (5%)
48	3PE	L	703	-	41,41,50	0.95	4 (9%)	44,46,55	1.08	2 (4%)
43	SF4	I	202	9	0,12,12	-	-	-	-	-
54	EHZ	T	201	19	29,36,37	1.87	5 (17%)	35,44,47	1.45	3 (8%)
49	CDL	M	501	-	58,58,99	1.07	4 (6%)	63,69,111	1.06	3 (4%)
49	CDL	L	702	-	73,73,99	1.04	7 (9%)	79,85,111	1.13	4 (5%)
50	LMT	L	705	-	36,36,36	1.17	6 (16%)	47,47,47	0.95	1 (2%)
43	SF4	I	201	9	0,12,12	-	-	-	-	-
48	3PE	L	701	-	48,48,50	0.88	2 (4%)	51,53,55	1.03	2 (3%)
48	3PE	J	201	-	32,32,50	1.05	4 (12%)	35,37,55	1.13	2 (5%)
52	NDP	P	501	-	45,52,52	2.22	5 (11%)	53,80,80	1.68	10 (18%)
43	SF4	B	201	2	0,12,12	-	-	-	-	-
49	CDL	h	201	-	69,69,99	1.06	7 (10%)	75,81,111	1.17	5 (6%)
44	PC1	H	402	-	41,41,53	1.42	6 (14%)	47,49,61	1.11	3 (6%)
46	FMN	F	502	-	33,33,33	4.64	19 (57%)	48,50,50	4.81	22 (45%)
45	FES	G	803	7	0,4,4	-	-	-	-	-
49	CDL	d	201	-	66,66,99	1.09	7 (10%)	72,78,111	1.17	4 (5%)
51	GTP	O	401	-	26,33,34	2.65	10 (38%)	32,52,54	1.61	9 (28%)
48	3PE	H	403	-	50,50,50	0.86	4 (8%)	53,55,55	1.08	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	PC1	B	202	-	-	19/44/44/57	-
48	3PE	Y	401	-	-	14/44/44/54	-
43	SF4	F	501	6	-	-	0/6/5/5
48	3PE	i	201	-	-	16/45/45/54	-
49	CDL	N	402	-	-	34/73/73/110	-
43	SF4	G	802	7	-	-	0/6/5/5
43	SF4	G	801	7	-	-	0/6/5/5
50	LMT	L	704	-	-	13/21/61/61	0/2/2/2
48	3PE	Z	401	-	-	17/47/47/54	-
47	UQ9	H	401	-	-	15/50/50/81	-
45	FES	E	301	5	-	-	0/1/1/1
54	EHZ	U	201	19	-	17/42/44/45	-
49	CDL	N	401	-	-	41/75/75/110	-
48	3PE	L	703	-	-	18/45/45/54	-
54	EHZ	T	201	19	-	13/42/44/45	-
43	SF4	I	202	9	-	-	0/6/5/5
49	CDL	M	501	-	-	42/67/67/110	-
49	CDL	L	702	-	-	32/84/84/110	-
50	LMT	L	705	-	-	10/21/61/61	0/2/2/2
43	SF4	I	201	9	-	-	0/6/5/5
48	3PE	L	701	-	-	16/52/52/54	-
48	3PE	J	201	-	-	10/36/36/54	-
52	NDP	P	501	-	-	12/30/77/77	0/5/5/5
43	SF4	B	201	2	-	-	0/6/5/5
49	CDL	h	201	-	-	41/80/80/110	-
44	PC1	H	402	-	-	17/45/45/57	-
46	FMN	F	502	-	-	6/18/18/18	0/3/3/3
49	CDL	d	201	-	-	31/77/77/110	-
45	FES	G	803	7	-	-	0/1/1/1
51	GTP	O	401	-	-	4/18/34/38	0/3/3/3
48	3PE	H	403	-	-	22/54/54/54	-

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	P	501	NDP	P2B-O2B	12.31	1.82	1.59
46	F	502	FMN	C6-C5A	11.57	1.58	1.40
46	F	502	FMN	C9A-C5A	10.28	1.58	1.41
46	F	502	FMN	C9-C8	-9.89	1.25	1.39
46	F	502	FMN	O2-C2	8.65	1.40	1.24
46	F	502	FMN	O4-C4	8.47	1.39	1.23
51	O	401	GTP	O6-C6	8.24	1.40	1.23
46	F	502	FMN	C8-C7	-6.85	1.23	1.40
54	U	201	EHZ	C15-N2	6.16	1.47	1.33
46	F	502	FMN	C4A-C4	6.13	1.67	1.44
54	T	201	EHZ	C15-N2	5.91	1.46	1.33
54	T	201	EHZ	C12-N1	5.81	1.46	1.33
54	U	201	EHZ	C12-N1	5.81	1.46	1.33
46	F	502	FMN	C2-N3	-5.43	1.26	1.39
46	F	502	FMN	C4A-N5	4.83	1.40	1.30
51	O	401	GTP	C2-N2	4.67	1.45	1.34
51	O	401	GTP	C2-N1	4.43	1.48	1.37
51	O	401	GTP	C2-N3	4.03	1.43	1.33
52	P	501	NDP	PN-O5D	3.88	1.75	1.59
44	B	202	PC1	O31-C31	3.75	1.44	1.33
44	H	402	PC1	O31-C31	3.70	1.44	1.33
44	H	402	PC1	O21-C21	3.49	1.44	1.34
44	B	202	PC1	O21-C21	3.46	1.44	1.34
46	F	502	FMN	C8M-C8	3.39	1.57	1.51
46	F	502	FMN	C4A-C10	3.35	1.54	1.44
52	P	501	NDP	O2B-C2B	-3.03	1.33	1.44
46	F	502	FMN	C9A-N10	2.98	1.46	1.41
50	L	705	LMT	O3'-C3'	-2.82	1.36	1.43
54	U	201	EHZ	C9-S1	2.79	1.82	1.76
54	T	201	EHZ	C9-S1	2.75	1.82	1.76
49	L	702	CDL	OB8-CB7	2.74	1.41	1.33
48	L	701	3PE	O21-C2	-2.73	1.39	1.46
49	d	201	CDL	OB8-CB7	2.73	1.41	1.33
50	L	704	LMT	O3'-C3'	-2.73	1.36	1.43
49	h	201	CDL	OA6-CA4	-2.71	1.39	1.46
49	N	402	CDL	OB8-CB7	2.67	1.41	1.33
51	O	401	GTP	C5-C6	-2.65	1.42	1.47
49	M	501	CDL	OB8-CB7	2.65	1.41	1.33
49	h	201	CDL	OB8-CB7	2.64	1.41	1.33
49	N	401	CDL	OB8-CB7	2.64	1.41	1.33
51	O	401	GTP	O4'-C1'	2.61	1.48	1.42
44	B	202	PC1	O21-C2	-2.59	1.40	1.46
48	H	403	3PE	O21-C2	-2.59	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	N	401	CDL	OA6-CA4	-2.57	1.40	1.46
49	M	501	CDL	OB6-CB5	2.57	1.41	1.34
46	F	502	FMN	C5A-N5	2.56	1.44	1.39
50	L	705	LMT	O2'-C2'	-2.56	1.36	1.43
49	L	702	CDL	OB6-CB4	-2.53	1.40	1.46
49	d	201	CDL	OB6-CB5	2.51	1.41	1.34
49	M	501	CDL	OA8-CA7	2.50	1.40	1.33
49	N	402	CDL	OA8-CA7	2.49	1.40	1.33
49	N	402	CDL	OB6-CB5	2.49	1.41	1.34
48	i	201	3PE	O21-C2	-2.49	1.40	1.46
48	J	201	3PE	O21-C2	-2.49	1.40	1.46
49	h	201	CDL	OB6-CB5	2.48	1.41	1.34
49	N	401	CDL	OA8-CA7	2.48	1.40	1.33
48	L	701	3PE	O31-C31	2.48	1.40	1.33
46	F	502	FMN	P-O2P	-2.47	1.45	1.54
51	O	401	GTP	C1'-N9	-2.47	1.42	1.49
49	d	201	CDL	OA6-CA4	-2.47	1.40	1.46
48	Y	401	3PE	O21-C2	-2.46	1.40	1.46
48	L	703	3PE	O21-C2	-2.46	1.40	1.46
44	H	402	PC1	O21-C2	-2.45	1.40	1.46
46	F	502	FMN	C10-N1	2.45	1.38	1.33
49	N	402	CDL	OB6-CB4	-2.44	1.40	1.46
48	Z	401	3PE	O31-C31	2.43	1.40	1.33
49	N	401	CDL	OB6-CB5	2.43	1.41	1.34
50	L	704	LMT	O2'-C2'	-2.42	1.37	1.43
49	N	401	CDL	OB6-CB4	-2.42	1.40	1.46
49	h	201	CDL	OA8-CA7	2.42	1.40	1.33
46	F	502	FMN	C1'-C2'	2.40	1.56	1.52
48	L	703	3PE	O31-C31	2.39	1.40	1.33
46	F	502	FMN	P-O3P	-2.39	1.45	1.54
54	U	201	EHZ	O4-C15	-2.39	1.18	1.23
54	T	201	EHZ	O4-C15	-2.39	1.18	1.23
51	O	401	GTP	C2'-C3'	-2.37	1.46	1.52
50	L	704	LMT	O3B-C3B	-2.36	1.37	1.43
49	L	702	CDL	OB6-CB5	2.36	1.41	1.34
49	d	201	CDL	OA8-CA7	2.36	1.40	1.33
48	H	403	3PE	O31-C3	-2.36	1.39	1.45
48	J	201	3PE	O31-C31	2.35	1.40	1.33
48	i	201	3PE	O31-C31	2.35	1.40	1.33
48	Y	401	3PE	O31-C31	2.34	1.40	1.33
49	h	201	CDL	OB6-CB4	-2.34	1.40	1.46
49	L	702	CDL	OA8-CA7	2.33	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	L	704	LMT	O2B-C2B	-2.33	1.37	1.43
49	N	402	CDL	OA6-CA4	-2.32	1.40	1.46
49	d	201	CDL	OB6-CB4	-2.32	1.40	1.46
50	L	705	LMT	O3B-C3B	-2.32	1.37	1.43
49	d	201	CDL	OA8-CA6	-2.31	1.39	1.45
49	L	702	CDL	OA6-CA4	-2.28	1.40	1.46
44	B	202	PC1	C22-C21	2.27	1.57	1.50
49	L	702	CDL	OA8-CA6	-2.27	1.40	1.45
44	H	402	PC1	P-O11	2.26	1.68	1.59
50	L	705	LMT	O2B-C2B	-2.23	1.37	1.43
48	Z	401	3PE	O21-C2	-2.23	1.41	1.46
51	O	401	GTP	PG-O2G	-2.23	1.46	1.54
46	F	502	FMN	C7M-C7	2.22	1.55	1.51
54	T	201	EHZ	O3-C12	-2.22	1.18	1.23
46	F	502	FMN	O4'-C4'	-2.21	1.38	1.43
44	H	402	PC1	C22-C21	2.20	1.57	1.50
51	O	401	GTP	PG-O3G	-2.20	1.46	1.54
48	i	201	3PE	O21-C21	2.19	1.40	1.34
49	L	702	CDL	OA6-CA5	2.19	1.40	1.34
49	h	201	CDL	OA8-CA6	-2.19	1.40	1.45
48	Y	401	3PE	O31-C3	-2.18	1.40	1.45
48	Z	401	3PE	O31-C3	-2.17	1.40	1.45
48	Y	401	3PE	O21-C21	2.17	1.40	1.34
48	Z	401	3PE	O21-C21	2.16	1.40	1.34
49	d	201	CDL	OA6-CA5	2.16	1.40	1.34
44	B	202	PC1	P-O11	2.16	1.68	1.59
54	U	201	EHZ	O3-C12	-2.16	1.18	1.23
49	N	402	CDL	OA6-CA5	2.13	1.40	1.34
49	N	401	CDL	OA6-CA5	2.13	1.40	1.34
48	L	703	3PE	O21-C21	2.13	1.40	1.34
48	H	403	3PE	O31-C31	2.13	1.39	1.33
48	J	201	3PE	O21-C21	2.12	1.40	1.34
50	L	704	LMT	O4'-C4B	-2.12	1.38	1.43
48	L	703	3PE	O31-C3	-2.11	1.40	1.45
48	J	201	3PE	O31-C3	-2.11	1.40	1.45
50	L	705	LMT	O4'-C4B	-2.11	1.38	1.43
50	L	705	LMT	O1'-C1'	-2.11	1.36	1.40
44	H	402	PC1	P-O13	2.10	1.67	1.59
48	i	201	3PE	O31-C3	-2.10	1.40	1.45
49	N	402	CDL	OA8-CA6	-2.07	1.40	1.45
52	P	501	NDP	O5D-C5D	-2.07	1.36	1.44
48	H	403	3PE	O21-C21	2.05	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	B	202	PC1	P-O13	2.04	1.67	1.59
52	P	501	NDP	C2A-N1A	2.01	1.37	1.33
49	h	201	CDL	OA6-CA5	2.01	1.40	1.34
49	M	501	CDL	OB6-CB4	-2.01	1.41	1.46
49	N	401	CDL	OA8-CA6	-2.01	1.40	1.45

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	F	502	FMN	C4-C4A-N5	15.31	140.02	118.23
46	F	502	FMN	C6-C5A-N5	15.30	145.22	118.51
46	F	502	FMN	C6-C5A-C9A	-12.12	101.79	118.94
46	F	502	FMN	C5A-N5-C4A	9.72	134.24	118.07
46	F	502	FMN	C9A-C5A-N5	-8.69	112.99	122.43
46	F	502	FMN	C9A-N10-C10	7.82	132.95	120.77
46	F	502	FMN	C10-N1-C2	6.81	130.51	116.90
52	P	501	NDP	PN-O3-PA	-6.78	109.56	132.83
46	F	502	FMN	C5A-C9A-N10	-6.49	111.25	117.95
46	F	502	FMN	C10-C4A-N5	-6.13	111.84	124.86
54	U	201	EHZ	C8-C9-S1	5.75	120.75	113.63
46	F	502	FMN	C4-C4A-C10	-5.15	108.14	116.79
47	H	401	UQ9	C40-C39-C41	4.95	123.60	115.27
47	H	401	UQ9	C35-C34-C36	4.86	123.45	115.27
54	T	201	EHZ	C8-C9-S1	4.82	119.59	113.63
49	d	201	CDL	OA6-CA5-C11	4.73	121.69	111.50
44	H	402	PC1	O21-C21-C22	4.72	121.67	111.50
48	i	201	3PE	O21-C21-C22	4.53	121.27	111.50
49	M	501	CDL	OB6-CB5-C51	4.36	120.90	111.50
49	L	702	CDL	OA6-CA5-C11	4.23	120.62	111.50
47	H	401	UQ9	C20-C19-C21	4.11	122.19	115.27
44	B	202	PC1	O21-C21-C22	4.10	120.33	111.50
48	J	201	3PE	O21-C21-C22	4.04	120.20	111.50
49	N	401	CDL	OB6-CB5-C51	3.98	120.09	111.50
49	N	402	CDL	OA6-CA5-C11	3.97	120.06	111.50
49	h	201	CDL	OB6-CB5-C51	3.95	120.02	111.50
48	Z	401	3PE	O21-C21-C22	3.94	120.00	111.50
48	H	403	3PE	O21-C21-C22	3.90	119.91	111.50
48	L	703	3PE	O21-C21-C22	3.89	119.89	111.50
49	h	201	CDL	OA6-CA5-C11	3.87	119.84	111.50
49	N	401	CDL	OA6-CA5-C11	3.87	119.84	111.50
46	F	502	FMN	C9-C9A-N10	3.82	127.00	121.84
48	Y	401	3PE	O21-C21-C22	3.77	119.62	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	d	201	CDL	OB6-CB5-C51	3.69	119.45	111.50
49	N	402	CDL	OB6-CB5-C51	3.65	119.38	111.50
49	L	702	CDL	OB6-CB5-C51	3.64	119.34	111.50
47	H	401	UQ9	C45-C44-C46	3.45	121.08	115.27
47	H	401	UQ9	C25-C24-C26	3.43	121.05	115.27
48	L	701	3PE	O21-C21-C22	3.40	118.82	111.50
52	P	501	NDP	O2B-P2B-O1X	-3.33	96.52	109.39
48	Z	401	3PE	O31-C31-C32	3.30	122.28	111.91
51	O	401	GTP	PA-O3A-PB	-3.21	121.82	132.83
51	O	401	GTP	C2-N1-C6	-3.16	119.28	125.10
52	P	501	NDP	PA-O5B-C5B	-3.14	103.24	121.68
51	O	401	GTP	C5-C6-N1	3.11	119.44	113.95
47	H	401	UQ9	C20-C19-C18	-3.06	115.82	123.68
47	H	401	UQ9	C35-C34-C33	-3.05	115.85	123.68
46	F	502	FMN	C9A-C9-C8	3.05	125.43	119.30
49	N	402	CDL	OB8-CB7-C71	3.00	121.31	111.91
47	H	401	UQ9	C30-C29-C31	2.95	120.24	115.27
46	F	502	FMN	C4A-C10-N1	-2.91	117.98	124.73
48	L	701	3PE	O31-C31-C32	2.89	120.98	111.91
46	F	502	FMN	O3P-P-O5'	2.89	114.42	106.73
49	h	201	CDL	OB8-CB7-C71	2.84	120.82	111.91
49	L	702	CDL	OB8-CB7-C71	2.83	120.78	111.91
49	h	201	CDL	OA8-CA7-C31	2.81	120.71	111.91
51	O	401	GTP	O2G-PG-O3B	2.81	114.05	104.64
47	H	401	UQ9	C42-C43-C44	-2.80	120.91	127.66
47	H	401	UQ9	C37-C38-C39	-2.80	120.92	127.66
51	O	401	GTP	O3G-PG-O3B	2.79	114.00	104.64
49	N	401	CDL	OA8-CA7-C31	2.78	120.63	111.91
49	M	501	CDL	OB8-CB7-C71	2.78	120.62	111.91
48	Y	401	3PE	O31-C31-C32	2.77	120.61	111.91
46	F	502	FMN	O2P-P-O5'	2.77	114.09	106.73
49	N	402	CDL	OA8-CA7-C31	2.76	120.57	111.91
51	O	401	GTP	PB-O3B-PG	-2.74	123.44	132.83
54	T	201	EHZ	C10-S1-C9	2.72	110.35	101.87
48	J	201	3PE	O31-C31-C32	2.72	120.44	111.91
49	d	201	CDL	OA8-CA7-C31	2.72	120.43	111.91
50	L	704	LMT	C1'-O5'-C5'	-2.71	108.37	113.69
52	P	501	NDP	PN-O5D-C5D	-2.70	105.85	121.68
47	H	401	UQ9	C10-C9-C11	2.70	119.81	115.27
49	d	201	CDL	OB8-CB7-C71	2.69	120.35	111.91
54	U	201	EHZ	C16-C15-N2	2.69	121.93	116.58
48	H	403	3PE	O31-C31-C32	2.65	120.23	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	N	401	CDL	OB8-CB7-C71	2.61	120.11	111.91
46	F	502	FMN	C1'-N10-C9A	-2.61	116.17	120.51
50	L	705	LMT	C3'-C4'-C5'	-2.59	104.99	110.93
49	M	501	CDL	OA8-CA7-C31	2.59	120.03	111.91
46	F	502	FMN	C5A-C6-C7	2.57	125.42	120.71
48	L	703	3PE	O31-C31-C32	2.55	119.91	111.91
52	P	501	NDP	O3X-P2B-O2X	2.54	117.36	107.64
54	U	201	EHZ	C10-S1-C9	2.54	109.79	101.87
46	F	502	FMN	O5'-P-O1P	2.53	113.57	106.47
47	H	401	UQ9	C7-C8-C9	-2.51	120.80	126.57
54	U	201	EHZ	C14-C13-C12	-2.50	108.19	112.36
46	F	502	FMN	N10-C10-N1	2.41	125.29	118.35
52	P	501	NDP	C2A-N1A-C6A	-2.39	114.67	118.75
54	U	201	EHZ	C7-C8-C9	-2.36	108.51	113.89
54	U	201	EHZ	O2-C9-S1	-2.35	119.56	122.61
44	B	202	PC1	O31-C31-C32	2.34	119.25	111.91
49	L	702	CDL	OA8-CA7-C31	2.34	119.25	111.91
54	U	201	EHZ	C13-C12-N1	2.31	120.31	116.42
44	H	402	PC1	O31-C31-C32	2.31	119.15	111.91
47	H	401	UQ9	C12-C13-C14	-2.31	122.10	127.66
48	i	201	3PE	O31-C31-C32	2.30	119.14	111.91
49	h	201	CDL	CA4-OA6-CA5	-2.29	112.14	117.79
47	H	401	UQ9	C22-C23-C24	-2.28	122.16	127.66
46	F	502	FMN	C9-C8-C7	2.27	122.91	119.67
51	O	401	GTP	O2A-PA-O1A	-2.25	101.13	112.24
51	O	401	GTP	O2B-PB-O1B	-2.22	101.28	112.24
46	F	502	FMN	C4-N3-C2	2.21	129.73	125.64
54	T	201	EHZ	C13-C12-N1	2.20	120.13	116.42
52	P	501	NDP	O2N-PN-O1N	2.16	122.90	112.24
52	P	501	NDP	O4B-C4B-C3B	2.16	109.38	105.11
52	P	501	NDP	C5B-C4B-C3B	-2.12	107.23	115.18
46	F	502	FMN	C6-C7-C8	2.11	122.69	119.67
50	L	704	LMT	O5B-C5B-C4B	2.10	113.51	109.69
51	O	401	GTP	O6-C6-C5	-2.08	120.30	124.37
44	H	402	PC1	C2-O21-C21	-2.07	112.70	117.79
47	H	401	UQ9	C50-C49-C51	2.05	119.14	114.60
50	L	704	LMT	O5B-C5B-C6B	2.05	111.53	106.44
52	P	501	NDP	C3N-C2N-N1N	-2.02	120.22	123.10
47	H	401	UQ9	C32-C33-C34	-2.01	122.83	127.66

