



Full wwPDB EM Validation Report ⓘ

Nov 30, 2022 – 01:30 pm GMT

PDB ID : 7ZMG
EMDB ID : EMD-14797
Title : CryoEM structure of mitochondrial complex I from *Chaetomium thermophilum* (state 1)
Authors : Laube, E.; Kuehlbrandt, W.
Deposited on : 2022-04-19
Resolution : 2.44 Å (reported)
Based on initial models : 6RFQ, 6RFR

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

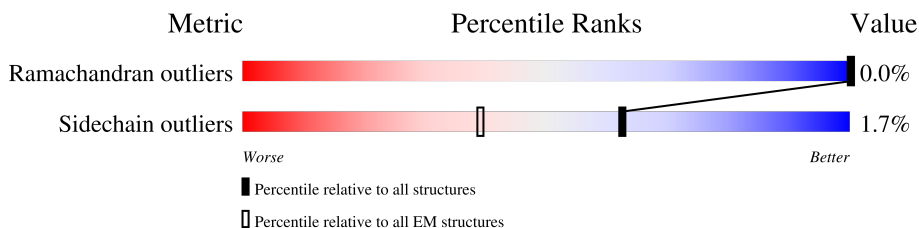
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.44 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.





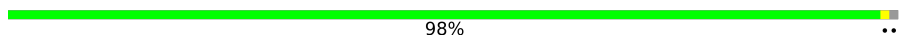







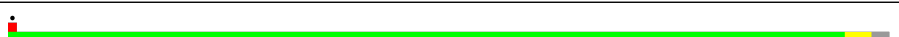


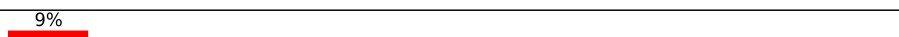
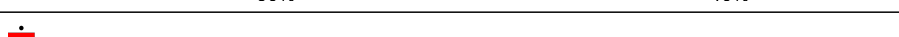
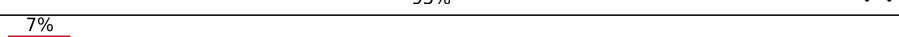
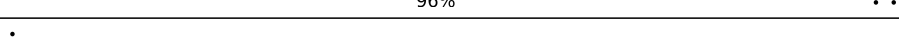
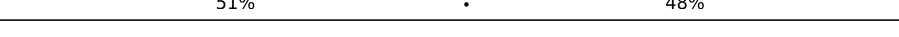

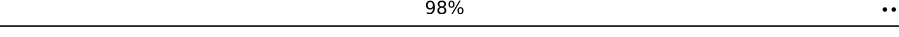
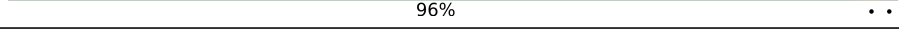

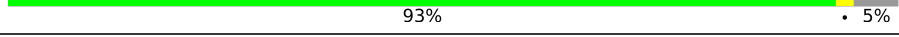


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1	378	87% 12%
2	2	571	96%
3	3	146	79% 20%
4	4	542	90% 9%
5	5	679	96%
6	6	224	83% 15%
7	8	86	88% 10%
8	9	785	13% 87%
9	A	749	93% 5%

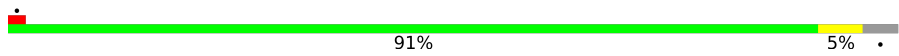

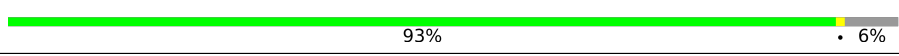
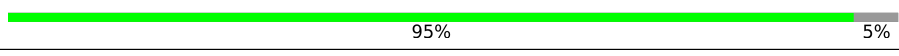
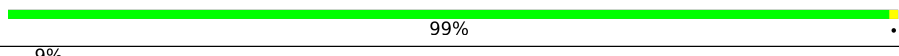

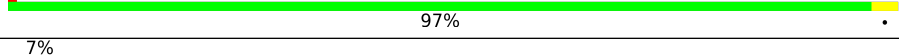

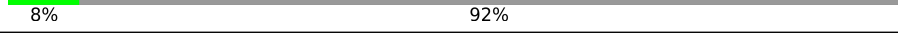
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Mol	Chain	Length	Quality of chain
10	B	507	
11	C	499	
12	D	86	
13	E	378	
14	F	261	
15	G	293	
16	H	318	
17	I	223	
18	J	199	
19	K	230	
20	L	89	
21	M	168	
22	O	141	
22	Q	141	
23	P	124	
24	R	99	
25	S	143	
26	U	186	
27	W	121	
28	X	191	
29	Y	210	
30	Z	196	
31	a	203	
32	b	94	
33	c	93	

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Mol	Chain	Length	Quality of chain
34	d	105	 <p>91% 5%</p>
35	e	46	 <p>78% 17%</p>
36	f	95	 <p>93% 6%</p>
37	g	82	 <p>95% 5%</p>
38	h	134	 <p>99%</p>
39	i	93	 <p>9% 86% 13%</p>
40	j	75	 <p>97%</p>
41	n	184	 <p>7% 73% 26%</p>
42	o	380	 <p>8% 92%</p>

2 Entry composition i

There are 53 unique types of molecules in this entry. The entry contains 70825 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	334	2573	1728	388	446	11	0	0

- Molecule 2 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	558	4459	2994	672	782	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	117	894	608	130	154	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	494	3904	2650	572	670	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	670	5273	3551	792	905	25	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	445	ARG	-	insertion	UNP G1DJA3
5	446	LEU	-	insertion	UNP G1DJA3
5	447	ALA	-	insertion	UNP G1DJA3

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Chain	Residue	Modelled	Actual	Comment	Reference
5	448	ILE	-	insertion	UNP G1DJA3
5	449	ASP	-	insertion	UNP G1DJA3
5	450	ASN	-	insertion	UNP G1DJA3
5	451	PHE	-	insertion	UNP G1DJA3
5	452	PHE	-	insertion	UNP G1DJA3
5	453	SER	-	insertion	UNP G1DJA3
5	454	ALA	-	insertion	UNP G1DJA3
5	455	GLN	-	insertion	UNP G1DJA3
5	456	ALA	-	insertion	UNP G1DJA3
5	457	ILE	-	insertion	UNP G1DJA3
5	458	LYS	-	insertion	UNP G1DJA3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	190	1465	985	221	253	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	8	77	658	408	126	118	6	0	0

- Molecule 8 is a protein called Subunit NDUFS5 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	9	103	807	500	147	154	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	100	VAL	-	insertion	UNP G0SG48

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	A	711	5476	3444	966	1035	31	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP G0RYA1
A	72	TYR	VAL	conflict	UNP G0RYA1
A	73	CYS	SER	conflict	UNP G0RYA1
A	74	TYR	MET	conflict	UNP G0RYA1
A	75	HIS	ARG	conflict	UNP G0RYA1
A	76	GLU	ARG	conflict	UNP G0RYA1

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	B	456	3538	2225	638	648	27	0	0

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase 49 kDa subunit-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C	425	3376	2152	587	618	19	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LYS	deletion	UNP G0SCG0
C	?	-	LEU	deletion	UNP G0SCG0
C	?	-	THR	deletion	UNP G0SCG0
C	?	-	ILE	deletion	UNP G0SCG0
C	?	-	ALA	deletion	UNP G0SCG0
C	?	-	PRO	deletion	UNP G0SCG0
C	?	-	LYS	deletion	UNP G0SCG0

- Molecule 12 is a protein called Subunit NDUFA1 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	D	85	678	432	127	115	4	0	0

- Molecule 13 is a protein called NADH dehydrogenase (Ubiquinone)-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	E	353	2886	1832	511	533	10	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	103	GLU	-	insertion	UNP G0SB35
E	104	PHE	-	insertion	UNP G0SB35
E	105	ASP	-	insertion	UNP G0SB35
E	106	LEU	-	insertion	UNP G0SB35
E	107	ARG	-	insertion	UNP G0SB35
E	108	ASN	-	insertion	UNP G0SB35
E	109	THR	-	insertion	UNP G0SB35
E	110	GLN	-	insertion	UNP G0SB35
E	233	HIS	-	insertion	UNP G0SB35
E	234	VAL	-	insertion	UNP G0SB35

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	F	238	1899	1198	330	370	1	0	0

- Molecule 15 is a protein called NADH-ubiquinone oxidoreductase 30.4 kDa subunit-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	G	242	1968	1271	329	361	7	0	0

- Molecule 16 is a protein called Subunit NDUFV2 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	H	221	1702	1071	288	329	14	0	0

- Molecule 17 is a protein called Oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	I	185	1487	941	252	282	12	0	0

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	J	186	1388	877	259	250	2	0	0

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	K	182	1446	922	254	255	15	0	0

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	L	87	673	453	102	115	3	0	0

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	M	118	935	584	178	168	5	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	149	ALA	SER	conflict	UNP G0S6J1
M	150	ASN	-	insertion	UNP G0S6J1
M	151	GLU	-	insertion	UNP G0S6J1
M	152	HIS	-	insertion	UNP G0S6J1
M	153	HIS	-	insertion	UNP G0S6J1
M	154	ARG	-	insertion	UNP G0S6J1
M	155	LYS	-	insertion	UNP G0S6J1
M	156	TYR	-	insertion	UNP G0S6J1
M	157	LEU	-	insertion	UNP G0S6J1
M	158	GLU	-	insertion	UNP G0S6J1
M	159	SER	-	insertion	UNP G0S6J1
M	160	LEU	-	insertion	UNP G0S6J1
M	161	PRO	-	insertion	UNP G0S6J1
M	162	GLN	-	insertion	UNP G0S6J1
M	163	THR	-	insertion	UNP G0S6J1
M	164	SER	-	insertion	UNP G0S6J1
M	165	TYR	-	insertion	UNP G0S6J1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	166	PRO	-	insertion	UNP G0S6J1
M	167	LEU	-	insertion	UNP G0S6J1
M	168	ASN	-	insertion	UNP G0S6J1

- Molecule 22 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	O	80	Total	C	N	O	S	0	0
			633	398	101	133	1		
22	Q	85	Total	C	N	O	S	0	0
			673	422	109	141	1		

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase B14 subunit-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	P	122	Total	C	N	O	S	0	0
			1033	656	197	177	3		

- Molecule 24 is a protein called Complex I-B22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	R	98	Total	C	N	O	S	0	0
			807	520	149	137	1		

- Molecule 25 is a protein called Complex I-ESSS.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	S	74	Total	C	N	O	0	0
			612	402	98	112		

- Molecule 26 is a protein called NADH-ubiquinone oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	U	167	Total	C	N	O	S	0	0
			1357	854	253	241	9		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	W	120	980	625	182	170	3	0	0

- Molecule 28 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	X	187	1484	943	268	265	8	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Y	154	1240	788	219	229	4	0	0

- Molecule 30 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Z	186	1428	895	253	278	2	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	189	SER	-	insertion	UNP G0SEF0
Z	190	TYR	-	insertion	UNP G0SEF0
Z	191	PRO	-	insertion	UNP G0SEF0
Z	192	CYS	-	insertion	UNP G0SEF0
Z	193	ARG	-	insertion	UNP G0SEF0
Z	194	SER	-	insertion	UNP G0SEF0
Z	195	PHE	-	insertion	UNP G0SEF0
Z	196	VAL	-	insertion	UNP G0SEF0

- Molecule 31 is a protein called NADH dehydrogenase (Ubiquinone)-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	a	144	1172	753	196	218	5	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	166	VAL	ALA	conflict	UNP G0RXU4
a	168	ALA	MET	conflict	UNP G0RXU4
a	?	-	GLU	deletion	UNP G0RXU4
a	?	-	GLY	deletion	UNP G0RXU4
a	?	-	ASP	deletion	UNP G0RXU4
a	?	-	PRO	deletion	UNP G0RXU4
a	?	-	ASP	deletion	UNP G0RXU4
a	?	-	PRO	deletion	UNP G0RXU4

- Molecule 32 is a protein called Subunit NDUFC2 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	b	81	683	445	125	110	3	0	0

- Molecule 33 is a protein called Subunit NDUF3 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	c	61	505	329	91	83	2	0	0

- Molecule 34 is a protein called Subunit NDUF10 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	d	101	843	535	149	155	4	0	0

- Molecule 35 is a protein called Subunit NDUF2 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	e	38	317	215	55	46	1	0	0

- Molecule 36 is a protein called NADH dehydrogenase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	f	89	722	462	128	129	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	?	-	ALA	deletion	UNP G0S1P3

- Molecule 37 is a protein called Subunit NDUFA3 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	g	78	610	399	105	105	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	h	134	1132	731	198	201	2	0	0

- Molecule 39 is a protein called Subunit NDUF6 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	i	81	682	450	118	112	2	0	0

- Molecule 40 is a protein called Subunit NDUF4 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	j	75	616	399	110	103	4	0	0

- Molecule 41 is a protein called Subunit NDUF5 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	n	136	1067	683	187	196	1	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	1	MET	-	initiating methionine	UNP G0S086

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Chain	Residue	Modelled	Actual	Comment	Reference
n	2	LEU	-	insertion	UNP G0S086
n	3	ALA	-	insertion	UNP G0S086
n	4	LEU	-	insertion	UNP G0S086
n	5	ARG	-	insertion	UNP G0S086
n	6	GLN	-	insertion	UNP G0S086
n	7	ARG	-	insertion	UNP G0S086
n	8	ALA	-	insertion	UNP G0S086
n	9	ALA	-	insertion	UNP G0S086
n	10	LEU	-	insertion	UNP G0S086
n	11	LEU	-	insertion	UNP G0S086
n	12	ALA	-	insertion	UNP G0S086
n	13	ARG	-	insertion	UNP G0S086
n	14	ARG	-	insertion	UNP G0S086
n	15	VAL	-	insertion	UNP G0S086
n	16	ARG	-	insertion	UNP G0S086
n	17	PRO	-	insertion	UNP G0S086
n	18	THR	-	insertion	UNP G0S086
n	19	VAL	-	insertion	UNP G0S086
n	20	VAL	-	insertion	UNP G0S086
n	21	VAL	-	insertion	UNP G0S086
n	22	PRO	-	insertion	UNP G0S086
n	23	ARG	-	insertion	UNP G0S086
n	24	ASN	-	insertion	UNP G0S086
n	25	ALA	-	insertion	UNP G0S086
n	26	ARG	-	insertion	UNP G0S086
n	27	THR	-	insertion	UNP G0S086
n	28	TYR	-	insertion	UNP G0S086
n	29	ALA	-	insertion	UNP G0S086
n	30	SER	-	insertion	UNP G0S086
n	31	SER	-	insertion	UNP G0S086
n	32	HIS	-	insertion	UNP G0S086
n	33	ASP	-	insertion	UNP G0S086
n	34	HIS	-	insertion	UNP G0S086
n	35	ASP	-	insertion	UNP G0S086
n	36	HIS	-	insertion	UNP G0S086
n	37	HIS	-	insertion	UNP G0S086
n	38	ASP	-	insertion	UNP G0S086
n	39	HIS	-	insertion	UNP G0S086
n	40	HIS	-	insertion	UNP G0S086
n	41	HIS	-	insertion	UNP G0S086
n	42	ASP	-	insertion	UNP G0S086
n	43	HIS	-	insertion	UNP G0S086

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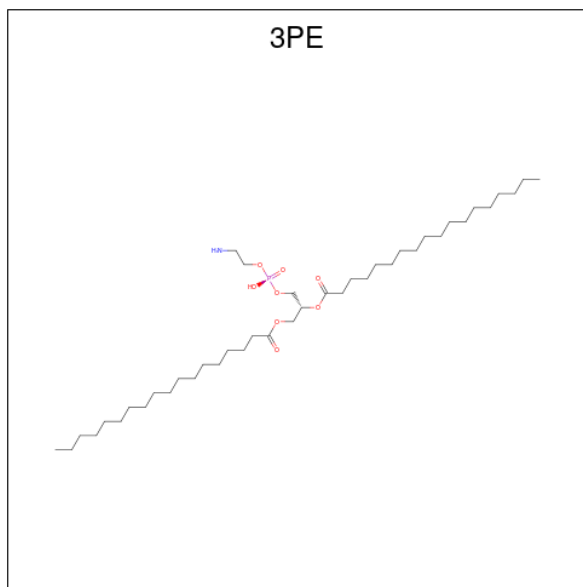
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Chain	Residue	Modelled	Actual	Comment	Reference
n	44	GLY	-	insertion	UNP G0S086
n	45	HIS	-	insertion	UNP G0S086
n	46	ASN	-	insertion	UNP G0S086
n	47	VAL	-	insertion	UNP G0S086
n	48	GLU	-	insertion	UNP G0S086
n	49	GLU	-	insertion	UNP G0S086
n	50	PRO	-	insertion	UNP G0S086
n	51	LEU	-	insertion	UNP G0S086
n	52	GLY	-	insertion	UNP G0S086

- Molecule 42 is a protein called Oxidoreductase-like domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	o	32	252	165	43	44	0	0

- Molecule 43 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P).