There are no chirality outliers.

All (460) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	B	202	PC1	C1-O11-P-O14
44	B	202	PC1	C12-C11-O13-P
44	B	202	PC1	O13-C11-C12-N
44	B	202	PC1	O11-C1-C2-O21
44	B	202	PC1	O22-C21-O21-C2
44	B	202	PC1	C22-C21-O21-C2
44	H	402	PC1	C1-O11-P-O13
46	F	502	FMN	N10-C1'-C2'-O2'
46	F	502	FMN	C1'-C2'-C3'-O3'
46	F	502	FMN	C1'-C2'-C3'-C4'
47	H	401	UQ9	C40-C39-C41-C42
47	H	401	UQ9	C38-C39-C41-C42
47	H	401	UQ9	C35-C34-C36-C37
47	H	401	UQ9	C29-C31-C32-C33
48	H	403	3PE	C1-O11-P-O14
48	H	403	3PE	C11-O13-P-O14
48	L	703	3PE	C11-O13-P-O11
48	L	703	3PE	C11-O13-P-O14
48	L	703	3PE	O11-C1-C2-O21
48	L	703	3PE	C22-C21-O21-C2
48	Y	401	3PE	C1-O11-P-O14
48	Z	401	3PE	C11-O13-P-O14
48	Z	401	3PE	C22-C21-O21-C2
48	i	201	3PE	C1-O11-P-O14
48	i	201	3PE	C22-C21-O21-C2
49	L	702	CDL	CA2-OA2-PA1-OA4
49	L	702	CDL	CA2-OA2-PA1-OA5
49	L	702	CDL	CB2-OB2-PB2-OB3
49	L	702	CDL	CB2-OB2-PB2-OB4
49	L	702	CDL	CB2-OB2-PB2-OB5
49	L	702	CDL	C51-CB5-OB6-CB4
49	M	501	CDL	O1-C1-CB2-OB2
49	M	501	CDL	CA2-OA2-PA1-OA3
49	M	501	CDL	CA2-OA2-PA1-OA4
49	M	501	CDL	CA2-OA2-PA1-OA5
49	M	501	CDL	CA3-OA5-PA1-OA3
49	M	501	CDL	CB2-OB2-PB2-OB3
49	N	401	CDL	O1-C1-CB2-OB2
49	N	401	CDL	C1-CA2-OA2-PA1
49	N	401	CDL	CA2-OA2-PA1-OA3
49	N	401	CDL	CA2-OA2-PA1-OA4
49	N	401	CDL	CA2-OA2-PA1-OA5
49	N	401	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
49	N	401	CDL	CA3-OA5-PA1-OA4
49	N	401	CDL	C51-CB5-OB6-CB4
49	N	402	CDL	C1-CA2-OA2-PA1
49	N	402	CDL	CA3-OA5-PA1-OA3
49	N	402	CDL	CB2-OB2-PB2-OB3
49	N	402	CDL	CB2-OB2-PB2-OB4
49	N	402	CDL	CB2-OB2-PB2-OB5
49	d	201	CDL	CB2-OB2-PB2-OB3
49	d	201	CDL	CB2-OB2-PB2-OB4
49	d	201	CDL	CB2-OB2-PB2-OB5
49	d	201	CDL	C51-CB5-OB6-CB4
49	h	201	CDL	CA2-OA2-PA1-OA3
49	h	201	CDL	CA3-OA5-PA1-OA3
49	h	201	CDL	CA3-OA5-PA1-OA4
49	h	201	CDL	CB2-OB2-PB2-OB3
49	h	201	CDL	CB2-OB2-PB2-OB4
49	h	201	CDL	CB2-OB2-PB2-OB5
49	h	201	CDL	C51-CB5-OB6-CB4
50	L	704	LMT	C2'-C1'-O1'-C1
50	L	704	LMT	O5'-C1'-O1'-C1
50	L	705	LMT	C2'-C1'-O1'-C1
50	L	705	LMT	O5'-C1'-O1'-C1
51	O	401	GTP	C5'-O5'-PA-O3A
51	O	401	GTP	C5'-O5'-PA-O1A
51	O	401	GTP	C5'-O5'-PA-O2A
52	P	501	NDP	O4B-C4B-C5B-O5B
52	P	501	NDP	C3B-C4B-C5B-O5B
54	T	201	EHZ	C6-C7-C8-C9
54	T	201	EHZ	S1-C10-C11-N1
54	T	201	EHZ	C16-C17-C20-O6
54	T	201	EHZ	O2-C9-S1-C10
54	T	201	EHZ	C8-C9-S1-C10
54	U	201	EHZ	C5-C6-C7-O1
54	U	201	EHZ	C5-C6-C7-C8
54	U	201	EHZ	S1-C10-C11-N1
54	U	201	EHZ	C12-C13-C14-N2
54	U	201	EHZ	C16-C15-N2-C14
54	U	201	EHZ	C15-C16-C17-C18
54	U	201	EHZ	C15-C16-C17-C19
54	U	201	EHZ	C15-C16-C17-C20
54	U	201	EHZ	O5-C16-C17-C18
54	U	201	EHZ	O5-C16-C17-C19

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Mol	Chain	Res	Type	Atoms
54	U	201	EHZ	O5-C16-C17-C20
54	U	201	EHZ	O2-C9-S1-C10
54	U	201	EHZ	C8-C9-S1-C10
48	Z	401	3PE	O32-C31-O31-C3
48	Z	401	3PE	C32-C31-O31-C3
49	L	702	CDL	C71-CB7-OB8-CB6
49	h	201	CDL	C31-CA7-OA8-CA6
48	Y	401	3PE	O32-C31-O31-C3
49	L	702	CDL	OB9-CB7-OB8-CB6
49	N	401	CDL	OB9-CB7-OB8-CB6
49	N	402	CDL	OA9-CA7-OA8-CA6
49	h	201	CDL	OA9-CA7-OA8-CA6
48	L	703	3PE	O22-C21-O21-C2
48	Z	401	3PE	O22-C21-O21-C2
48	i	201	3PE	O22-C21-O21-C2
49	L	702	CDL	OB7-CB5-OB6-CB4
49	N	401	CDL	OA7-CA5-OA6-CA4
49	N	401	CDL	OB7-CB5-OB6-CB4
49	d	201	CDL	OB7-CB5-OB6-CB4
49	h	201	CDL	OB7-CB5-OB6-CB4
49	N	401	CDL	C71-CB7-OB8-CB6
49	N	402	CDL	C31-CA7-OA8-CA6
49	N	401	CDL	C11-CA5-OA6-CA4
48	H	403	3PE	C32-C31-O31-C3
48	Y	401	3PE	C32-C31-O31-C3
49	d	201	CDL	C31-CA7-OA8-CA6
48	H	403	3PE	O32-C31-O31-C3
49	M	501	CDL	OB9-CB7-OB8-CB6
49	d	201	CDL	OA9-CA7-OA8-CA6
49	N	401	CDL	O1-C1-CA2-OA2
50	L	704	LMT	O5B-C1B-O1B-C4'
48	J	201	3PE	C32-C31-O31-C3
49	d	201	CDL	C71-CB7-OB8-CB6
50	L	704	LMT	C4'-C5'-C6'-O6'
54	U	201	EHZ	O4-C15-N2-C14
49	h	201	CDL	C11-CA5-OA6-CA4
49	N	402	CDL	C78-C79-C80-C81
50	L	704	LMT	O5'-C5'-C6'-O6'
49	M	501	CDL	C71-CB7-OB8-CB6
49	N	401	CDL	CA4-CA3-OA5-PA1
49	d	201	CDL	OB9-CB7-OB8-CB6
47	H	401	UQ9	C20-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
47	H	401	UQ9	C33-C34-C36-C37
47	H	401	UQ9	C18-C19-C21-C22
48	J	201	3PE	O32-C31-O31-C3
47	H	401	UQ9	C44-C46-C47-C48
44	B	202	PC1	C32-C31-O31-C3
44	H	402	PC1	C32-C31-O31-C3
49	N	402	CDL	C71-CB7-OB8-CB6
49	N	401	CDL	C71-C72-C73-C74
49	M	501	CDL	CB2-C1-CA2-OA2
49	M	501	CDL	CA2-C1-CB2-OB2
49	N	401	CDL	CA2-C1-CB2-OB2
49	h	201	CDL	OA7-CA5-OA6-CA4
44	H	402	PC1	O32-C31-O31-C3
50	L	705	LMT	O5B-C1B-O1B-C4'
50	L	705	LMT	C2B-C1B-O1B-C4'
49	M	501	CDL	O1-C1-CA2-OA2
48	H	403	3PE	C22-C21-O21-C2
49	M	501	CDL	C51-CB5-OB6-CB4
49	M	501	CDL	CB5-C51-C52-C53
49	N	401	CDL	CA7-C31-C32-C33
48	H	403	3PE	C21-C22-C23-C24
54	T	201	EHZ	C5-C6-C7-O1
46	F	502	FMN	O2'-C2'-C3'-C4'
49	d	201	CDL	CB5-C51-C52-C53
44	B	202	PC1	O32-C31-O31-C3
48	L	701	3PE	C2-C3-O31-C31
47	H	401	UQ9	C24-C26-C27-C28
49	N	402	CDL	O1-C1-CA2-OA2
49	M	501	CDL	OB7-CB5-OB6-CB4
49	N	402	CDL	OB9-CB7-OB8-CB6
48	H	403	3PE	C11-O13-P-O11
48	L	703	3PE	C1-O11-P-O13
49	M	501	CDL	CA3-OA5-PA1-OA2
49	M	501	CDL	CB2-OB2-PB2-OB5
49	N	401	CDL	CA3-OA5-PA1-OA2
49	N	401	CDL	CB2-OB2-PB2-OB5
49	d	201	CDL	CB3-OB5-PB2-OB2
49	h	201	CDL	CA2-OA2-PA1-OA5
49	h	201	CDL	CA3-OA5-PA1-OA2
49	h	201	CDL	CB3-OB5-PB2-OB2
48	L	701	3PE	C32-C31-O31-C3
49	N	402	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
48	H	403	3PE	O22-C21-O21-C2
50	L	704	LMT	C3'-C4'-O1B-C1B
50	L	704	LMT	C5'-C4'-O1B-C1B
49	h	201	CDL	C71-CB7-OB8-CB6
46	F	502	FMN	O2'-C2'-C3'-O3'
49	M	501	CDL	C53-C54-C55-C56
49	N	402	CDL	C11-CA5-OA6-CA4
48	i	201	3PE	C25-C26-C27-C28
49	N	401	CDL	C75-C76-C77-C78
49	h	201	CDL	C20-C21-C22-C23
54	T	201	EHZ	C18-C17-C20-O6
54	T	201	EHZ	C19-C17-C20-O6
49	N	402	CDL	OA7-CA5-OA6-CA4
48	Z	401	3PE	C34-C35-C36-C37
50	L	705	LMT	O5'-C5'-C6'-O6'
49	N	402	CDL	C75-C76-C77-C78
49	h	201	CDL	O1-C1-CA2-OA2
49	N	402	CDL	C72-C73-C74-C75
48	L	703	3PE	C3B-C3C-C3D-C3E
49	L	702	CDL	C52-C53-C54-C55
49	N	402	CDL	CA5-C11-C12-C13
49	L	702	CDL	OA7-CA5-OA6-CA4
49	L	702	CDL	C11-CA5-OA6-CA4
48	H	403	3PE	C2D-C2E-C2F-C2G
49	N	401	CDL	C83-C84-C85-C86
48	L	703	3PE	C35-C36-C37-C38
44	B	202	PC1	C37-C38-C39-C3A
49	N	401	CDL	C51-C52-C53-C54
48	L	701	3PE	O32-C31-O31-C3
44	B	202	PC1	C35-C36-C37-C38
49	d	201	CDL	C31-C32-C33-C34
48	H	403	3PE	C25-C26-C27-C28
49	L	702	CDL	C77-C78-C79-C80
44	H	402	PC1	C27-C28-C29-C2A
48	H	403	3PE	C3C-C3D-C3E-C3F
48	H	403	3PE	C37-C38-C39-C3A
49	h	201	CDL	OB9-CB7-OB8-CB6
49	N	402	CDL	C51-C52-C53-C54
48	Y	401	3PE	C31-C32-C33-C34
48	L	703	3PE	C3A-C3B-C3C-C3D
50	L	704	LMT	C11-C10-C9-C8
49	M	501	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
49	h	201	CDL	CA5-C11-C12-C13
44	H	402	PC1	C33-C34-C35-C36
48	H	403	3PE	C3A-C3B-C3C-C3D
49	d	201	CDL	C57-C58-C59-C60
44	H	402	PC1	C24-C25-C26-C27
48	i	201	3PE	C33-C34-C35-C36
49	N	402	CDL	C71-C72-C73-C74
49	N	402	CDL	C51-CB5-OB6-CB4
49	N	402	CDL	OB7-CB5-OB6-CB4
48	Y	401	3PE	O21-C2-C3-O31
49	L	702	CDL	OB6-CB4-CB6-OB8
49	N	401	CDL	OA6-CA4-CA6-OA8
49	M	501	CDL	C75-C76-C77-C78
52	P	501	NDP	O4D-C4D-C5D-O5D
49	N	401	CDL	C76-C77-C78-C79
49	d	201	CDL	C55-C56-C57-C58
48	H	403	3PE	C1-O11-P-O13
48	Y	401	3PE	C1-O11-P-O13
48	Z	401	3PE	C11-O13-P-O11
49	N	401	CDL	CB5-C51-C52-C53
50	L	704	LMT	C1-C2-C3-C4
48	L	701	3PE	O11-C1-C2-C3
48	L	703	3PE	O11-C1-C2-C3
49	M	501	CDL	OA5-CA3-CA4-CA6
48	i	201	3PE	C24-C25-C26-C27
49	N	401	CDL	C78-C79-C80-C81
49	M	501	CDL	OA5-CA3-CA4-OA6
49	N	401	CDL	CA3-CA4-CA6-OA8
49	N	401	CDL	CB3-CB4-CB6-OB8
48	L	701	3PE	C27-C28-C29-C2A
49	h	201	CDL	C51-C52-C53-C54
49	L	702	CDL	CB5-C51-C52-C53
49	M	501	CDL	C31-C32-C33-C34
49	N	401	CDL	CA5-C11-C12-C13
48	Z	401	3PE	C32-C33-C34-C35
50	L	705	LMT	C6-C7-C8-C9
48	Z	401	3PE	C3-C2-O21-C21
49	M	501	CDL	CB6-CB4-OB6-CB5
49	d	201	CDL	CB3-CB4-OB6-CB5
49	L	702	CDL	C75-C76-C77-C78
49	N	401	CDL	C53-C54-C55-C56
49	N	402	CDL	C76-C77-C78-C79