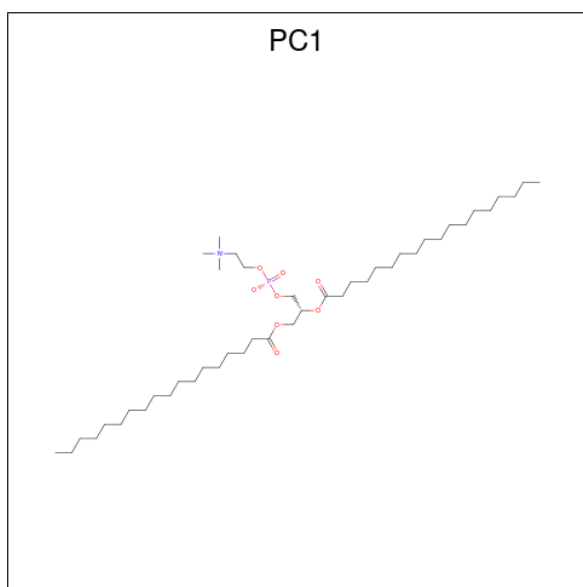
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
43	1	1	32	22	1	8	1	0
43	4	1	118	88	3	24	3	0
43	4	1	118	88	3	24	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
43	4	1	Total 118	C 88	N 3	O 24	P 3	0
43	5	1	Total 142	C 102	N 4	O 32	P 4	0
43	5	1	Total 142	C 102	N 4	O 32	P 4	0
43	5	1	Total 142	C 102	N 4	O 32	P 4	0
43	5	1	Total 142	C 102	N 4	O 32	P 4	0
43	E	1	Total 31	C 21	N 1	O 8	P 1	0
43	I	1	Total 86	C 66	N 2	O 16	P 2	0
43	I	1	Total 86	C 66	N 2	O 16	P 2	0
43	J	1	Total 30	C 20	N 1	O 8	P 1	0
43	W	1	Total 74	C 54	N 2	O 16	P 2	0
43	W	1	Total 74	C 54	N 2	O 16	P 2	0
43	g	1	Total 36	C 26	N 1	O 8	P 1	0
43	i	1	Total 92	C 72	N 2	O 16	P 2	0
43	i	1	Total 92	C 72	N 2	O 16	P 2	0
43	n	1	Total 39	C 29	N 1	O 8	P 1	0

- Molecule 44 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C₄₄H₈₈NO₈P).



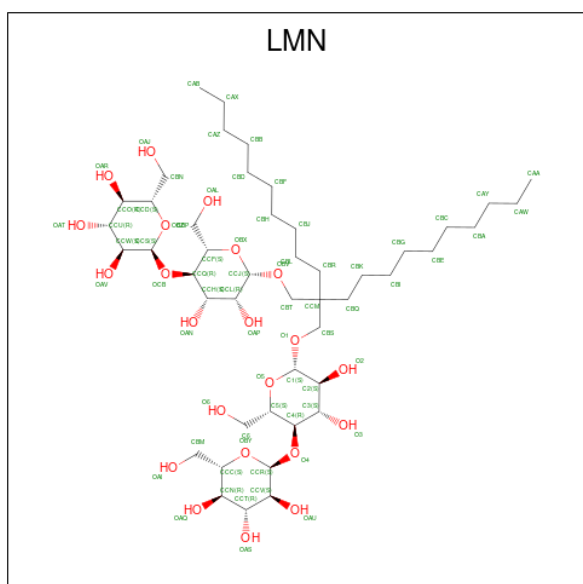
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
44	1	1	Total 43	C 33	N 1	O 8	P 1	0
44	3	1	Total 48	C 38	N 1	O 8	P 1	0
44	4	1	Total 50	C 40	N 1	O 8	P 1	0
44	5	1	Total 97	C 77	N 2	O 16	P 2	0
44	5	1	Total 97	C 77	N 2	O 16	P 2	0
44	K	1	Total 47	C 37	N 1	O 8	P 1	0
44	S	1	Total 51	C 41	N 1	O 8	P 1	0
44	X	1	Total 71	C 51	N 2	O 16	P 2	0
44	X	1	Total 71	C 51	N 2	O 16	P 2	0

- Molecule 45 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



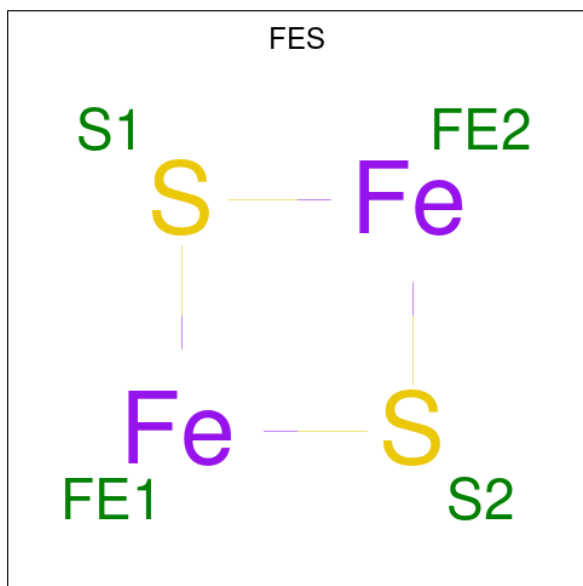
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
45	2	1	74	55	17	2	0
45	D	1	74	55	17	2	0
45	S	1	79	60	17	2	0
45	X	1	77	58	17	2	0
45	g	1	70	51	17	2	0

- Molecule 46 is Lauryl Maltose Neopentyl Glycol (three-letter code: LMN) (formula: $C_{47}H_{88}O_{22}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
46	2	1	58	41	17	0
46	4	1	47	35	12	0
46	5	1	69	47	22	0

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



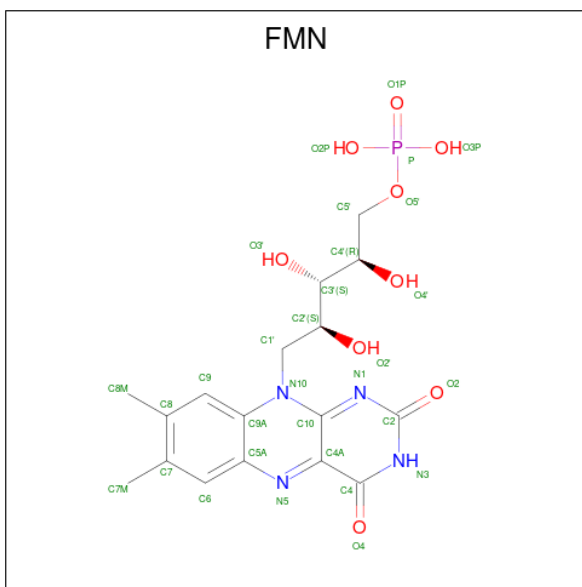
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	A	1	4	2	2	0
47	H	1	4	2	2	0

- Molecule 48 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



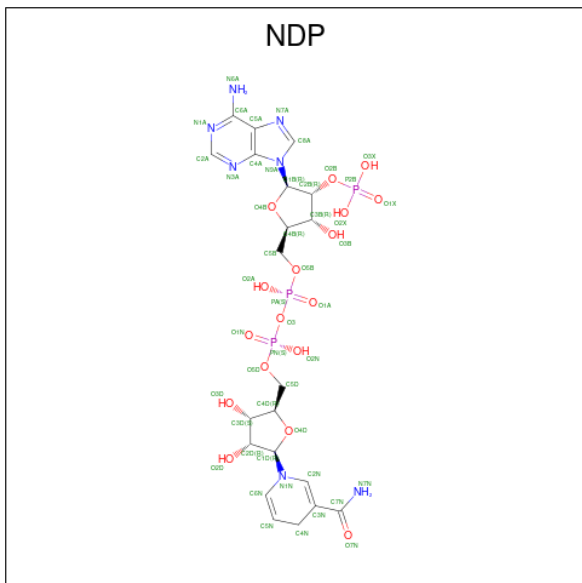
Mol	Chain	Residues	Atoms			AltConf
48	A	1	Total	Fe	S	0
			16	8	8	
48	A	1	Total	Fe	S	0
			16	8	8	
48	B	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			16	8	8	
48	I	1	Total	Fe	S	0
			16	8	8	
48	K	1	Total	Fe	S	0
			8	4	4	

- Molecule 49 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



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

- Molecule 50 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

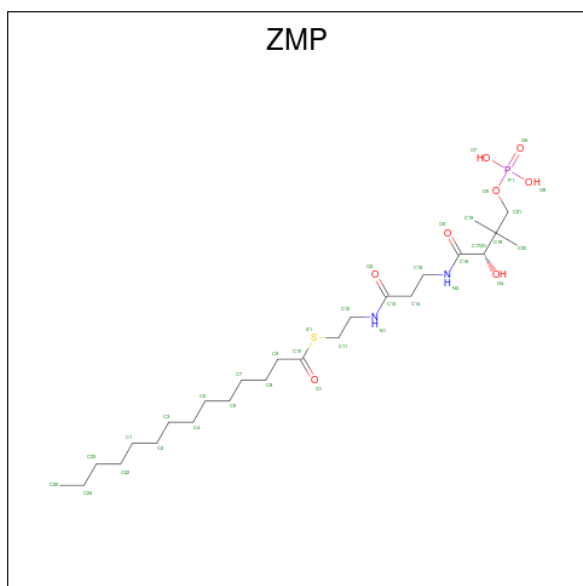


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
50	E	1	48	21	7	17	3	0

- Molecule 51 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
51	M	1	Total	Zn	0
			1	1	

- Molecule 52 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
52	O	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	
52	Q	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	

- Molecule 53 is water.