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Mol	Chain	Res	Type	Atoms
50	L	704	LMT	C5-C6-C7-C8
48	L	701	3PE	C22-C23-C24-C25
54	T	201	EHZ	C2-C3-C4-C5
49	L	702	CDL	C14-C15-C16-C17
48	i	201	3PE	C22-C23-C24-C25
54	T	201	EHZ	C5-C6-C7-C8
49	N	401	CDL	CB2-C1-CA2-OA2
48	Z	401	3PE	C36-C37-C38-C39
49	L	702	CDL	C55-C56-C57-C58
52	P	501	NDP	C3D-C4D-C5D-O5D
48	H	403	3PE	O11-C1-C2-C3
48	J	201	3PE	O11-C1-C2-C3
49	L	702	CDL	OB5-CB3-CB4-CB6
48	L	703	3PE	C37-C38-C39-C3A
49	M	501	CDL	C31-CA7-OA8-CA6
49	h	201	CDL	C73-C74-C75-C76
54	U	201	EHZ	C2-C3-C4-C5
48	Y	401	3PE	C33-C34-C35-C36
48	Y	401	3PE	C1-C2-C3-O31
49	L	702	CDL	CB3-CB4-CB6-OB8
49	L	702	CDL	C13-C14-C15-C16
49	M	501	CDL	CA3-CA4-CA6-OA8
49	M	501	CDL	OA6-CA4-CA6-OA8
44	B	202	PC1	C1-O11-P-O13
48	i	201	3PE	C1-O11-P-O13
48	J	201	3PE	O11-C1-C2-O21
48	L	701	3PE	O11-C1-C2-O21
49	L	702	CDL	OB5-CB3-CB4-OB6
49	d	201	CDL	OA5-CA3-CA4-OA6
49	M	501	CDL	C52-C51-CB5-OB6
49	d	201	CDL	O1-C1-CA2-OA2
49	h	201	CDL	CB5-C51-C52-C53
49	N	401	CDL	C84-C85-C86-C87
52	P	501	NDP	PN-O3-PA-O5B
49	M	501	CDL	C51-C52-C53-C54
44	B	202	PC1	O11-C1-C2-C3
48	L	701	3PE	C32-C33-C34-C35
50	L	705	LMT	C5-C6-C7-C8
48	L	701	3PE	C26-C27-C28-C29
49	L	702	CDL	CA6-CA4-OA6-CA5
49	N	402	CDL	CA6-CA4-OA6-CA5
48	L	703	3PE	C3D-C3E-C3F-C3G

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Mol	Chain	Res	Type	Atoms
49	M	501	CDL	CB3-CB4-CB6-OB8
49	M	501	CDL	OA9-CA7-OA8-CA6
48	H	403	3PE	O11-C1-C2-O21
49	h	201	CDL	C72-C73-C74-C75
50	L	705	LMT	C9-C10-C11-C12
54	T	201	EHZ	O1-C7-C8-C9
48	H	403	3PE	O21-C2-C3-O31
49	N	402	CDL	OB6-CB4-CB6-OB8
44	B	202	PC1	C3C-C3D-C3E-C3F
49	N	401	CDL	C79-C80-C81-C82
44	H	402	PC1	C34-C35-C36-C37
48	L	703	3PE	C22-C23-C24-C25
49	L	702	CDL	C73-C74-C75-C76
54	U	201	EHZ	C22-C23-C24-C25
49	N	402	CDL	C74-C75-C76-C77
49	M	501	CDL	CA4-CA6-OA8-CA7
44	B	202	PC1	C11-O13-P-O11
48	Y	401	3PE	C11-O13-P-O11
49	L	702	CDL	C1-CA2-OA2-PA1
49	d	201	CDL	C1-CA2-OA2-PA1
48	J	201	3PE	C1-O11-P-O12
48	L	703	3PE	C1-O11-P-O12
48	L	703	3PE	C1-O11-P-O14
48	Z	401	3PE	C11-O13-P-O12
48	i	201	3PE	C1-O11-P-O12
49	L	702	CDL	CA2-OA2-PA1-OA3
49	M	501	CDL	CA3-OA5-PA1-OA4
49	M	501	CDL	CB2-OB2-PB2-OB4
49	N	401	CDL	CB2-OB2-PB2-OB3
49	d	201	CDL	CB3-OB5-PB2-OB4
49	h	201	CDL	CA2-OA2-PA1-OA4
49	h	201	CDL	CB3-OB5-PB2-OB3
49	h	201	CDL	CB3-OB5-PB2-OB4
49	M	501	CDL	OB5-CB3-CB4-CB6
49	N	401	CDL	OB5-CB3-CB4-CB6
44	B	202	PC1	C3F-C3G-C3H-C3I
48	H	403	3PE	C12-C11-O13-P
48	Z	401	3PE	C12-C11-O13-P
44	B	202	PC1	C3B-C3C-C3D-C3E
48	H	403	3PE	C35-C36-C37-C38
44	H	402	PC1	C31-C32-C33-C34
48	Y	401	3PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
44	H	402	PC1	O11-C1-C2-O21
48	L	701	3PE	C36-C37-C38-C39
48	i	201	3PE	O21-C21-C22-C23
49	d	201	CDL	C51-C52-C53-C54
44	H	402	PC1	O13-C11-C12-N
44	B	202	PC1	O21-C2-C3-O31
49	d	201	CDL	C62-C63-C64-C65
48	H	403	3PE	C34-C35-C36-C37
49	M	501	CDL	C1-CB2-OB2-PB2
50	L	704	LMT	C4-C5-C6-C7
48	L	703	3PE	C32-C31-O31-C3
49	L	702	CDL	C71-C72-C73-C74
44	H	402	PC1	C39-C3A-C3B-C3C
49	M	501	CDL	C58-C59-C60-C61
49	d	201	CDL	C54-C55-C56-C57
48	i	201	3PE	C3-C2-O21-C21
48	L	703	3PE	O32-C31-O31-C3
48	L	701	3PE	C34-C35-C36-C37
47	H	401	UQ9	C25-C24-C26-C27
49	N	401	CDL	C81-C82-C83-C84
49	N	402	CDL	CB5-C51-C52-C53
49	M	501	CDL	OB6-CB4-CB6-OB8
49	N	401	CDL	OB6-CB4-CB6-OB8
48	J	201	3PE	C1-O11-P-O13
48	L	701	3PE	C11-O13-P-O11
49	N	402	CDL	CB3-OB5-PB2-OB2
49	d	201	CDL	CA3-OA5-PA1-OA2
44	H	402	PC1	C37-C38-C39-C3A
48	L	703	3PE	C32-C33-C34-C35
49	M	501	CDL	C54-C55-C56-C57
49	M	501	CDL	C73-C74-C75-C76
48	J	201	3PE	C25-C26-C27-C28
51	O	401	GTP	O4'-C4'-C5'-O5'
52	P	501	NDP	O4D-C1D-N1N-C6N
49	N	402	CDL	C32-C33-C34-C35
54	T	201	EHZ	C3-C4-C5-C6
54	T	201	EHZ	C21-C22-C23-C24
48	Z	401	3PE	C27-C28-C29-C2A
48	L	701	3PE	C24-C25-C26-C27
50	L	705	LMT	O5B-C5B-C6B-O6B
49	L	702	CDL	CA7-C31-C32-C33
48	i	201	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
49	N	402	CDL	CA2-C1-CB2-OB2
49	h	201	CDL	O1-C1-CB2-OB2
49	L	702	CDL	C56-C57-C58-C59
48	H	403	3PE	C32-C33-C34-C35
49	h	201	CDL	CB3-CB4-OB6-CB5
52	P	501	NDP	C2D-C1D-N1N-C6N
44	H	402	PC1	C35-C36-C37-C38
49	d	201	CDL	CA5-C11-C12-C13
44	H	402	PC1	O21-C2-C3-O31
48	i	201	3PE	C21-C22-C23-C24
47	H	401	UQ9	C39-C41-C42-C43
52	P	501	NDP	PN-O3-PA-O1A
48	L	701	3PE	O21-C21-C22-C23
49	N	402	CDL	CB3-CB4-CB6-OB8
48	H	403	3PE	C3F-C3G-C3H-C3I
48	Z	401	3PE	O11-C1-C2-O21
48	Y	401	3PE	C35-C36-C37-C38
48	J	201	3PE	O31-C31-C32-C33
49	d	201	CDL	C52-C53-C54-C55
44	H	402	PC1	O11-C1-C2-C3
49	d	201	CDL	OA5-CA3-CA4-CA6
54	U	201	EHZ	O4-C15-C16-O5
48	Z	401	3PE	O13-C11-C12-N
49	h	201	CDL	C17-C18-C19-C20
49	h	201	CDL	OA6-CA4-CA6-OA8
44	B	202	PC1	C38-C39-C3A-C3B
49	h	201	CDL	C12-C11-CA5-OA6
48	i	201	3PE	C23-C24-C25-C26
49	L	702	CDL	C78-C79-C80-C81
49	N	401	CDL	C12-C11-CA5-OA6
47	H	401	UQ9	C45-C44-C46-C47
48	L	701	3PE	C28-C29-C2A-C2B
49	L	702	CDL	C74-C75-C76-C77
44	H	402	PC1	O22-C21-O21-C2
44	B	202	PC1	C1-C2-C3-O31
49	h	201	CDL	CA3-CA4-CA6-OA8
49	M	501	CDL	C76-C77-C78-C79
49	M	501	CDL	C52-C51-CB5-OB7
49	N	402	CDL	OB5-CB3-CB4-OB6
48	Z	401	3PE	C38-C39-C3A-C3B
49	h	201	CDL	C21-C22-C23-C24
52	P	501	NDP	C5B-O5B-PA-O3

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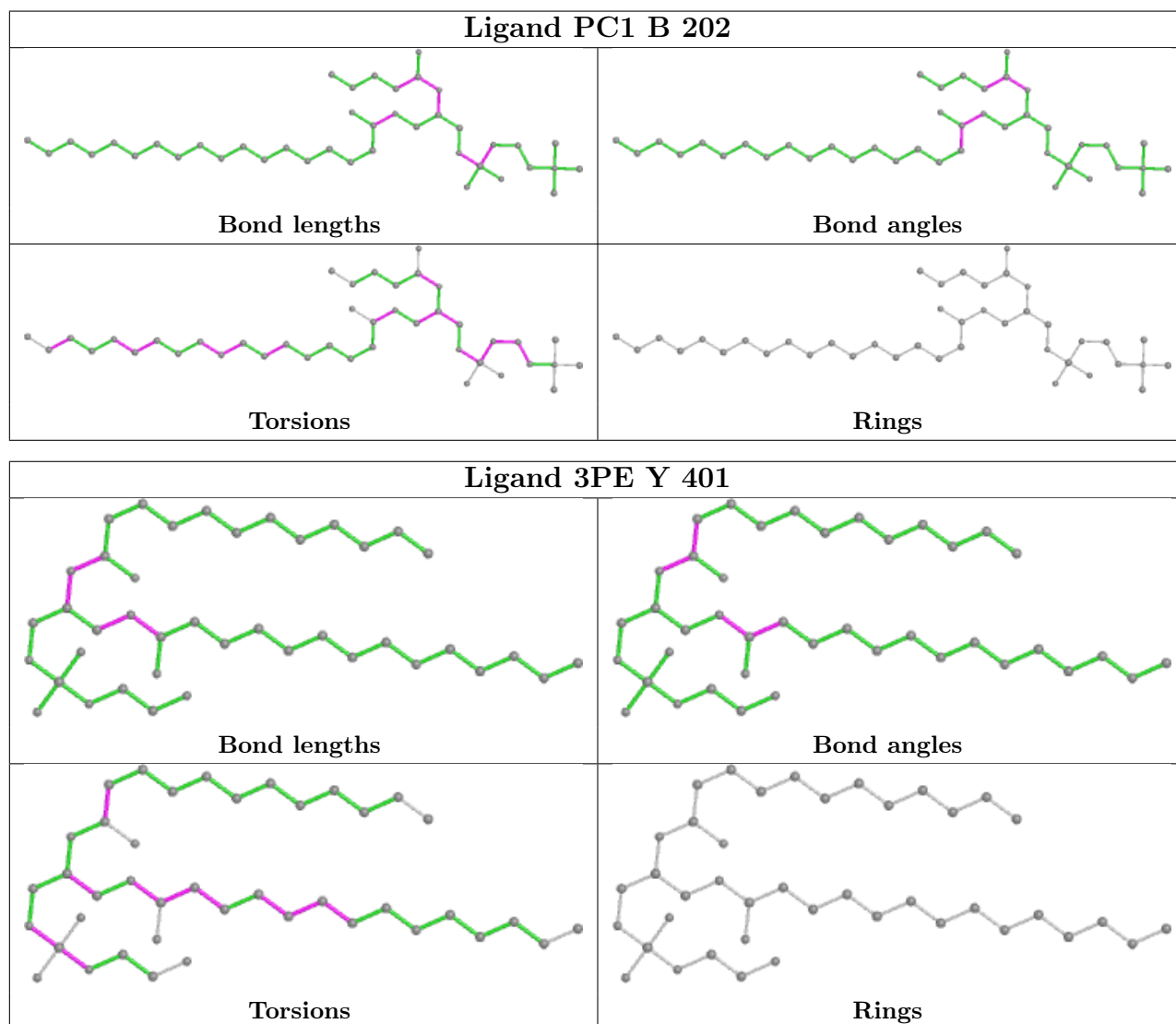
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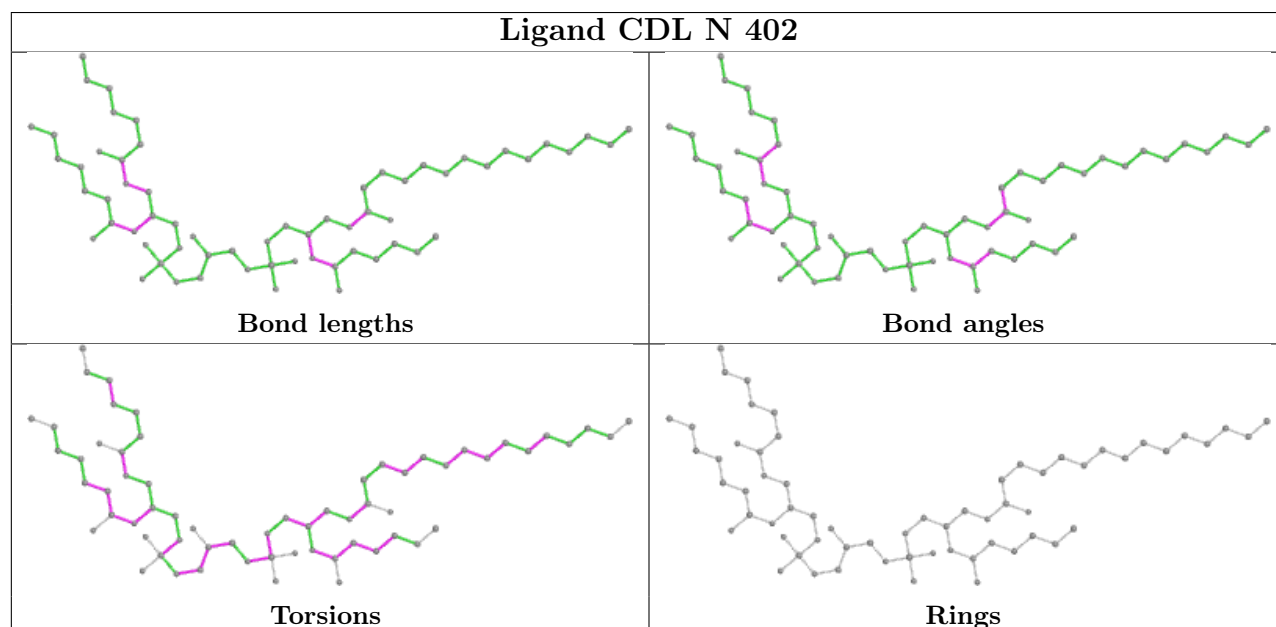
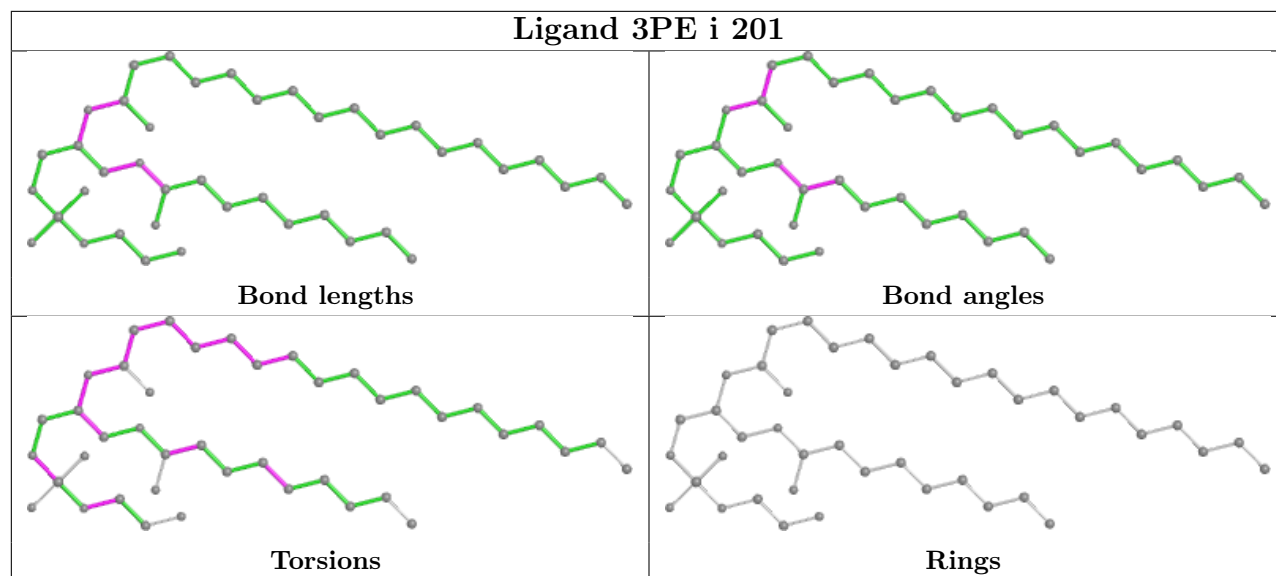
Mol	Chain	Res	Type	Atoms
52	P	501	NDP	C2B-O2B-P2B-O2X
52	P	501	NDP	C5D-O5D-PN-O3
49	d	201	CDL	C52-C51-CB5-OB6
50	L	705	LMT	C3-C4-C5-C6
44	H	402	PC1	C22-C21-O21-C2
47	H	401	UQ9	C36-C37-C38-C39
49	d	201	CDL	C32-C31-CA7-OA8
47	H	401	UQ9	C23-C24-C26-C27
49	N	401	CDL	C12-C11-CA5-OA7
49	h	201	CDL	CB2-C1-CA2-OA2
49	h	201	CDL	C12-C11-CA5-OA7
48	Y	401	3PE	O31-C31-C32-C33
48	L	701	3PE	C1-O11-P-O14
48	Z	401	3PE	C1-O11-P-O14
49	M	501	CDL	CB3-OB5-PB2-OB4
49	d	201	CDL	CA3-OA5-PA1-OA3
52	P	501	NDP	C5B-O5B-PA-O2A
47	H	401	UQ9	C15-C14-C16-C17
48	i	201	3PE	C12-C11-O13-P
49	h	201	CDL	CB6-CB4-OB6-CB5
48	Y	401	3PE	O21-C21-C22-C23
49	h	201	CDL	C52-C51-CB5-OB6
49	L	702	CDL	C36-C37-C38-C39
48	J	201	3PE	O21-C21-C22-C23
48	i	201	3PE	O31-C31-C32-C33
49	N	402	CDL	C52-C51-CB5-OB6
49	d	201	CDL	C52-C51-CB5-OB7
49	h	201	CDL	C32-C31-CA7-OA9
50	L	704	LMT	C2-C3-C4-C5
50	L	704	LMT	C9-C10-C11-C12
49	N	401	CDL	C1-CB2-OB2-PB2
46	F	502	FMN	N10-C1'-C2'-C3'
49	h	201	CDL	C32-C31-CA7-OA8
49	N	402	CDL	C12-C11-CA5-OA6
49	N	402	CDL	O1-C1-CB2-OB2
48	Y	401	3PE	O32-C31-C32-C33
49	h	201	CDL	C19-C20-C21-C22
48	J	201	3PE	O22-C21-C22-C23
49	d	201	CDL	C32-C31-CA7-OA9

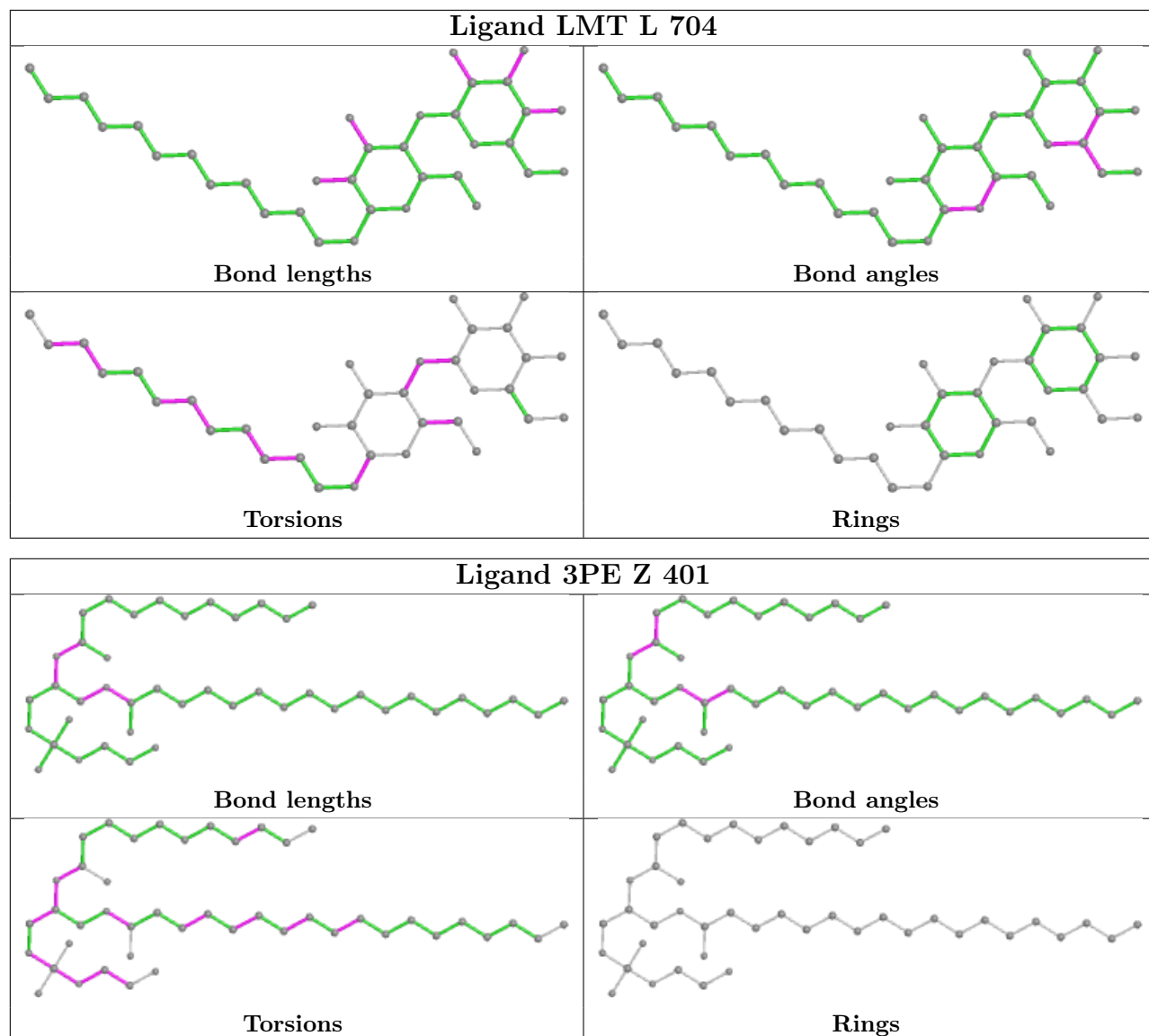
There are no ring outliers.

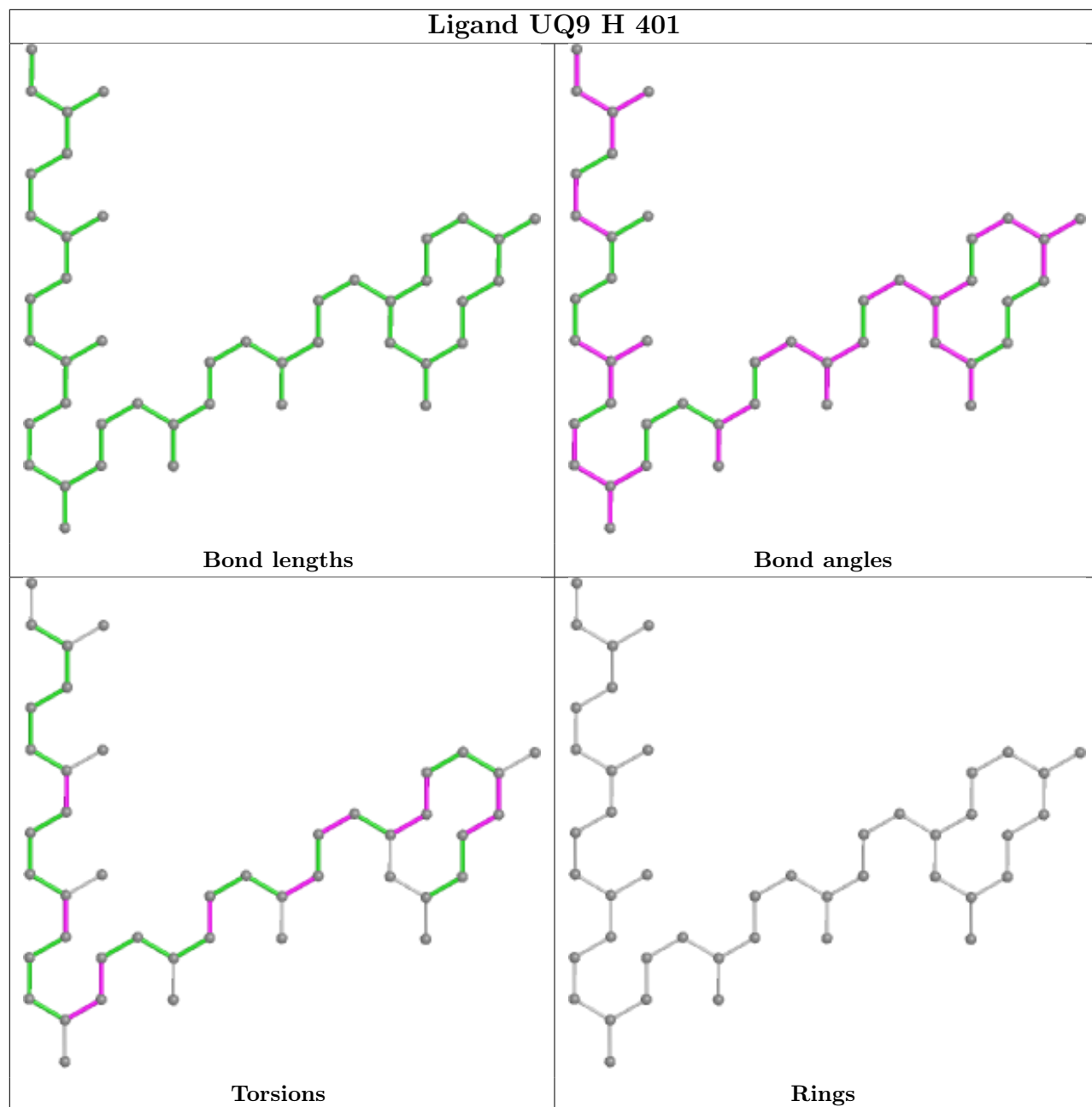
No monomer is involved in short contacts.

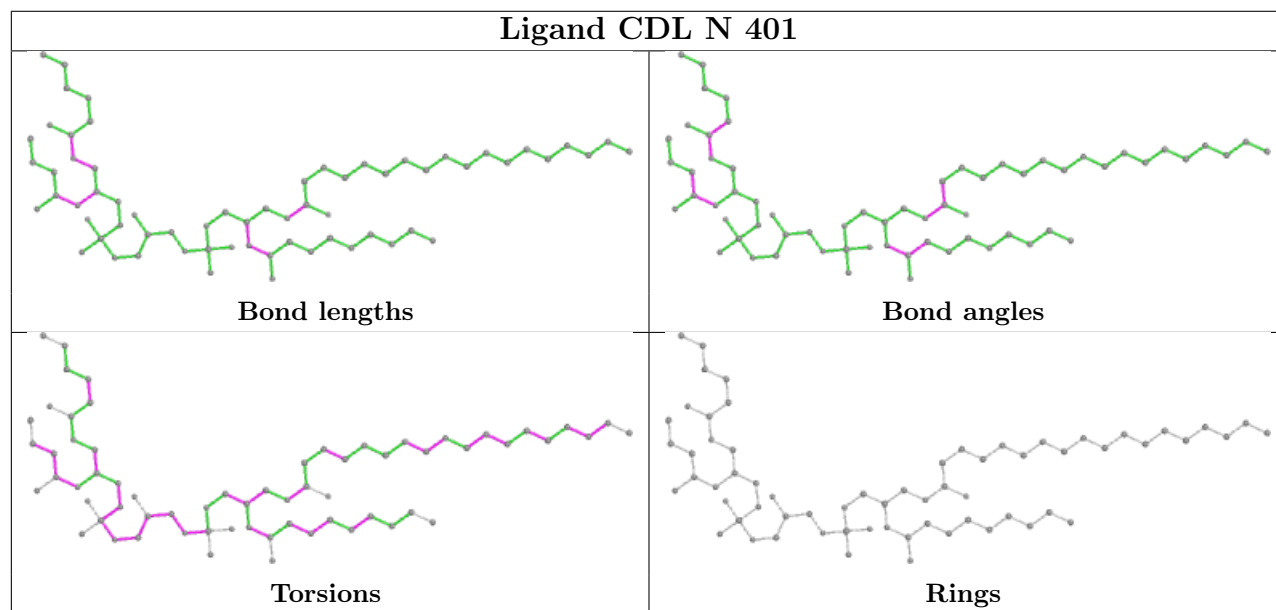
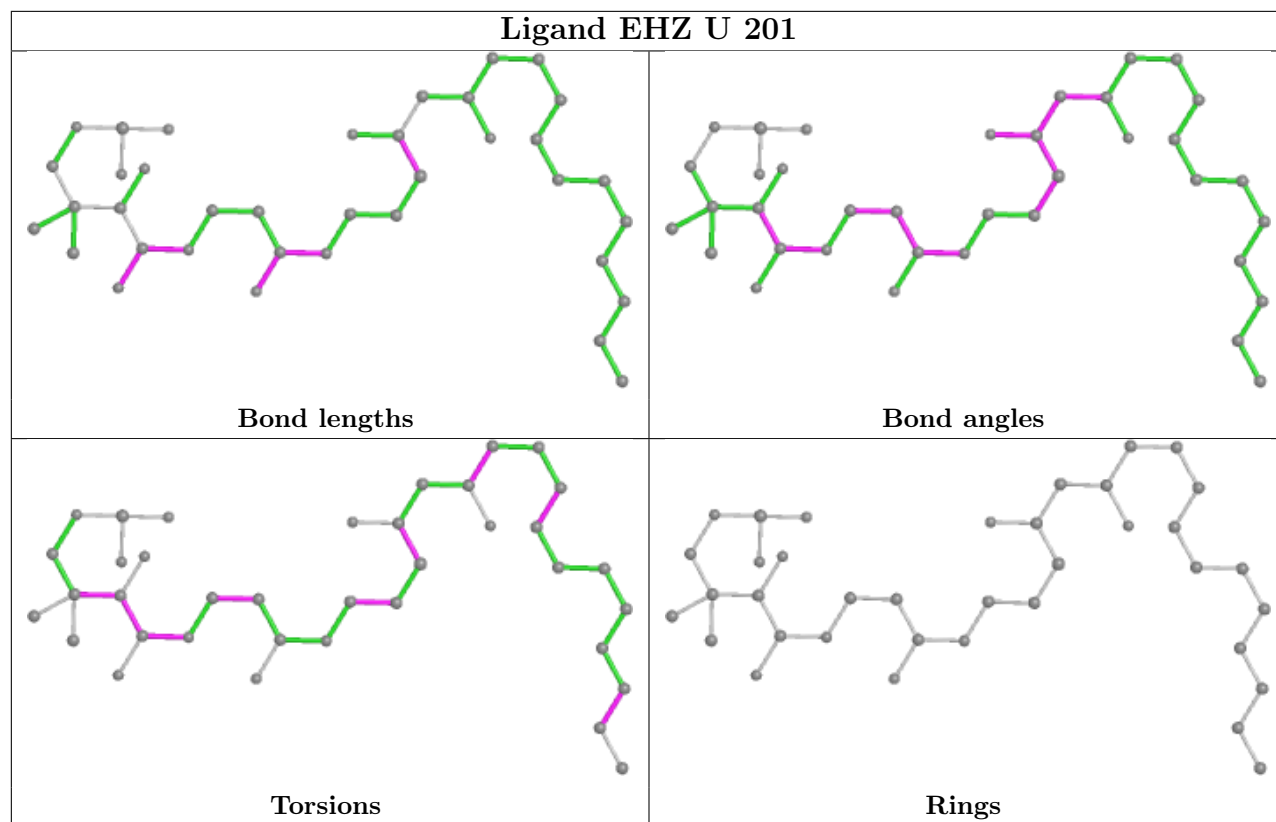
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