Mol	Chain	Residues	Atoms		AltConf
53	1	134	Total	O	0
			134	134	
53	2	214	Total	O	0
			214	214	
53	3	31	Total	O	0
			31	31	
53	4	115	Total	O	0
			115	115	
53	5	28	Total	O	0
			28	28	
53	6	56	Total	O	0
			56	56	

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Mol	Chain	Residues	Atoms		AltConf
53	9	19	Total 19	O 19	0
53	A	319	Total 319	O 319	0
53	B	73	Total 73	O 73	0
53	C	257	Total 257	O 257	0
53	D	41	Total 41	O 41	0
53	E	88	Total 88	O 88	0
53	F	65	Total 65	O 65	0
53	G	172	Total 172	O 172	0
53	H	34	Total 34	O 34	0
53	I	124	Total 124	O 124	0
53	J	1	Total 1	O 1	0
53	K	107	Total 107	O 107	0
53	L	25	Total 25	O 25	0
53	M	81	Total 81	O 81	0
53	P	42	Total 42	O 42	0
53	R	3	Total 3	O 3	0
53	S	3	Total 3	O 3	0
53	U	67	Total 67	O 67	0
53	W	64	Total 64	O 64	0
53	X	81	Total 81	O 81	0
53	Y	163	Total 163	O 163	0

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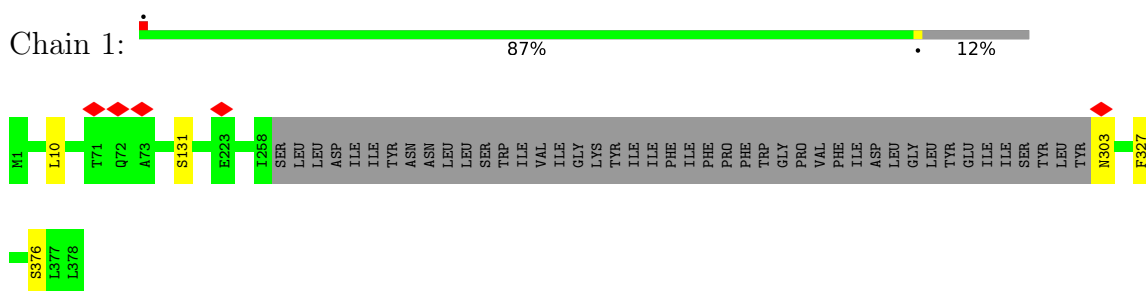
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Mol	Chain	Residues	Atoms		AltConf
53	Z	84	Total 84	O 84	0
53	a	8	Total 8	O 8	0
53	b	11	Total 11	O 11	0
53	d	8	Total 8	O 8	0
53	f	6	Total 6	O 6	0
53	g	20	Total 20	O 20	0
53	h	58	Total 58	O 58	0
53	j	9	Total 9	O 9	0
53	n	37	Total 37	O 37	0
53	o	1	Total 1	O 1	0

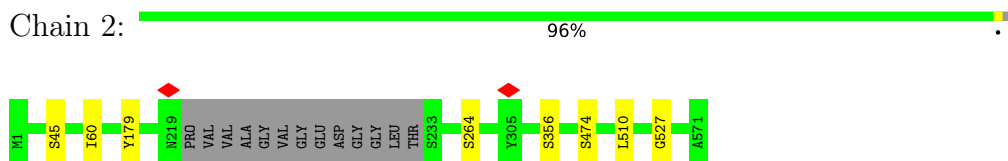
3 Residue-property plots [i](#)

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.

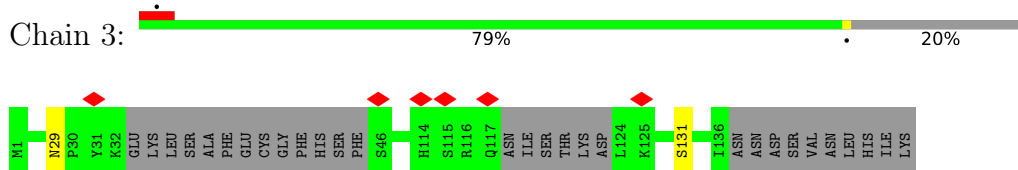
- Molecule 1: NADH-ubiquinone oxidoreductase chain 1



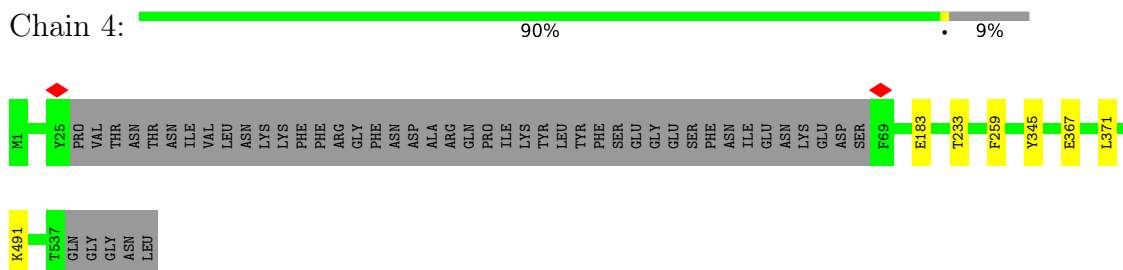
- Molecule 2: NADH dehydrogenase subunit 2



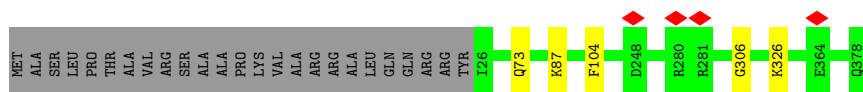
- Molecule 3: NADH-ubiquinone oxidoreductase chain 3



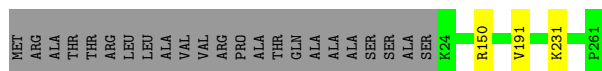
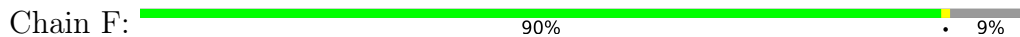
- Molecule 4: NADH-ubiquinone oxidoreductase chain 4



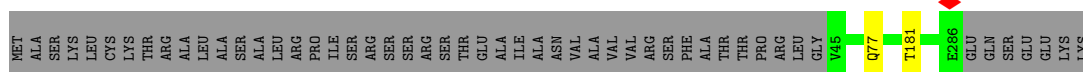
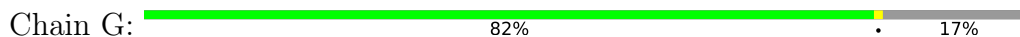
- Molecule 5: NADH-ubiquinone oxidoreductase chain 5



- Molecule 14: NADH-ubiquinone oxidoreductase-like protein



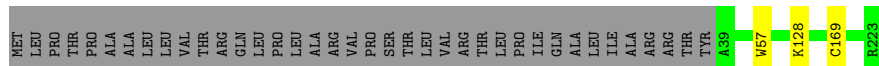
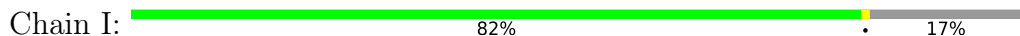
- Molecule 15: NADH-ubiquinone oxidoreductase 30.4 kDa subunit-like protein



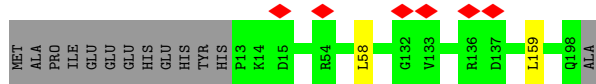
- Molecule 16: Subunit NDUFV2 of NADH-ubiquinone oxidoreductase (Complex I)



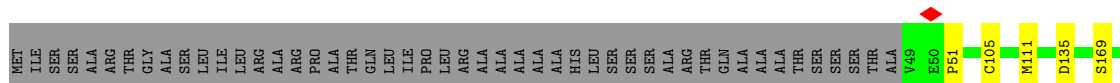
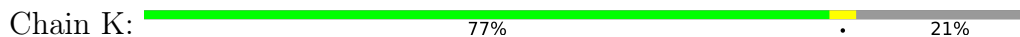
- Molecule 17: Oxidoreductase-like protein

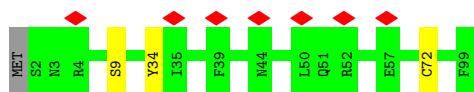


- Molecule 18: NADH-ubiquinone oxidoreductase-like protein

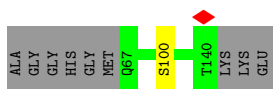


- Molecule 19: NADH-ubiquinone oxidoreductase-like protein

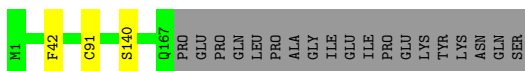
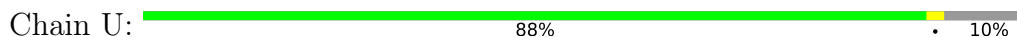




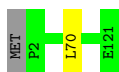
- Molecule 25: Complex I-ESSS



- Molecule 26: NADH-ubiquinone oxidoreductase



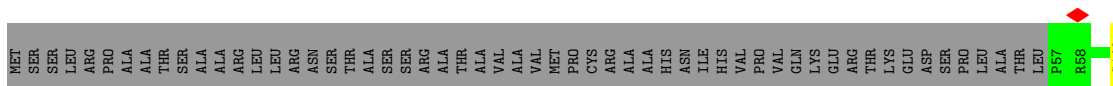
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



- Molecule 28: NADH-ubiquinone oxidoreductase-like protein



- Molecule 29: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

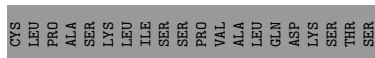
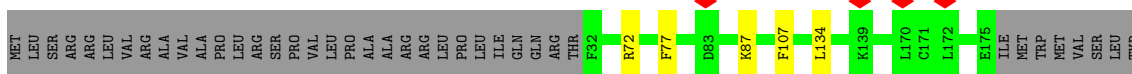


- Molecule 30: NADH-ubiquinone oxidoreductase-like protein

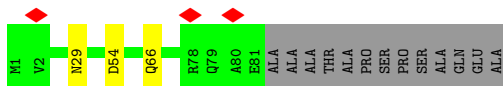
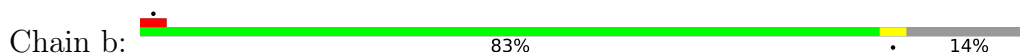




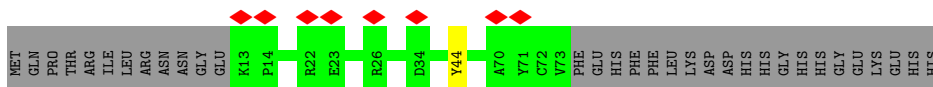
- Molecule 31: NADH dehydrogenase (Ubiquinone)-like protein



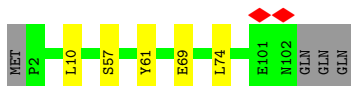
- Molecule 32: Subunit NDUFC2 of NADH-ubiquinone oxidoreductase (Complex I)



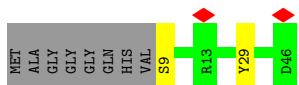
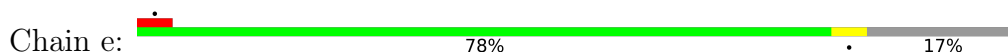
- Molecule 33: Subunit NDUF3 of NADH-ubiquinone oxidoreductase (Complex I)



- Molecule 34: Subunit NDUF10 of NADH-ubiquinone oxidoreductase (Complex I)



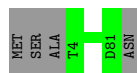
- Molecule 35: Subunit NDUF2 of NADH-ubiquinone oxidoreductase (Complex I)



- Molecule 36: NADH dehydrogenase-like protein



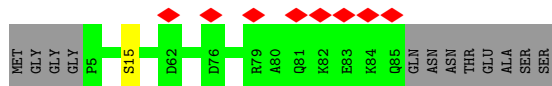
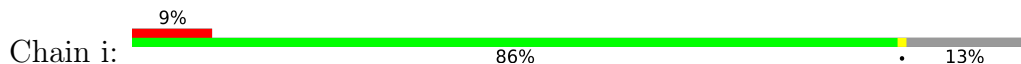
- Molecule 37: Subunit NDUFA3 of NADH-ubiquinone oxidoreductase (Complex I)



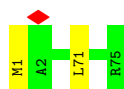
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit



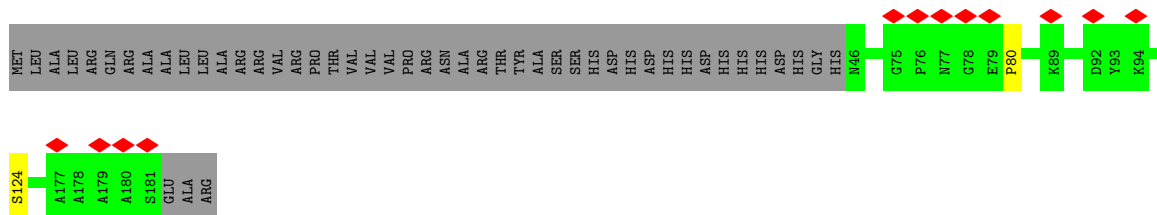
- Molecule 39: Subunit NDUFB6 of NADH-ubiquinone oxidoreductase (Complex I)



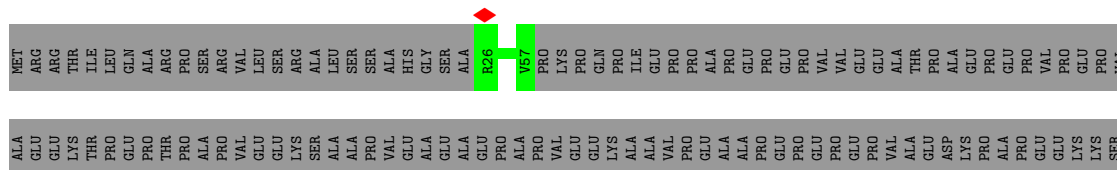
- Molecule 40: Subunit NDUFB4 of NADH-ubiquinone oxidoreductase (Complex I)



- Molecule 41: Subunit NDUFB5 of NADH-ubiquinone oxidoreductase (Complex I)



- Molecule 42: Oxidoreductase-like domain-containing protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	153568	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.669	Depositor
Minimum map value	-3.480	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.142	Depositor
Recommended contour level	0.12	Depositor
Map size (\AA)	159.03, 221.80501, 319.734	wwPDB
Map dimensions	382, 265, 190	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.837, 0.837, 0.837	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 2MR, FMN, 3PE, FES, SF4, NDP, ZMP, PC1, LMN, CDL, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.38	0/2633	0.57	0/3593
2	2	0.38	2/4565 (0.0%)	0.54	1/6209 (0.0%)
3	3	0.37	0/915	0.47	0/1246
4	4	0.42	0/4002	0.57	2/5454 (0.0%)
5	5	0.39	2/5415 (0.0%)	0.56	3/7372 (0.0%)
6	6	0.37	0/1492	0.57	0/2034
7	8	0.34	0/671	0.44	0/896
8	9	0.35	0/824	0.51	0/1112
9	A	0.39	0/5589	0.61	1/7579 (0.0%)
10	B	0.37	0/3621	0.56	2/4878 (0.0%)
11	C	0.39	1/3449 (0.0%)	0.59	0/4677
12	D	0.47	0/674	0.67	0/911
13	E	0.40	1/2954 (0.0%)	0.59	0/4002
14	F	0.35	1/1939 (0.1%)	0.50	0/2626
15	G	0.35	0/2026	0.51	0/2759
16	H	0.36	0/1741	0.57	0/2367
17	I	0.49	1/1527 (0.1%)	0.71	1/2070 (0.0%)
18	J	0.35	0/1413	0.49	0/1908
19	K	0.35	0/1485	0.57	0/2017
20	L	0.43	0/680	0.60	0/921
21	M	0.36	0/966	0.55	0/1316
22	O	0.53	0/642	0.59	0/871
22	Q	0.54	0/683	0.58	0/926
23	P	0.38	0/1060	0.50	0/1429
24	R	0.38	0/832	0.53	0/1133
25	S	0.33	0/637	0.48	0/872
26	U	0.40	0/1394	0.61	1/1890 (0.1%)
27	W	0.38	0/1005	0.53	0/1359
28	X	0.47	2/1523 (0.1%)	0.65	1/2058 (0.0%)
29	Y	0.36	0/1277	0.50	0/1731
30	Z	0.38	0/1462	0.56	0/1993
31	a	0.46	1/1209 (0.1%)	0.56	0/1639