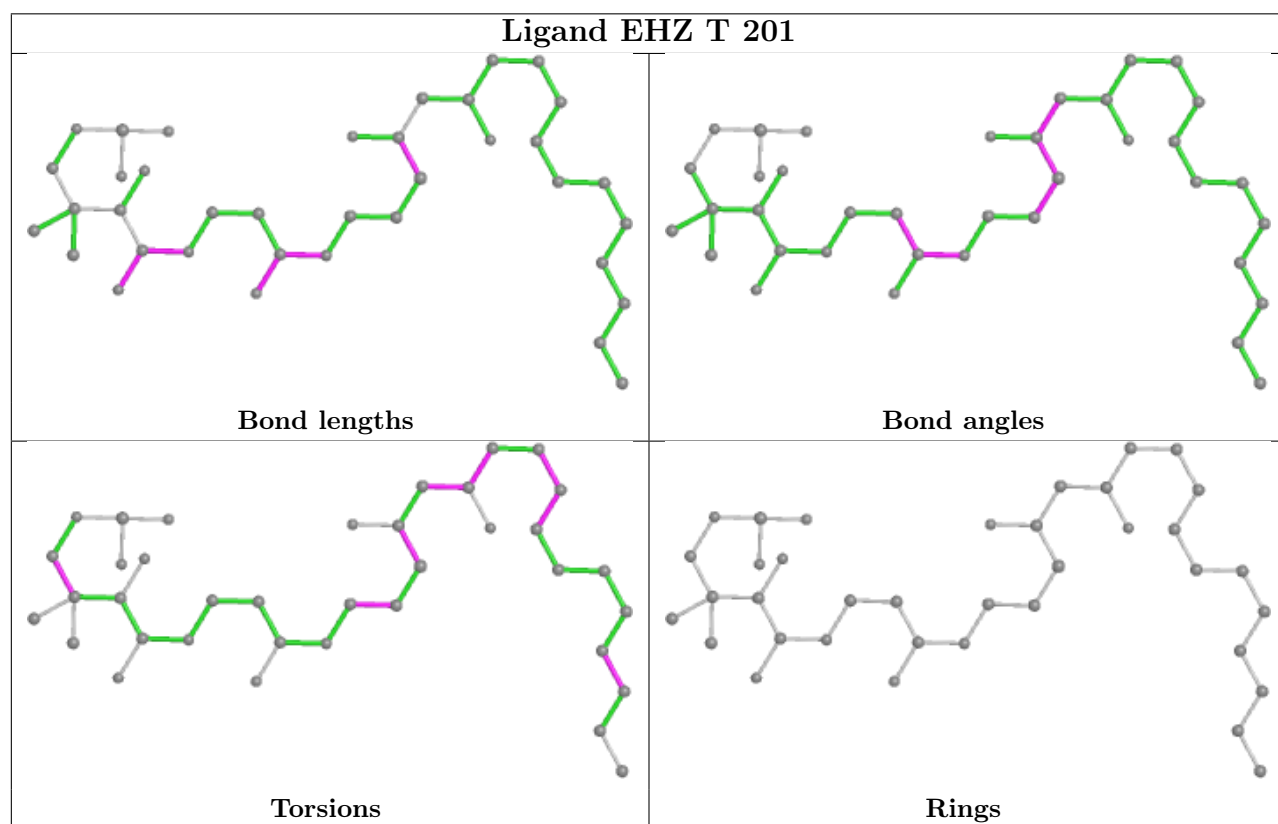
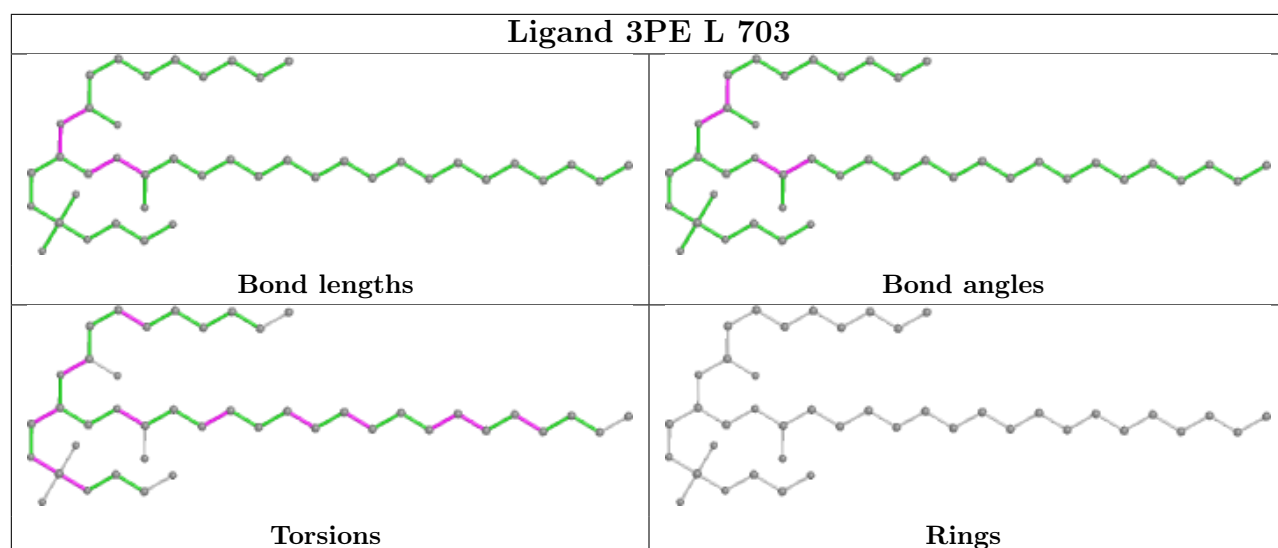


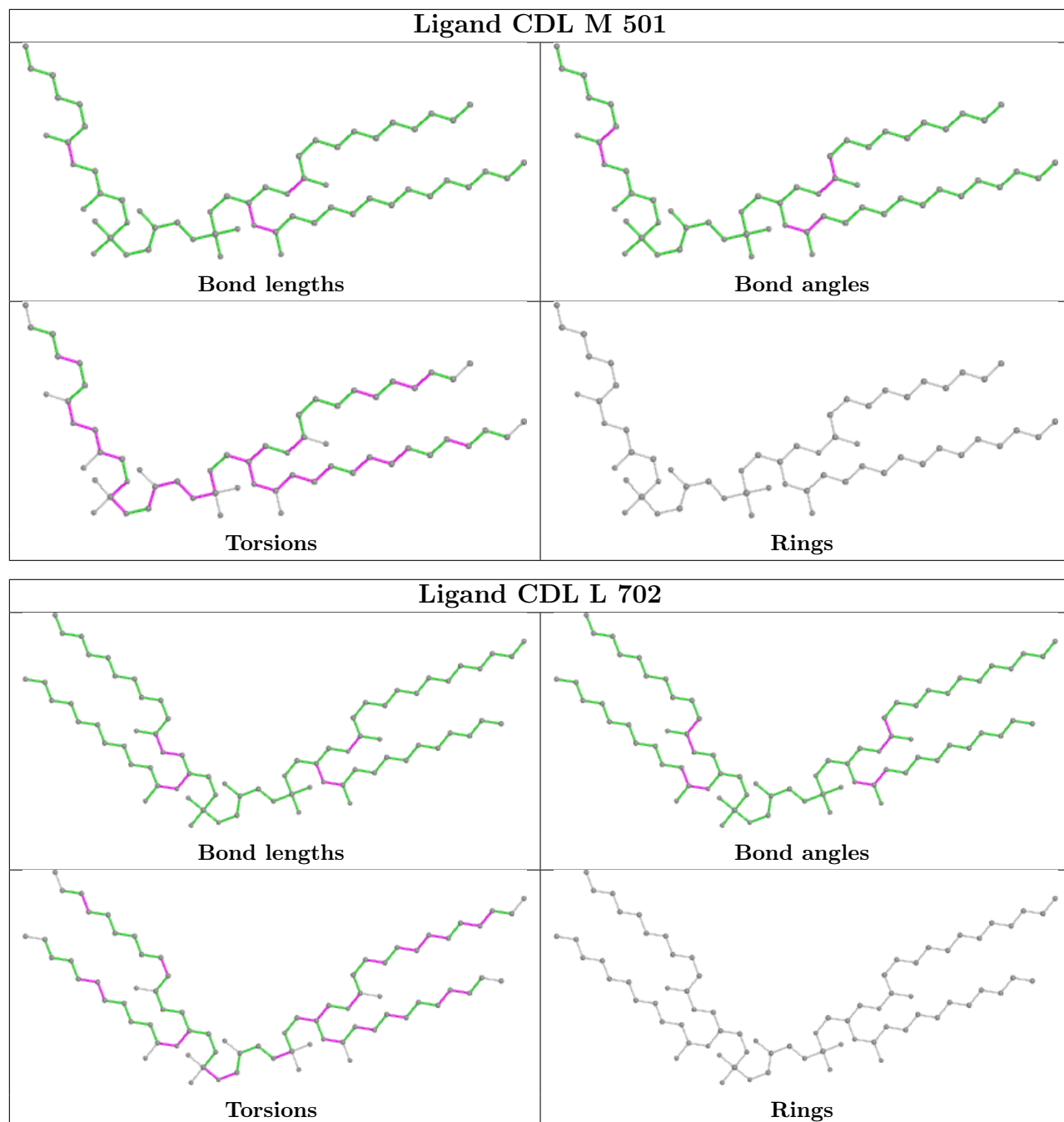


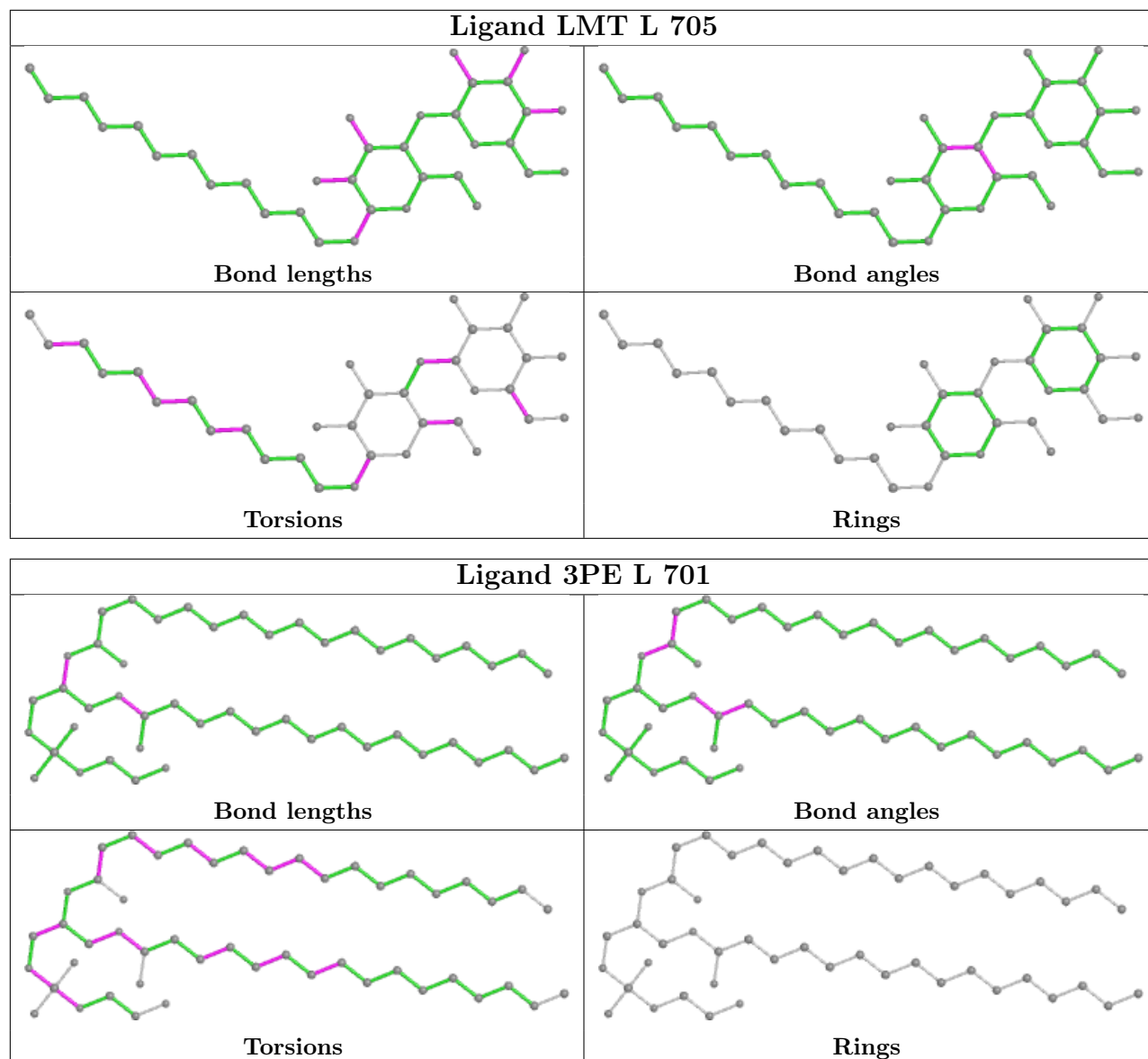


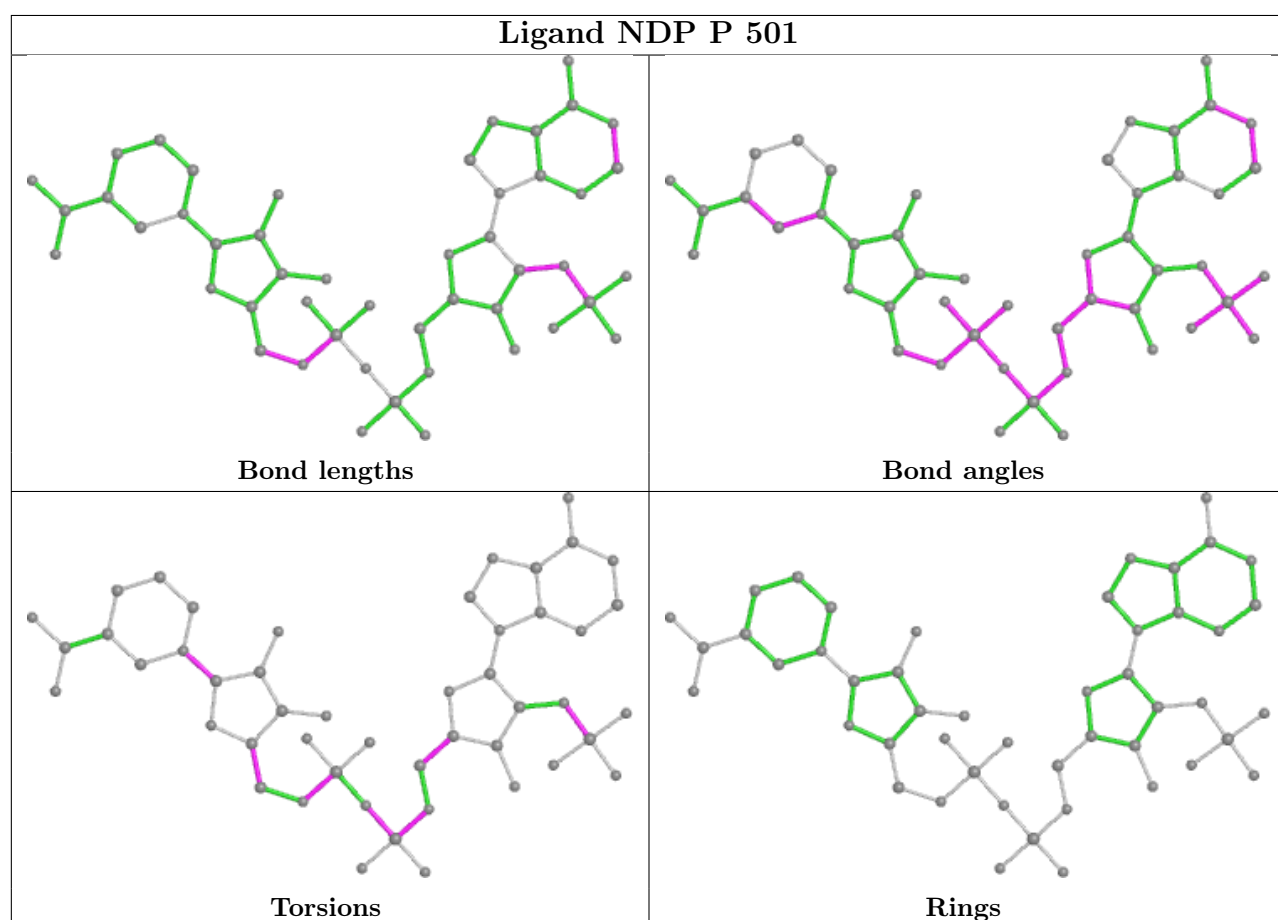
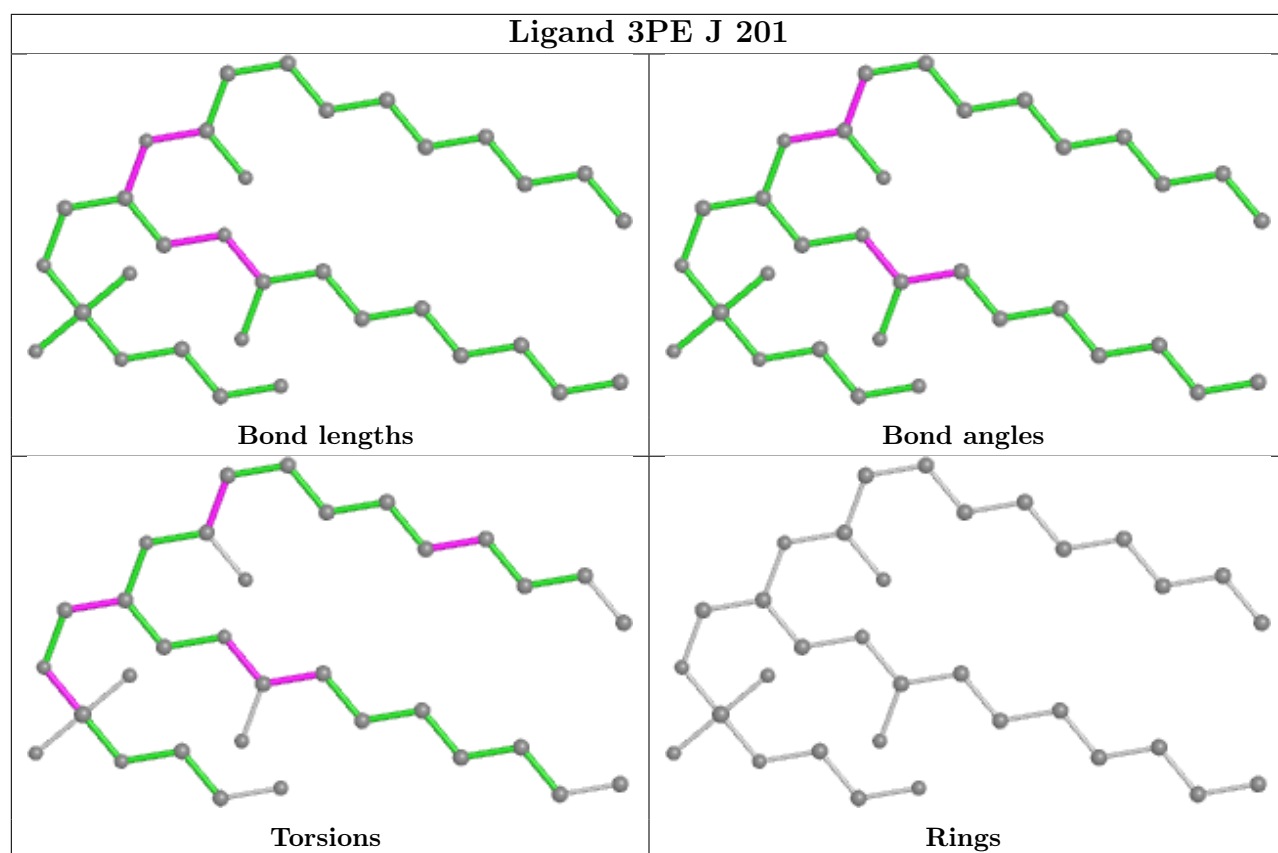


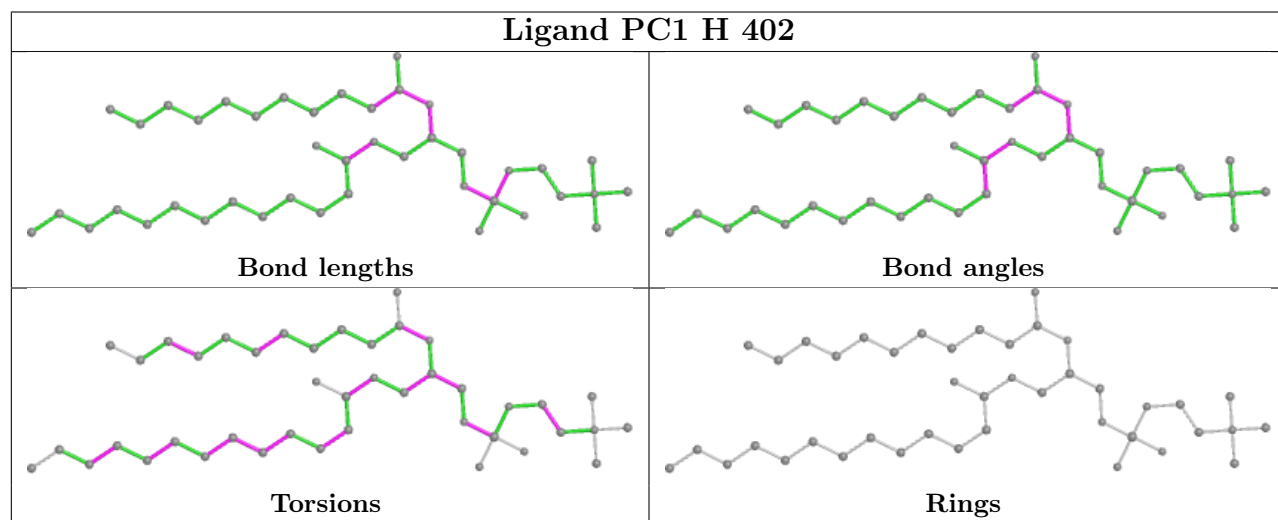
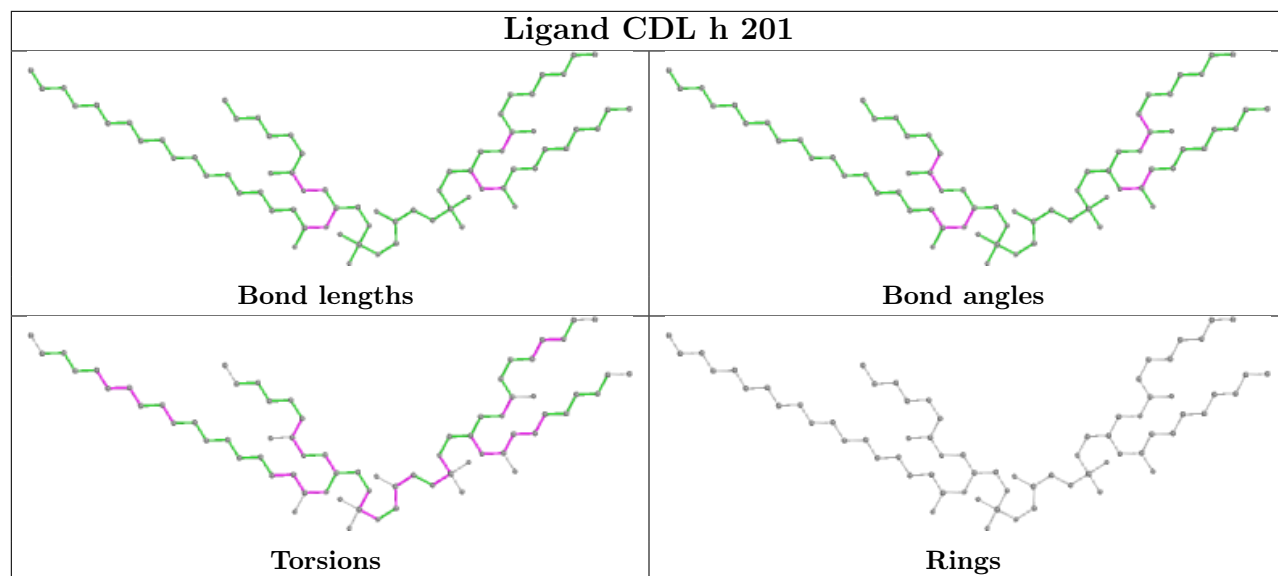


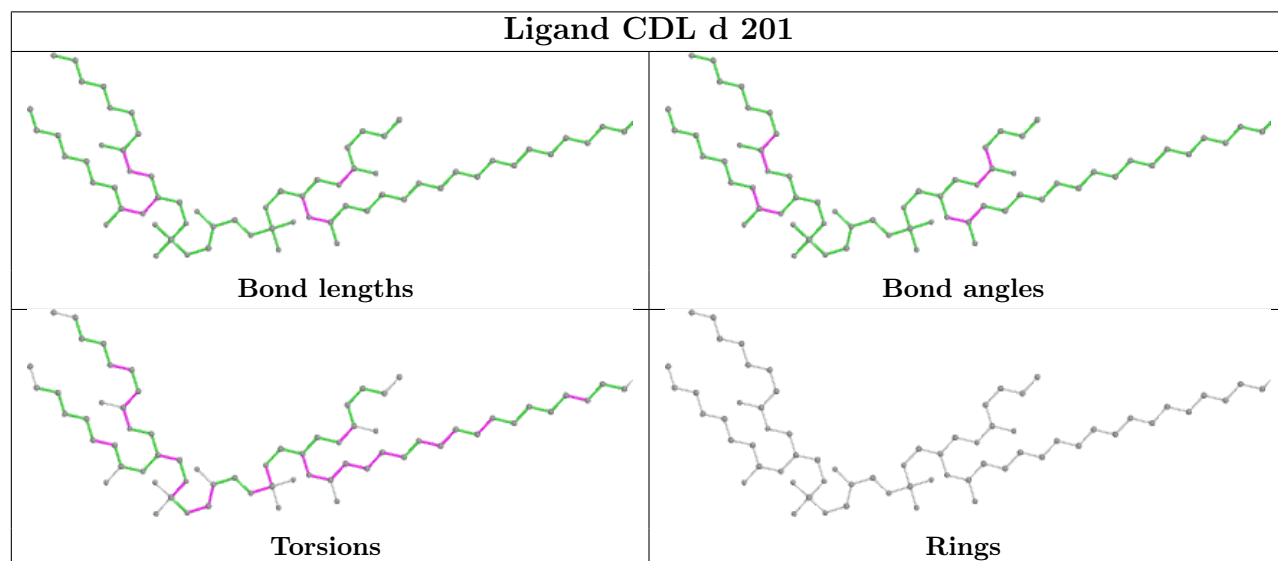
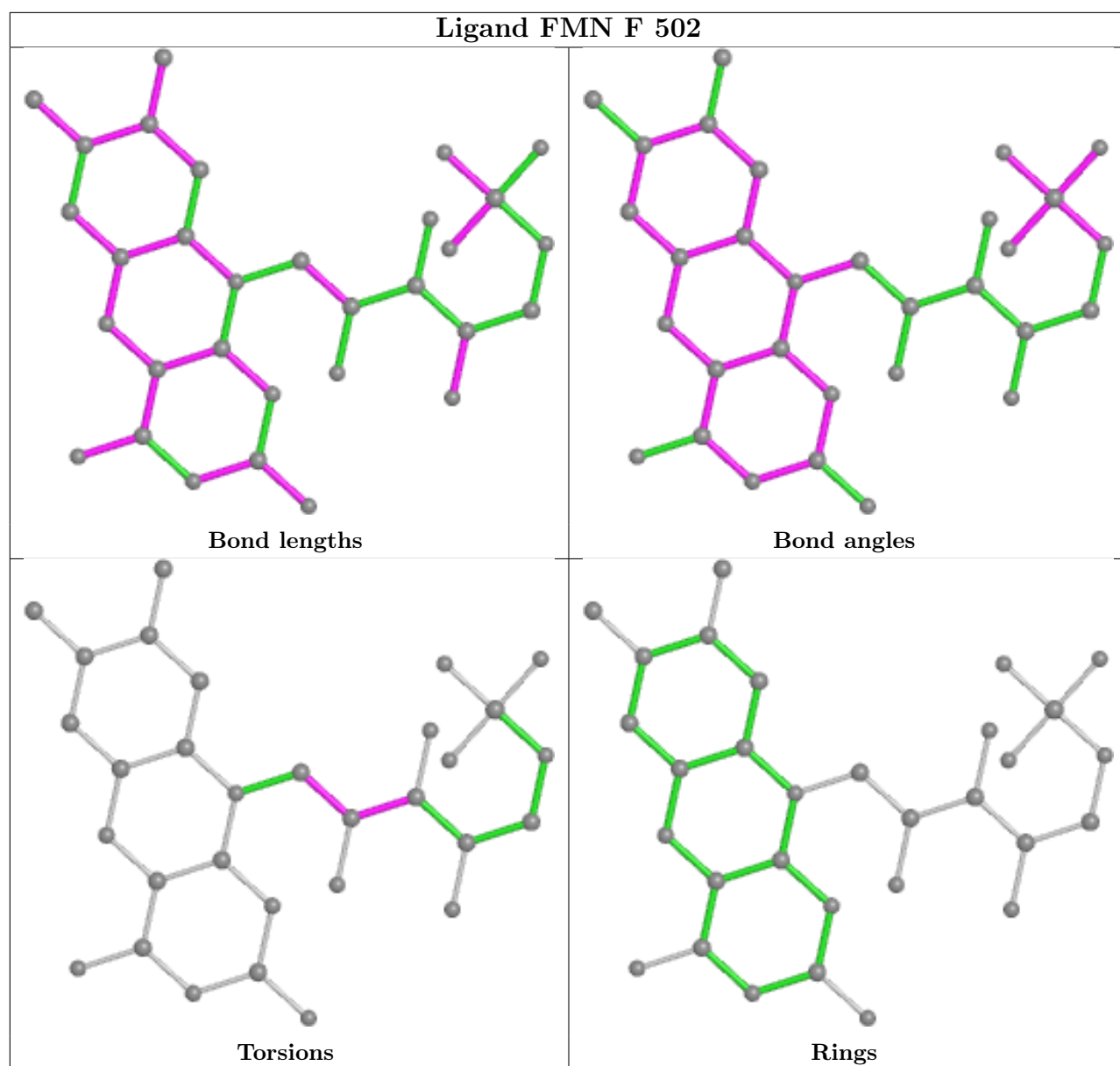


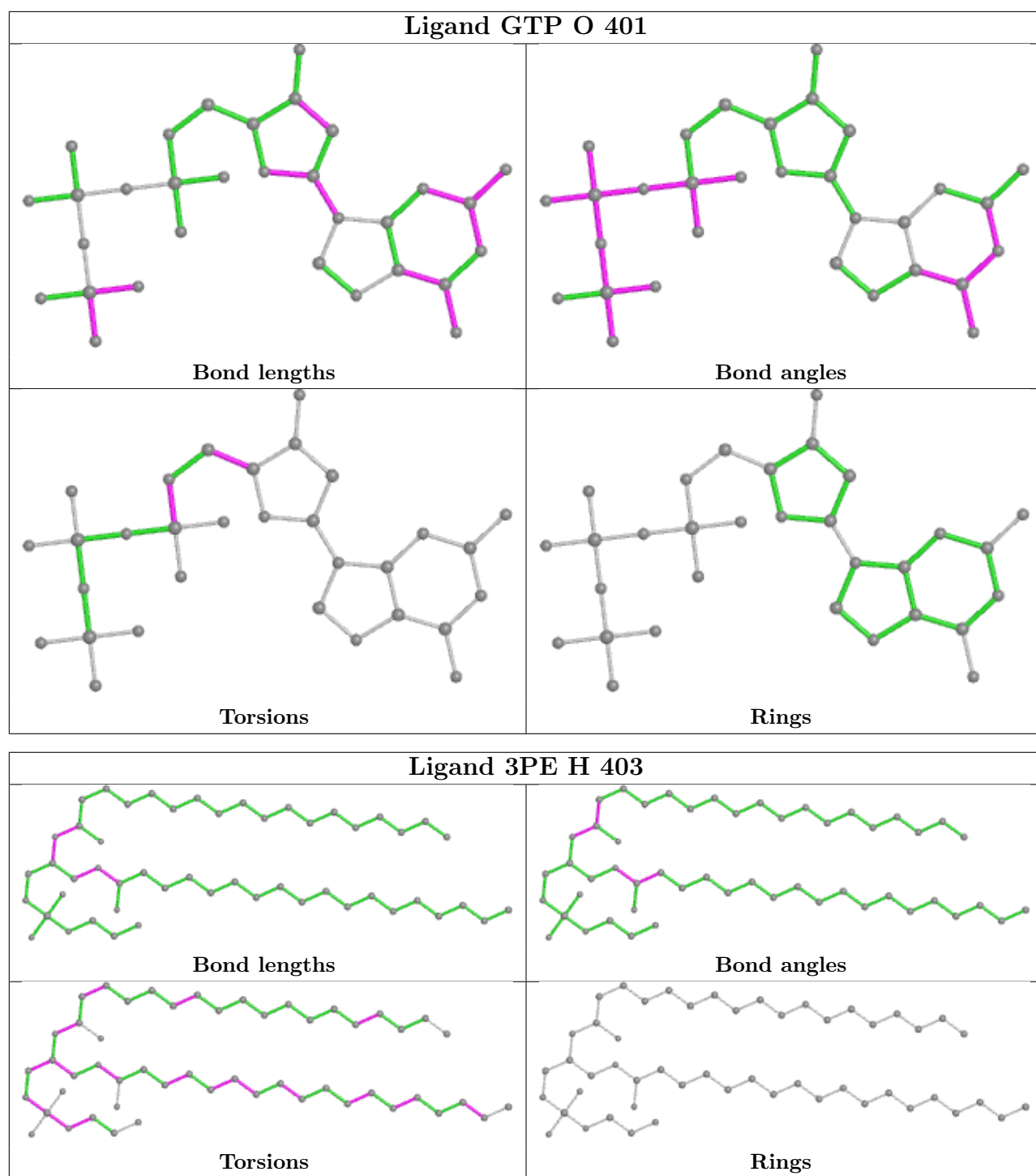












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

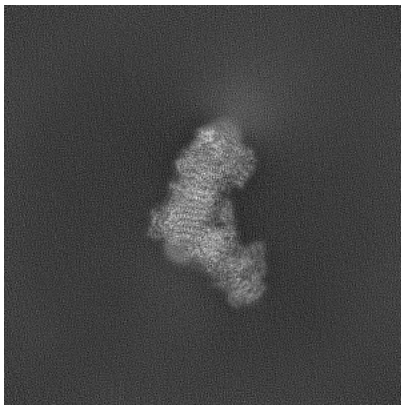
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16516. These allow visual inspection of the internal detail of the map and identification of artifacts.

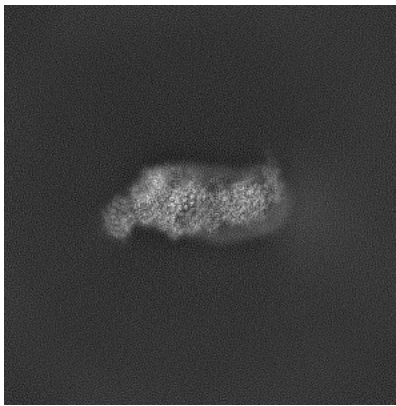
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

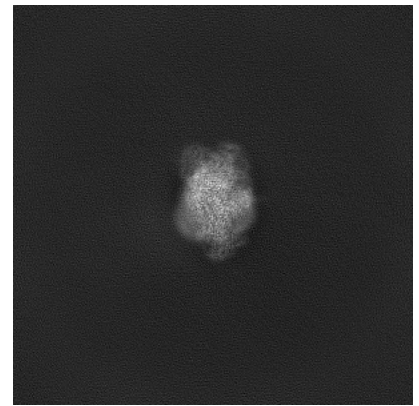
6.1.1 Primary map



X

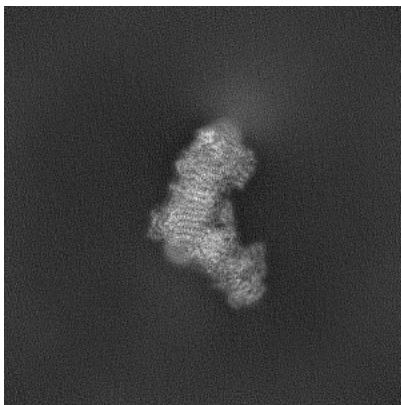


Y

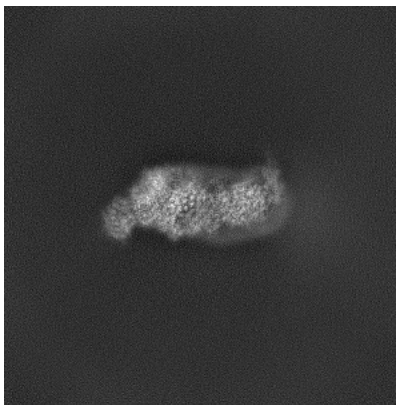


Z

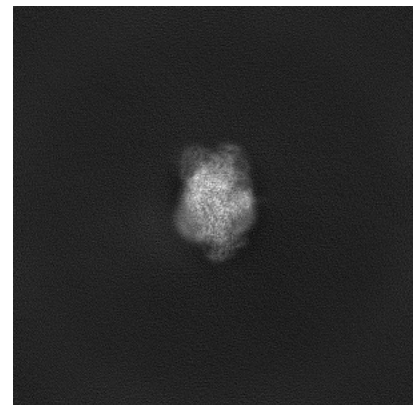
6.1.2 Raw map



X



Y

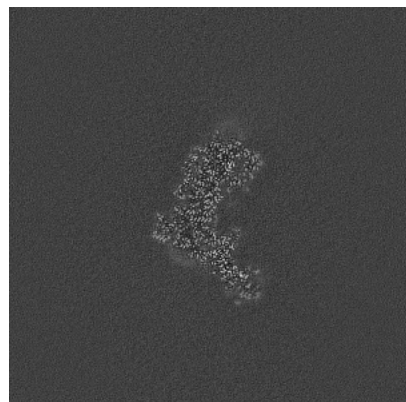


Z

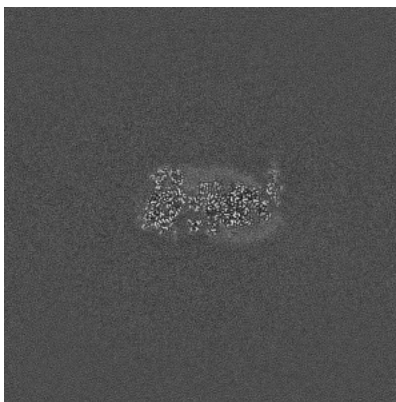
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