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	b	0.28	0/701	0.45	0/939
33	c	0.34	0/524	0.46	0/710
34	d	0.31	0/861	0.50	1/1157 (0.1%)
35	e	0.26	0/332	0.38	0/451
36	f	0.40	1/736 (0.1%)	0.58	1/988 (0.1%)
37	g	0.38	0/631	0.49	0/868
38	h	0.38	0/1172	0.61	1/1594 (0.1%)
39	i	0.33	0/711	0.45	0/967
40	j	0.40	0/630	0.51	0/847
41	n	0.35	1/1098 (0.1%)	0.46	0/1489
42	o	0.33	0/262	0.48	0/360
All	All	0.39	13/67963 (0.0%)	0.56	15/92218 (0.0%)

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
10	B	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	232	ALA	C-N	5.97	1.47	1.34
2	2	527	GLY	C-N	-5.86	1.20	1.34
36	f	38	ILE	C-N	-5.85	1.20	1.34
28	X	175	ALA	C-N	5.72	1.47	1.34
31	a	77	PHE	C-N	5.46	1.46	1.34
17	I	57	TRP	C-N	5.36	1.46	1.34
2	2	510	LEU	C-N	5.35	1.46	1.34
41	n	80	PRO	C-N	5.34	1.46	1.34
13	E	306	GLY	C-N	5.33	1.46	1.34
28	X	9	TYR	C-N	5.24	1.46	1.34
5	5	488	THR	C-N	-5.12	1.22	1.34
5	5	548	SER	C-N	-5.12	1.22	1.34
14	F	191	VAL	C-N	-5.08	1.24	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	259	PHE	CB-CA-C	6.51	123.42	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	f	38	ILE	O-C-N	-6.43	112.42	122.70
5	5	304	TYR	CB-CA-C	6.13	122.66	110.40
2	2	527	GLY	O-C-N	-6.00	113.10	122.70
28	X	25	ASN	CB-CA-C	-5.92	98.56	110.40
5	5	335	TYR	CB-CA-C	5.78	121.96	110.40
10	B	253	PRO	N-CA-C	5.54	126.52	112.10
10	B	254	PRO	N-CA-C	-5.35	98.19	112.10
17	I	128	LYS	CB-CA-C	5.28	120.96	110.40
38	h	10	ASN	CB-CA-C	5.25	120.91	110.40
4	4	367	GLU	CB-CA-C	5.22	120.84	110.40
9	A	403	SER	N-CA-C	-5.14	97.13	111.00
34	d	61	TYR	CB-CA-C	5.10	120.61	110.40
5	5	488	THR	O-C-N	-5.09	114.55	122.70
26	U	42	PHE	CB-CA-C	5.06	120.51	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	B	252	LYS	Peptide

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	1	330/378 (87%)	317 (96%)	13 (4%)	0	100	100
2	2	554/571 (97%)	548 (99%)	6 (1%)	0	100	100
3	3	111/146 (76%)	107 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	4	490/542 (90%)	476 (97%)	14 (3%)	0	100	100
5	5	668/679 (98%)	635 (95%)	33 (5%)	0	100	100
6	6	186/224 (83%)	181 (97%)	5 (3%)	0	100	100
7	8	75/86 (87%)	73 (97%)	2 (3%)	0	100	100
8	9	101/785 (13%)	100 (99%)	1 (1%)	0	100	100
9	A	709/749 (95%)	683 (96%)	26 (4%)	0	100	100
10	B	454/507 (90%)	437 (96%)	17 (4%)	0	100	100
11	C	420/499 (84%)	406 (97%)	14 (3%)	0	100	100
12	D	79/86 (92%)	75 (95%)	4 (5%)	0	100	100
13	E	351/378 (93%)	342 (97%)	9 (3%)	0	100	100
14	F	236/261 (90%)	233 (99%)	3 (1%)	0	100	100
15	G	240/293 (82%)	233 (97%)	7 (3%)	0	100	100
16	H	219/318 (69%)	207 (94%)	12 (6%)	0	100	100
17	I	183/223 (82%)	180 (98%)	3 (2%)	0	100	100
18	J	184/199 (92%)	180 (98%)	4 (2%)	0	100	100
19	K	180/230 (78%)	174 (97%)	5 (3%)	1 (1%)	25	29
20	L	85/89 (96%)	85 (100%)	0	0	100	100
21	M	116/168 (69%)	111 (96%)	5 (4%)	0	100	100
22	O	78/141 (55%)	76 (97%)	2 (3%)	0	100	100
22	Q	83/141 (59%)	82 (99%)	1 (1%)	0	100	100
23	P	120/124 (97%)	116 (97%)	4 (3%)	0	100	100
24	R	96/99 (97%)	93 (97%)	3 (3%)	0	100	100
25	S	72/143 (50%)	71 (99%)	1 (1%)	0	100	100
26	U	165/186 (89%)	162 (98%)	3 (2%)	0	100	100
27	W	118/121 (98%)	117 (99%)	1 (1%)	0	100	100
28	X	185/191 (97%)	182 (98%)	3 (2%)	0	100	100
29	Y	152/210 (72%)	148 (97%)	4 (3%)	0	100	100
30	Z	184/196 (94%)	179 (97%)	5 (3%)	0	100	100
31	a	142/203 (70%)	138 (97%)	4 (3%)	0	100	100
32	b	79/94 (84%)	78 (99%)	1 (1%)	0	100	100
33	c	59/93 (63%)	55 (93%)	4 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	d	99/105 (94%)	95 (96%)	4 (4%)	0	100	100
35	e	36/46 (78%)	35 (97%)	1 (3%)	0	100	100
36	f	87/95 (92%)	84 (97%)	3 (3%)	0	100	100
37	g	76/82 (93%)	74 (97%)	2 (3%)	0	100	100
38	h	132/134 (98%)	131 (99%)	1 (1%)	0	100	100
39	i	79/93 (85%)	77 (98%)	2 (2%)	0	100	100
40	j	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
41	n	134/184 (73%)	129 (96%)	5 (4%)	0	100	100
42	o	30/380 (8%)	28 (93%)	2 (7%)	0	100	100
All	All	8250/10547 (78%)	8005 (97%)	244 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	K	51	PRO

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	1	284/326 (87%)	279 (98%)	5 (2%)	59	71
2	2	510/518 (98%)	504 (99%)	6 (1%)	71	81
3	3	93/128 (73%)	91 (98%)	2 (2%)	52	64
4	4	431/477 (90%)	426 (99%)	5 (1%)	71	81
5	5	580/596 (97%)	568 (98%)	12 (2%)	53	66
6	6	167/203 (82%)	163 (98%)	4 (2%)	49	61
7	8	69/75 (92%)	68 (99%)	1 (1%)	67	78
8	9	84/687 (12%)	84 (100%)	0	100	100
9	A	577/602 (96%)	566 (98%)	11 (2%)	57	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	B	366/401 (91%)	355 (97%)	11 (3%)	41	53
11	C	356/416 (86%)	351 (99%)	5 (1%)	67	78
12	D	68/69 (99%)	67 (98%)	1 (2%)	65	76
13	E	315/335 (94%)	311 (99%)	4 (1%)	69	80
14	F	203/219 (93%)	201 (99%)	2 (1%)	76	84
15	G	215/257 (84%)	213 (99%)	2 (1%)	78	87
16	H	191/272 (70%)	188 (98%)	3 (2%)	62	74
17	I	158/191 (83%)	157 (99%)	1 (1%)	86	91
18	J	129/146 (88%)	127 (98%)	2 (2%)	62	74
19	K	156/191 (82%)	151 (97%)	5 (3%)	39	50
20	L	74/76 (97%)	71 (96%)	3 (4%)	30	40
21	M	97/135 (72%)	95 (98%)	2 (2%)	53	66
22	O	71/119 (60%)	70 (99%)	1 (1%)	67	78
22	Q	75/119 (63%)	74 (99%)	1 (1%)	69	80
23	P	108/110 (98%)	104 (96%)	4 (4%)	34	45
24	R	87/89 (98%)	84 (97%)	3 (3%)	37	48
25	S	60/111 (54%)	59 (98%)	1 (2%)	60	73
26	U	149/167 (89%)	147 (99%)	2 (1%)	69	80
27	W	101/102 (99%)	100 (99%)	1 (1%)	76	84
28	X	146/152 (96%)	145 (99%)	1 (1%)	84	90
29	Y	131/176 (74%)	130 (99%)	1 (1%)	81	88
30	Z	151/155 (97%)	147 (97%)	4 (3%)	46	58
31	a	123/177 (70%)	119 (97%)	4 (3%)	38	49
32	b	67/74 (90%)	64 (96%)	3 (4%)	27	36
33	c	49/80 (61%)	48 (98%)	1 (2%)	55	67
34	d	90/94 (96%)	86 (96%)	4 (4%)	28	37
35	e	30/35 (86%)	28 (93%)	2 (7%)	16	20
36	f	76/80 (95%)	76 (100%)	0	100	100
37	g	65/69 (94%)	65 (100%)	0	100	100
38	h	119/119 (100%)	119 (100%)	0	100	100
39	i	68/78 (87%)	67 (98%)	1 (2%)	65	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	j	64/64 (100%)	62 (97%)	2 (3%)	40	52
41	n	107/150 (71%)	106 (99%)	1 (1%)	78	87
42	o	26/318 (8%)	26 (100%)	0	100	100
All	All	7086/8958 (79%)	6962 (98%)	124 (2%)	62	73