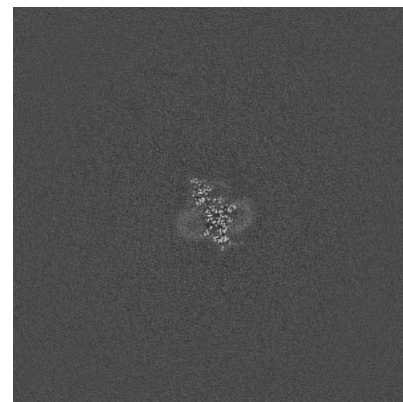
6.2.1 Primary map



X Index: 225

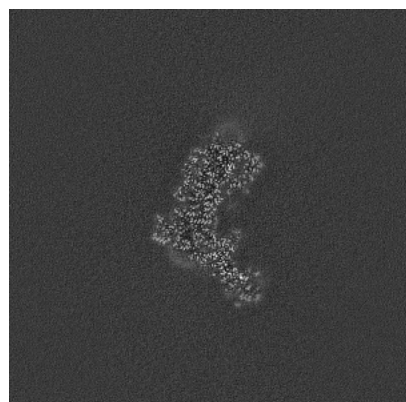


Y Index: 225

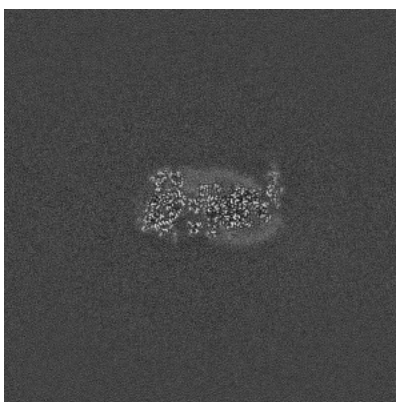


Z Index: 225

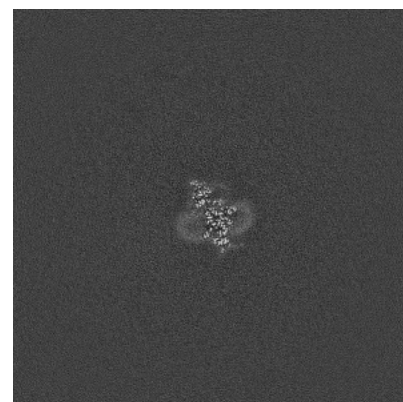
6.2.2 Raw map



X Index: 225



Y Index: 225

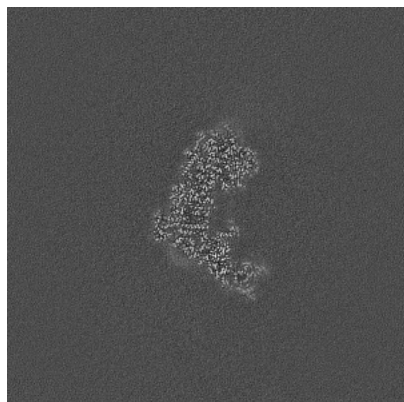


Z Index: 225

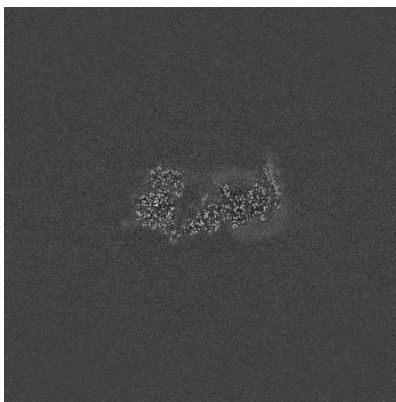
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

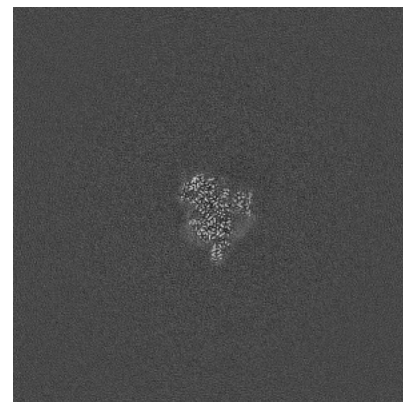
6.3.1 Primary map



X Index: 230

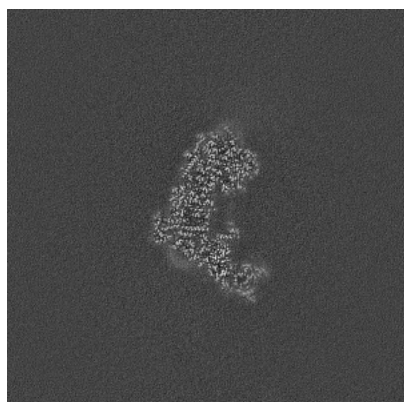


Y Index: 234



Z Index: 189

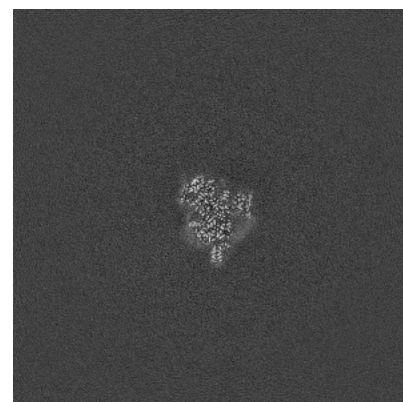
6.3.2 Raw map



X Index: 230



Y Index: 234

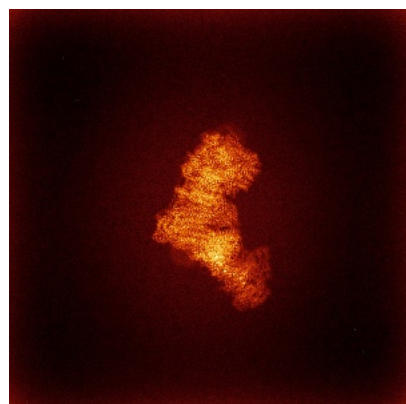


Z Index: 189

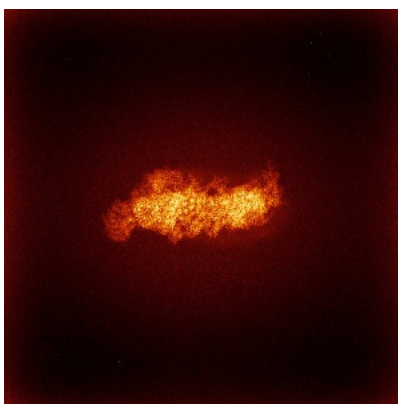
The images above show the largest variance slices of the map in three orthogonal directions.

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

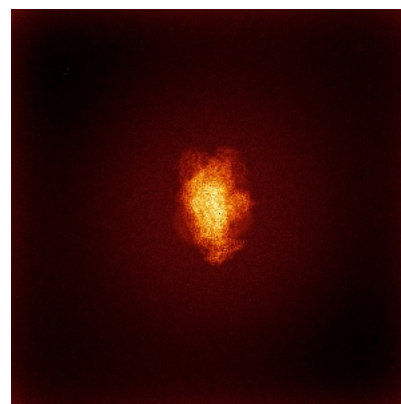
6.4.1 Primary map



X

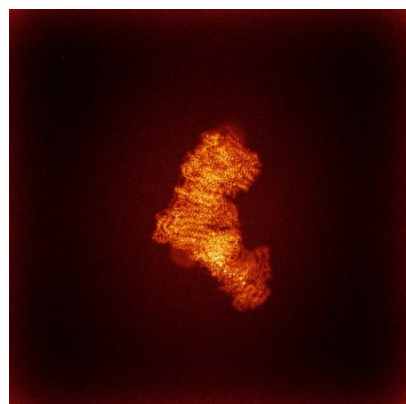


Y

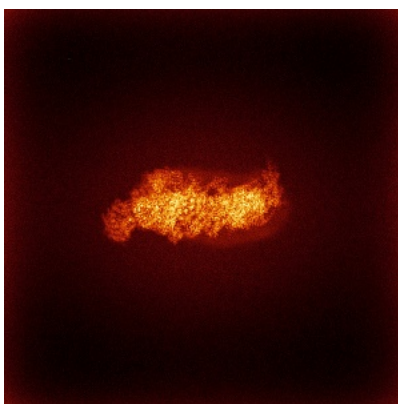


Z

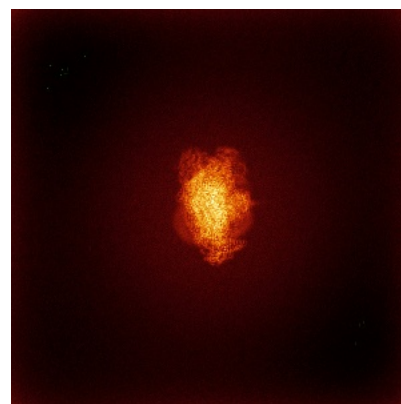
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

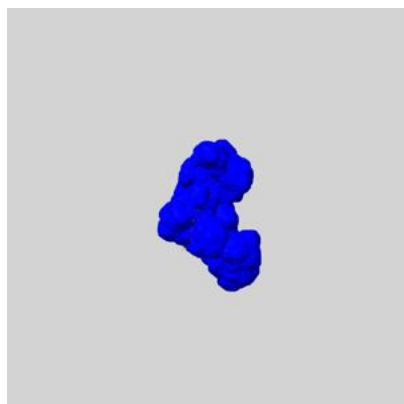
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

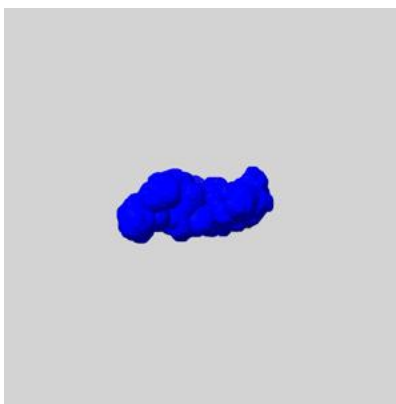
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

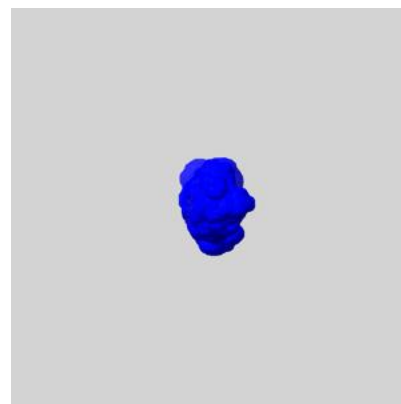
6.6.1 emd_16516_msk_1.map [i](#)



X



Y

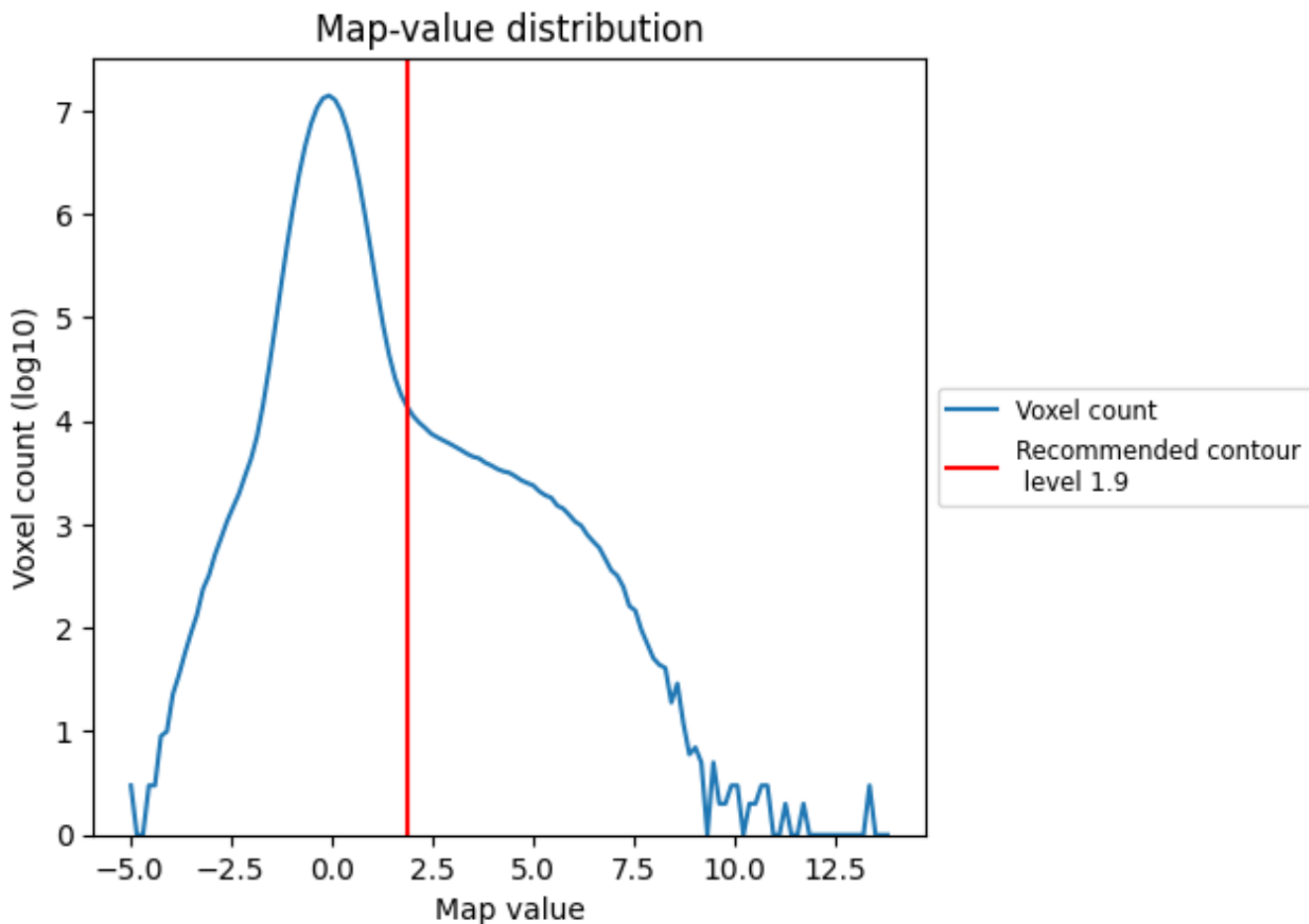


Z

7 Map analysis [i](#)

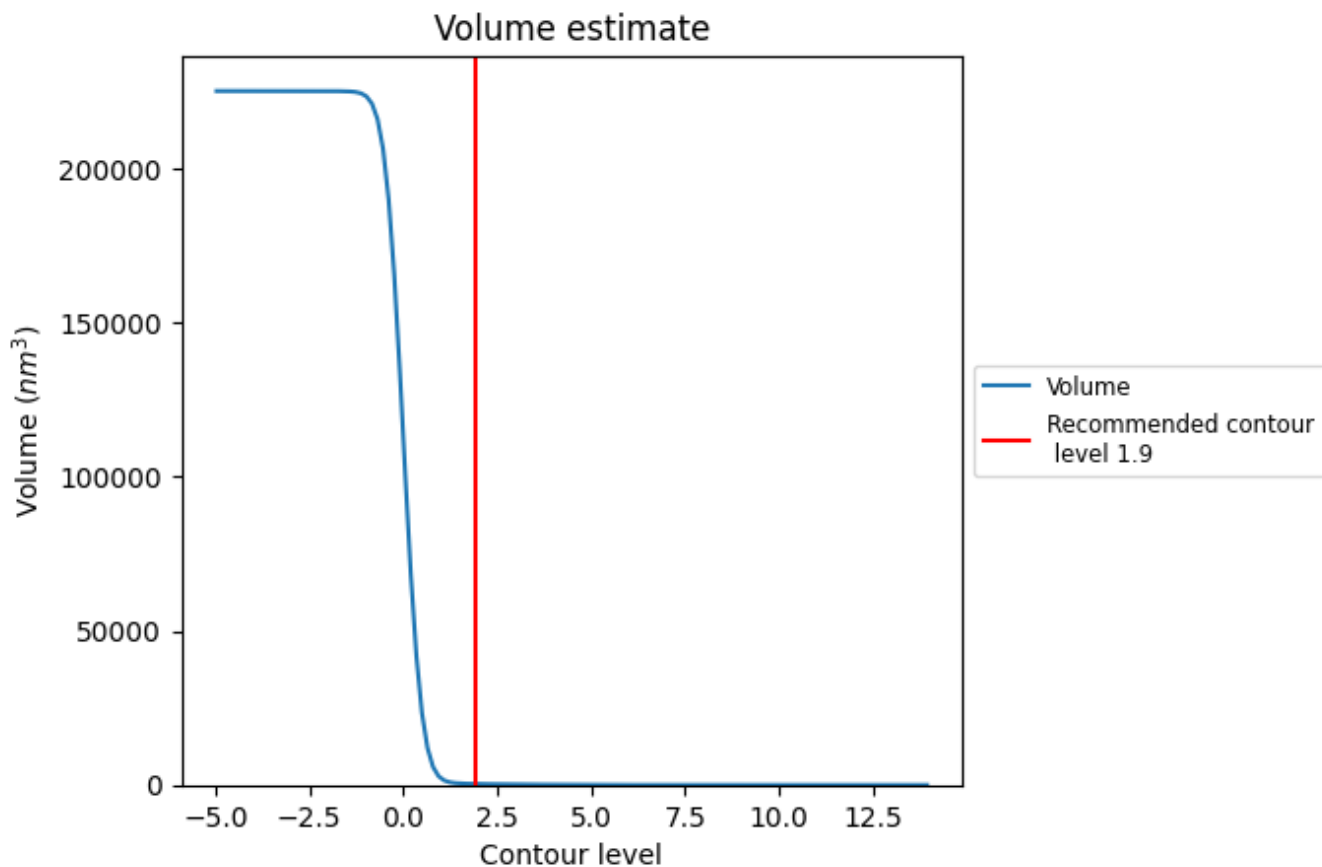
This section contains the results of statistical analysis of the map.

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.