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	10	LEU
1	1	131	SER
1	1	303	ASN
1	1	327	PHE
1	1	376	SER
2	2	45	SER
2	2	60	ILE
2	2	179	TYR
2	2	264	SER
2	2	356	SER
2	2	474	SER
3	3	29	ASN
3	3	131	SER
4	4	183	GLU
4	4	233	THR
4	4	345	TYR
4	4	371	LEU
4	4	491	LYS
5	5	90	LEU
5	5	96	VAL
5	5	136	MET
5	5	176	CYS
5	5	262	ARG
5	5	284	THR
5	5	306	THR
5	5	316	SER
5	5	340	PHE
5	5	400	TYR
5	5	444	TYR
5	5	538	VAL
6	6	58	SER
6	6	127	TYR
6	6	186	SER

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Mol	Chain	Res	Type
6	6	198	VAL
7	8	85	SER
9	A	43	LEU
9	A	71	ARG
9	A	98	VAL
9	A	228	GLU
9	A	271	ASN
9	A	359	GLU
9	A	387	GLN
9	A	403	SER
9	A	431	ARG
9	A	581	HIS
9	A	697	LYS
10	B	63	ARG
10	B	71	ARG
10	B	120	LEU
10	B	150	THR
10	B	152	LYS
10	B	279	THR
10	B	290	SER
10	B	294	GLU
10	B	338	ASP
10	B	373	SER
10	B	475	ARG
11	C	119	ASN
11	C	180	MET
11	C	225	SER
11	C	250	TYR
11	C	489	THR
12	D	81	VAL
13	E	73	GLN
13	E	87	LYS
13	E	104	PHE
13	E	326	LYS
14	F	150	ARG
14	F	231	LYS
15	G	77	GLN
15	G	181	THR
16	H	157	SER
16	H	211	ASP
16	H	251	VAL
17	I	169	CYS

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Mol	Chain	Res	Type
18	J	58	LEU
18	J	159	LEU
19	K	105	CYS
19	K	111	MET
19	K	135	ASP
19	K	169	SER
19	K	176	TYR
20	L	22	ILE
20	L	26	LEU
20	L	35	SER
21	M	112	ASP
21	M	134	ASP
22	O	134	ILE
23	P	23	GLN
23	P	41	THR
23	P	50	SER
23	P	113	SER
22	Q	75	PHE
24	R	9	SER
24	R	34	TYR
24	R	72	CYS
25	S	100	SER
26	U	91	CYS
26	U	140	SER
27	W	70	LEU
28	X	163	GLN
29	Y	149	SER
30	Z	17	THR
30	Z	30	ARG
30	Z	55	SER
30	Z	74	ASP
31	a	72	ARG
31	a	87	LYS
31	a	107	PHE
31	a	134	LEU
32	b	29	ASN
32	b	54	ASP
32	b	66	GLN
33	c	44	TYR
34	d	10	LEU
34	d	57	SER
34	d	69	GLU

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Mol	Chain	Res	Type
34	d	74	LEU
35	e	9	SER
35	e	29	TYR
39	i	15	SER
40	j	1	MET
40	j	71	LEU
41	n	124	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
5	5	402	GLN
5	5	503	ASN
5	5	583	ASN
5	5	647	ASN
11	C	185	GLN
11	C	473	HIS
13	E	30	HIS
14	F	42	HIS
14	F	253	GLN
15	G	266	GLN
16	H	128	GLN
17	I	112	HIS
22	Q	83	ASN
24	R	51	GLN
26	U	104	ASN
26	U	107	GLN
26	U	153	HIS
26	U	154	HIS
27	W	66	HIS
28	X	10	GLN
30	Z	12	ASN
34	d	67	HIS
40	j	24	ASN
41	n	84	HIS
41	n	113	HIS
42	o	38	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
11	2MR	C	154	11	10,12,13	0.39	0	5,13,15	1.31	1 (20%)

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
11	2MR	C	154	11	-	0/10/13/15	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
11	C	154	2MR	NE-CZ-NH2	-2.33	117.34	119.48

There are no chirality outliers.

There are no torsion outliers.

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 48 ligands modelled in this entry, 1 is monoatomic - leaving 47 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	S	202	-	50,50,53	0.96	4 (8%)	56,58,61	1.07	2 (3%)
46	LMN	2	602	-	60,60,72	1.70	12 (20%)	78,80,98	1.05	3 (3%)
44	PC1	5	706	-	42,42,53	1.06	4 (9%)	48,50,61	1.14	3 (6%)
48	SF4	B	601	10	0,12,12	-	-	-	-	-
48	SF4	I	302	17	0,12,12	-	-	-	-	-
48	SF4	A	803	9	0,12,12	-	-	-	-	-
43	3PE	W	201	-	34,34,50	1.03	4 (11%)	37,39,55	1.16	2 (5%)
43	3PE	g	102	-	35,35,50	1.00	4 (11%)	38,40,55	1.13	3 (7%)
44	PC1	X	203	-	31,31,53	1.21	4 (12%)	37,39,61	1.17	3 (8%)
45	CDL	g	101	-	69,69,99	1.03	8 (11%)	75,81,111	1.15	6 (8%)
43	3PE	5	703	-	34,34,50	1.03	4 (11%)	37,39,55	1.13	2 (5%)
44	PC1	5	701	-	53,53,53	0.95	5 (9%)	59,61,61	1.21	3 (5%)
52	ZMP	O	201	22	29,35,36	0.24	0	34,42,45	0.43	0
43	3PE	I	304	-	43,43,50	0.94	4 (9%)	46,48,55	1.10	2 (4%)
43	3PE	i	102	-	40,40,50	0.94	4 (10%)	43,45,55	1.11	2 (4%)
45	CDL	S	201	-	78,78,99	0.97	8 (10%)	84,90,111	1.10	4 (4%)
43	3PE	5	704	-	42,42,50	0.94	4 (9%)	45,47,55	1.14	2 (4%)
45	CDL	2	601	-	73,73,99	1.00	8 (10%)	79,85,111	1.23	4 (5%)
43	3PE	4	605	-	33,33,50	1.04	4 (12%)	36,38,55	1.12	2 (5%)
48	SF4	I	301	17	0,12,12	-	-	-	-	-
44	PC1	K	302	-	46,46,53	1.01	4 (8%)	52,54,61	1.15	2 (3%)
43	3PE	l	401	-	31,31,50	1.09	4 (12%)	34,36,55	1.34	3 (8%)
43	3PE	i	101	-	50,50,50	0.86	4 (8%)	53,55,55	1.06	2 (3%)
48	SF4	A	802	9	0,12,12	-	-	-	-	-
43	3PE	4	601	-	50,50,50	0.87	4 (8%)	53,55,55	1.19	2 (3%)
43	3PE	n	201	-	38,38,50	0.98	4 (10%)	41,43,55	1.14	2 (4%)
50	NDP	E	402	-	45,52,52	0.66	0	53,80,80	0.65	2 (3%)
43	3PE	E	401	-	30,30,50	1.10	4 (13%)	33,35,55	1.21	2 (6%)
44	PC1	X	202	-	38,38,53	1.10	4 (10%)	44,46,61	1.18	3 (6%)
43	3PE	I	303	-	41,41,50	0.92	2 (4%)	44,46,55	1.13	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	FMN	B	602	-	33,33,33	0.70	0	48,50,50	0.80	1 (2%)
43	3PE	5	702	-	30,30,50	1.11	4 (13%)	33,35,55	1.20	2 (6%)
47	FES	H	401	16	0,4,4	-	-	-	-	-
48	SF4	K	301	19	0,12,12	-	-	-	-	-
43	3PE	4	602	-	32,32,50	1.05	4 (12%)	35,37,55	1.18	2 (5%)
52	ZMP	Q	201	22	29,35,36	0.18	0	34,42,45	0.40	0
43	3PE	J	201	-	29,29,50	1.10	4 (13%)	32,34,55	1.17	2 (6%)
46	LMN	5	705	-	72,72,72	1.62	12 (16%)	96,98,98	1.08	5 (5%)
45	CDL	D	101	-	73,73,99	1.00	8 (10%)	79,85,111	1.16	4 (5%)
43	3PE	5	707	-	32,32,50	1.05	4 (12%)	35,37,55	1.11	2 (5%)
46	LMN	4	603	-	48,48,72	1.85	13 (27%)	60,62,98	0.99	2 (3%)
47	FES	A	801	9	0,4,4	-	-	-	-	-
43	3PE	W	202	-	38,38,50	0.97	4 (10%)	41,43,55	1.30	4 (9%)
44	PC1	4	604	-	49,49,53	0.99	4 (8%)	55,57,61	1.19	3 (5%)
45	CDL	X	201	-	76,76,99	0.98	6 (7%)	82,88,111	1.26	6 (7%)
44	PC1	3	201	-	47,47,53	1.01	4 (8%)	53,55,61	1.05	3 (5%)
44	PC1	1	402	-	42,42,53	1.09	4 (9%)	48,50,61	1.23	4 (8%)