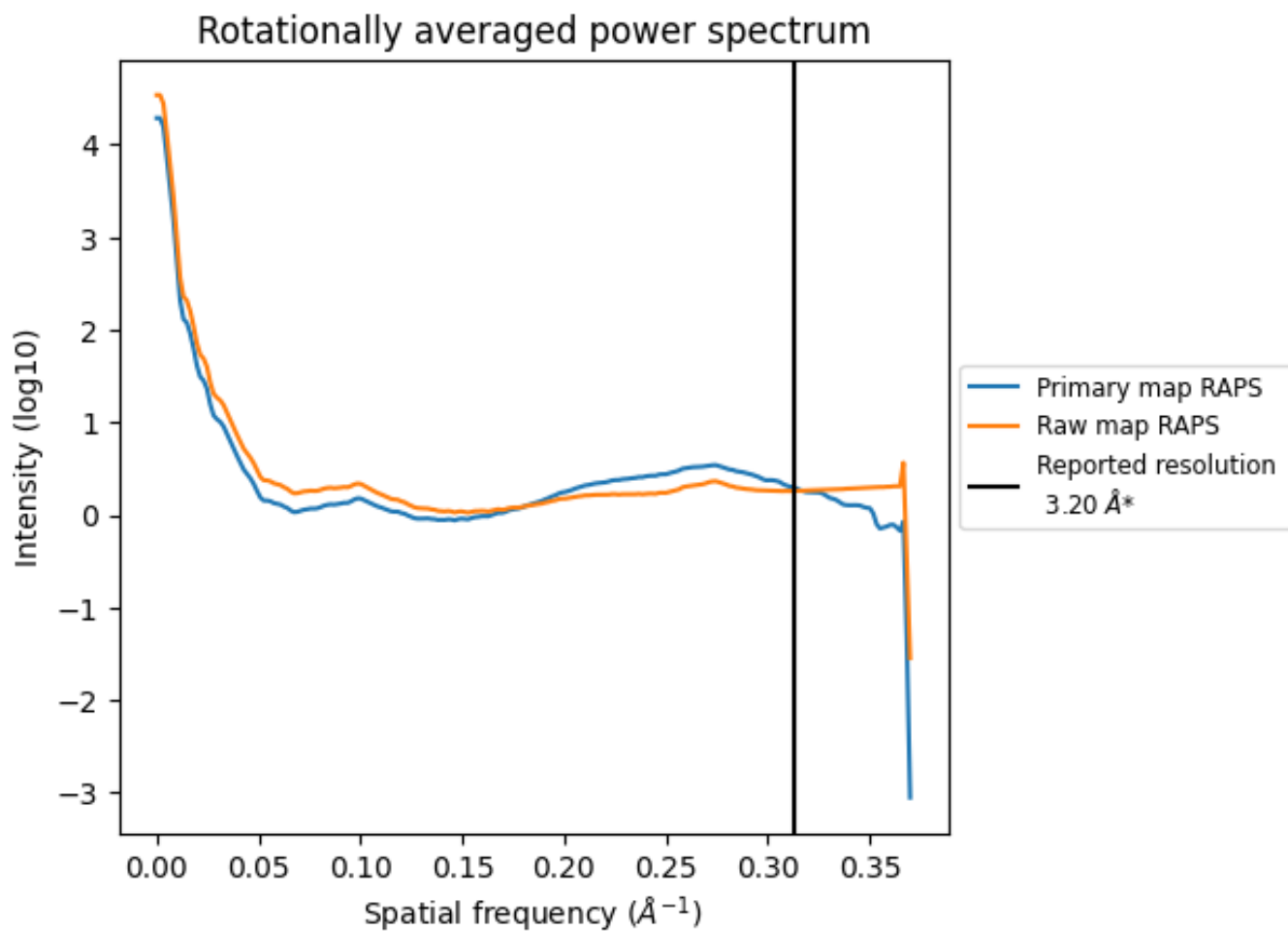
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 339 nm^3 ; this corresponds to an approximate mass of 306 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 [\(i\)](#)

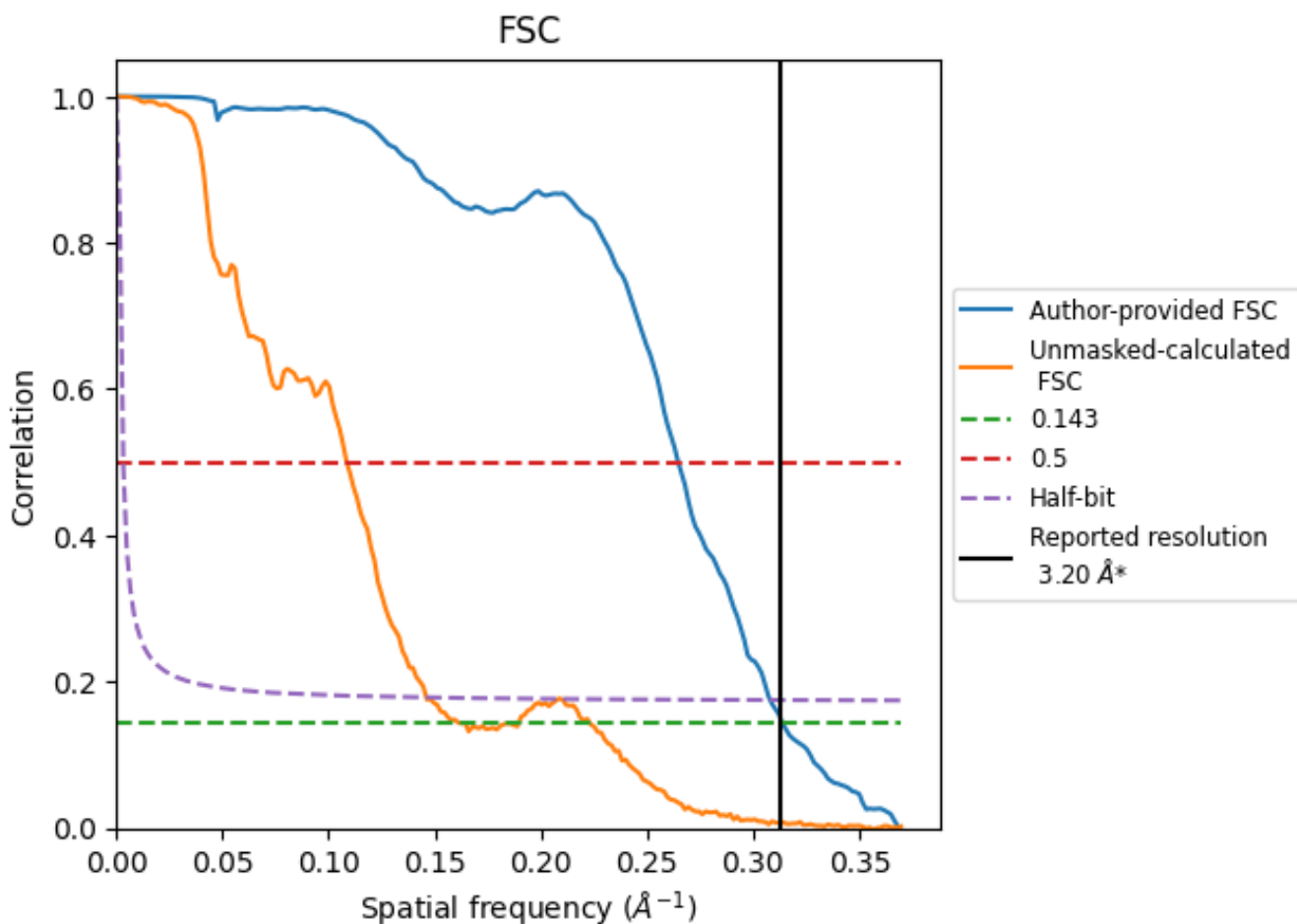


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

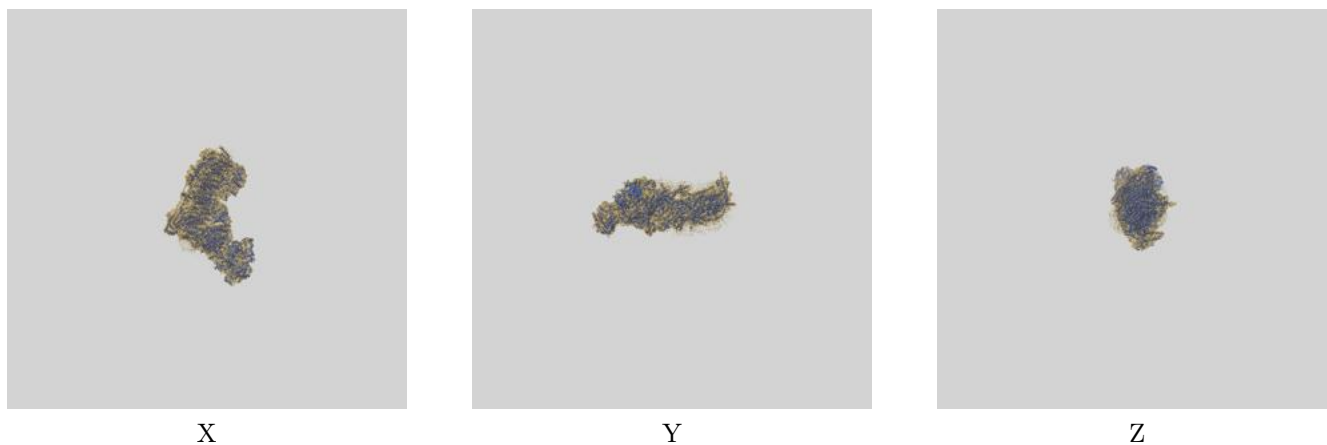
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.78	3.25
Unmasked-calculated*	6.17	9.22	6.85

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.17 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

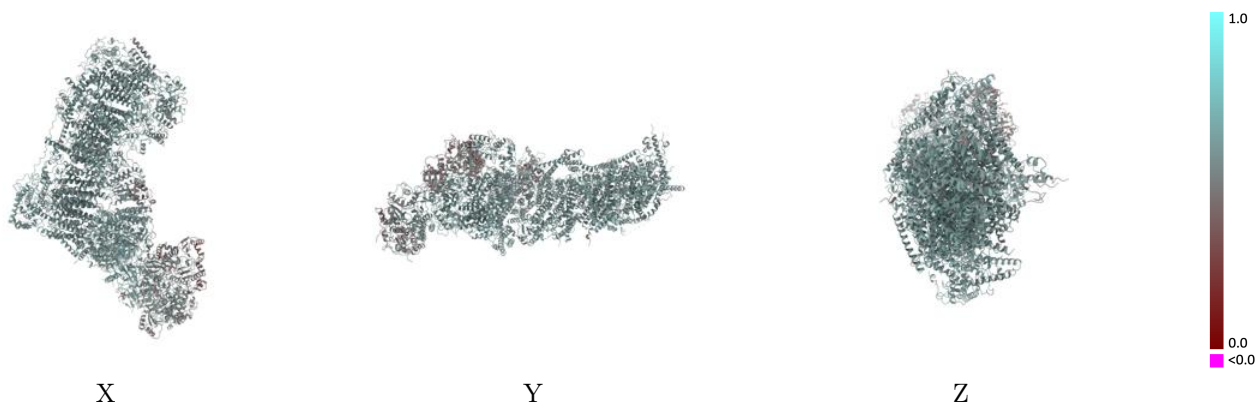
This section contains information regarding the fit between EMDB map EMD-16516 and PDB model 8CA3. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



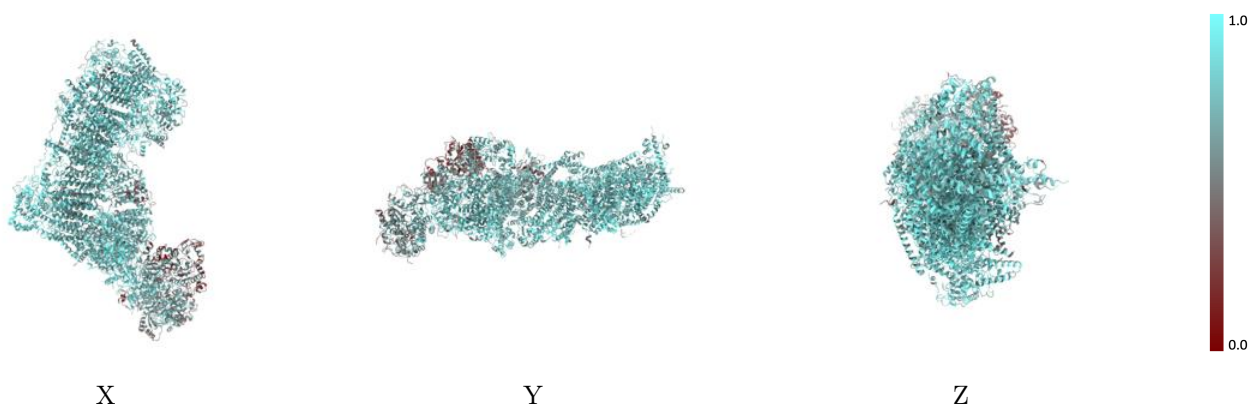
The images above show the 3D surface view of the map at the recommended contour level 1.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



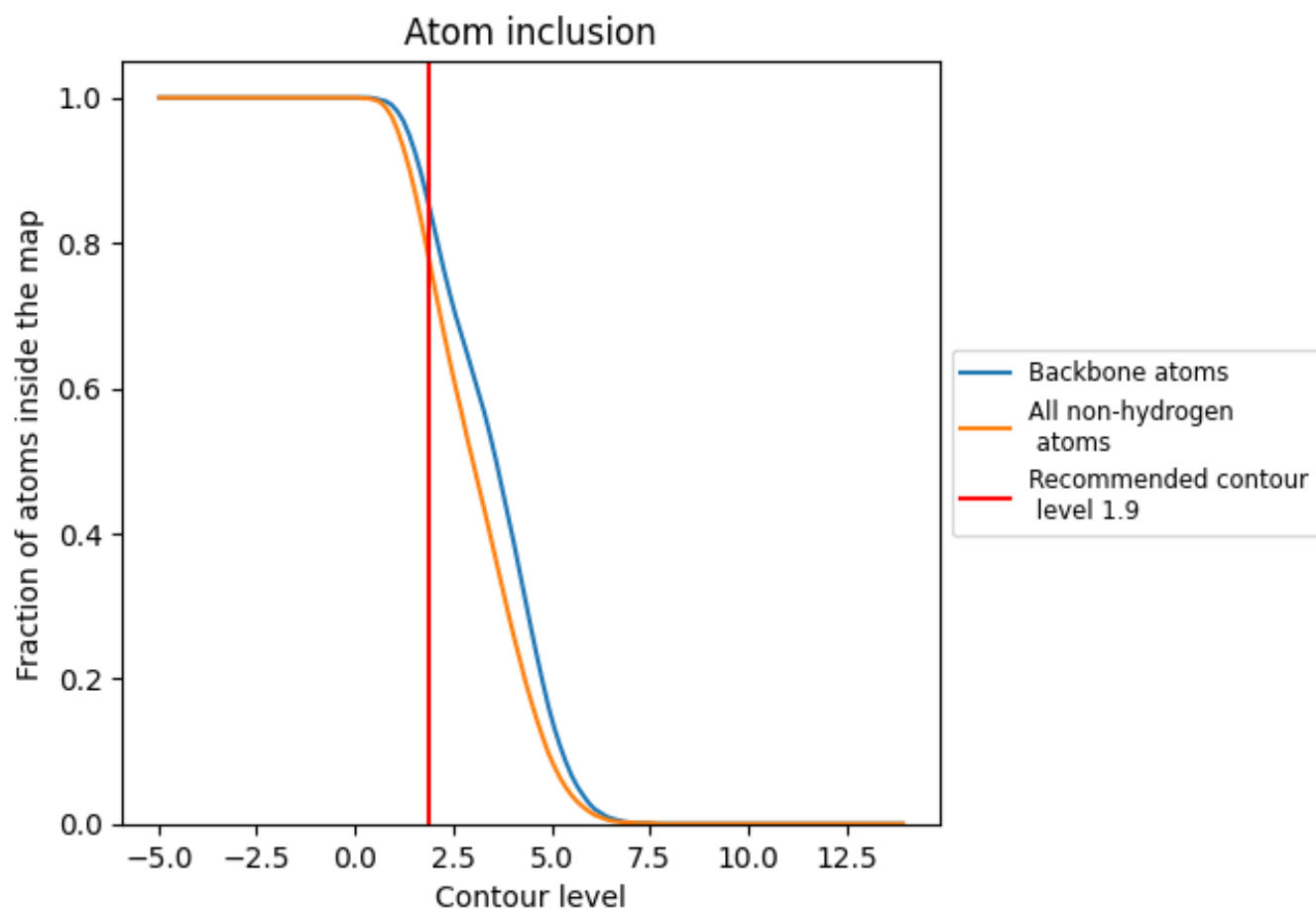
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.9).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 77% 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 (1.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7730	 0.5680
A	 0.8020	 0.5870
B	 0.8710	 0.6010
C	 0.8420	 0.6030
D	 0.8530	 0.6010
E	 0.6070	 0.5000
F	 0.6360	 0.5160
G	 0.5940	 0.5110
H	 0.8160	 0.5850
I	 0.8400	 0.5830
J	 0.7710	 0.5720
K	 0.8210	 0.5880
L	 0.8090	 0.5820
M	 0.8610	 0.5990
N	 0.8350	 0.5950
O	 0.8380	 0.5860
P	 0.7820	 0.5780
R	 0.6150	 0.5580
S	 0.4410	 0.4350
T	 0.4950	 0.4590
U	 0.7570	 0.5510
V	 0.7960	 0.5760
W	 0.7100	 0.5620
X	 0.8320	 0.5800
Y	 0.7610	 0.5640
Z	 0.8000	 0.5770
a	 0.8660	 0.5990
b	 0.8090	 0.5720
c	 0.7670	 0.5620
d	 0.8380	 0.5920
e	 0.8480	 0.5910
f	 0.7340	 0.5520
g	 0.8050	 0.5800
h	 0.8360	 0.5910
i	 0.7640	 0.5670



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
j	 0.7870	 0.5670
k	 0.7570	 0.5510
l	 0.8320	 0.5810
m	 0.8100	 0.5760
n	 0.8140	 0.5770
o	 0.7610	 0.5530
p	 0.8080	 0.5730
r	 0.7730	 0.5880
s	 0.5040	 0.4750