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	S	202	-	-	19/54/54/57	-
46	LMN	2	602	-	-	25/44/104/130	0/3/3/4
44	PC1	5	706	-	-	11/46/46/57	-
48	SF4	B	601	10	-	-	0/6/5/5
48	SF4	I	302	17	-	-	0/6/5/5
48	SF4	A	803	9	-	-	0/6/5/5
43	3PE	W	201	-	-	14/38/38/54	-
43	3PE	g	102	-	-	18/39/39/54	-
44	PC1	X	203	-	-	15/35/35/57	-
45	CDL	g	101	-	-	36/80/80/110	-
43	3PE	5	703	-	-	15/38/38/54	-
44	PC1	5	701	-	-	20/57/57/57	-
52	ZMP	O	201	22	-	16/40/42/43	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	3PE	I	304	-	-	20/47/47/54	-
43	3PE	i	102	-	-	17/44/44/54	-
45	CDL	S	201	-	-	30/89/89/110	-
43	3PE	5	704	-	-	10/46/46/54	-
45	CDL	2	601	-	-	36/84/84/110	-
43	3PE	4	605	-	-	18/37/37/54	-
48	SF4	I	301	17	-	-	0/6/5/5
44	PC1	K	302	-	-	11/50/50/57	-
43	3PE	1	401	-	-	15/35/35/54	-
43	3PE	i	101	-	-	16/54/54/54	-
48	SF4	A	802	9	-	-	0/6/5/5
43	3PE	4	601	-	-	19/54/54/54	-
43	3PE	n	201	-	-	19/42/42/54	-
50	NDP	E	402	-	-	6/30/77/77	0/5/5/5
43	3PE	E	401	-	-	18/34/34/54	-
44	PC1	X	202	-	-	14/42/42/57	-
43	3PE	I	303	-	-	20/45/45/54	-
49	FMN	B	602	-	-	9/18/18/18	0/3/3/3
43	3PE	5	702	-	-	14/34/34/54	-
47	FES	H	401	16	-	-	0/1/1/1
48	SF4	K	301	19	-	-	0/6/5/5
43	3PE	4	602	-	-	17/36/36/54	-
52	ZMP	Q	201	22	-	17/40/42/43	-
43	3PE	J	201	-	-	6/33/33/54	-
46	LMN	5	705	-	-	29/50/130/130	0/4/4/4
45	CDL	D	101	-	-	31/84/84/110	-
43	3PE	5	707	-	-	5/36/36/54	-
46	LMN	4	603	-	-	25/38/78/130	0/2/2/4
47	FES	A	801	9	-	-	0/1/1/1
43	3PE	W	202	-	-	18/42/42/54	-
44	PC1	4	604	-	-	18/53/53/57	-
45	CDL	X	201	-	-	44/87/87/110	-
44	PC1	3	201	-	-	17/51/51/57	-
44	PC1	1	402	-	-	16/46/46/57	-

All (182) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	5	705	LMN	O5-C1	4.68	1.53	1.41
46	4	603	LMN	O5-C1	4.64	1.53	1.41
46	2	602	LMN	O5-C1	4.59	1.53	1.41
46	5	705	LMN	CBS-CCM	4.32	1.63	1.53
46	4	603	LMN	CBT-CCM	4.03	1.62	1.53
46	2	602	LMN	CBS-CCM	3.99	1.62	1.53
46	4	603	LMN	CBS-CCM	3.91	1.62	1.53
46	4	603	LMN	O1-C1	-3.90	1.33	1.40
46	2	602	LMN	CBT-CCM	3.89	1.62	1.53
46	5	705	LMN	CBT-CCM	3.76	1.62	1.53
46	2	602	LMN	CBR-CCM	3.64	1.60	1.54
46	5	705	LMN	CBR-CCM	3.58	1.60	1.54
46	2	602	LMN	O1-C1	-3.58	1.34	1.40
46	4	603	LMN	O4-C4	3.53	1.51	1.43
46	5	705	LMN	O1-C1	-3.45	1.34	1.40
46	4	603	LMN	CBR-CCM	3.35	1.60	1.54
46	2	602	LMN	O4-C4	3.33	1.50	1.43
46	5	705	LMN	OBZ-CCS	2.92	1.49	1.41
46	5	705	LMN	O4-C4	2.85	1.51	1.43
46	5	705	LMN	OBY-CCR	2.82	1.49	1.41
43	I	303	3PE	O21-C2	-2.78	1.39	1.46
46	2	602	LMN	OBZ-CCS	2.71	1.48	1.41
43	4	605	3PE	O21-C2	-2.61	1.40	1.46
44	4	604	PC1	O21-C2	-2.61	1.40	1.46
43	E	401	3PE	O21-C2	-2.61	1.40	1.46
45	D	101	CDL	OA6-CA4	-2.59	1.40	1.46
43	5	702	3PE	O21-C2	-2.59	1.40	1.46
44	S	202	PC1	O21-C2	-2.58	1.40	1.46
46	2	602	LMN	C4-C3	-2.57	1.45	1.52
45	g	101	CDL	OB6-CB4	-2.57	1.40	1.46
46	4	603	LMN	OCB-CCQ	2.56	1.49	1.43
45	S	201	CDL	OB6-CB4	-2.56	1.40	1.46
44	3	201	PC1	O21-C2	-2.55	1.40	1.46
44	5	706	PC1	O21-C2	-2.55	1.40	1.46
43	5	707	3PE	O21-C2	-2.54	1.40	1.46
43	W	202	3PE	O21-C2	-2.54	1.40	1.46
45	D	101	CDL	OB6-CB4	-2.53	1.40	1.46
43	i	102	3PE	O21-C2	-2.53	1.40	1.46
43	5	704	3PE	O21-C2	-2.53	1.40	1.46
44	5	701	PC1	O21-C2	-2.52	1.40	1.46
43	J	201	3PE	O21-C2	-2.51	1.40	1.46
43	n	201	3PE	O21-C2	-2.51	1.40	1.46
43	5	703	3PE	O21-C2	-2.51	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	4	602	3PE	O21-C2	-2.50	1.40	1.46
43	W	201	3PE	O21-C2	-2.50	1.40	1.46
44	5	701	PC1	O31-C3	-2.50	1.39	1.45
43	i	101	3PE	O21-C2	-2.50	1.40	1.46
45	X	201	CDL	OB6-CB5	2.50	1.41	1.34
44	X	203	PC1	O21-C2	-2.47	1.40	1.46
43	5	704	3PE	O31-C31	2.47	1.40	1.33
45	X	201	CDL	OA6-CA4	-2.47	1.40	1.46
43	4	601	3PE	O21-C2	-2.46	1.40	1.46
45	2	601	CDL	OA8-CA7	2.46	1.40	1.33
45	2	601	CDL	OA6-CA4	-2.46	1.40	1.46
44	1	402	PC1	O21-C2	-2.46	1.40	1.46
45	S	201	CDL	OA8-CA7	2.45	1.40	1.33
45	X	201	CDL	OA8-CA6	-2.45	1.39	1.45
43	5	702	3PE	O31-C31	2.44	1.40	1.33
45	2	601	CDL	OB6-CB5	2.43	1.41	1.34
45	2	601	CDL	OB8-CB7	2.42	1.40	1.33
43	4	602	3PE	O31-C31	2.42	1.40	1.33
43	n	201	3PE	O31-C31	2.41	1.40	1.33
45	g	101	CDL	OA6-CA5	2.40	1.41	1.34
46	4	603	LMN	C4-C3	-2.40	1.46	1.52
43	1	401	3PE	O21-C2	-2.39	1.40	1.46
44	X	202	PC1	O31-C31	2.39	1.40	1.33
43	4	601	3PE	O31-C31	2.39	1.40	1.33
44	5	706	PC1	O31-C31	2.38	1.40	1.33
43	W	201	3PE	O31-C31	2.38	1.40	1.33
44	3	201	PC1	O31-C31	2.38	1.40	1.33
43	5	707	3PE	O31-C31	2.38	1.40	1.33
45	S	201	CDL	OA6-CA5	2.38	1.41	1.34
43	I	304	3PE	O31-C31	2.37	1.40	1.33
43	i	101	3PE	O31-C31	2.37	1.40	1.33
44	1	402	PC1	O31-C31	2.37	1.40	1.33
44	K	302	PC1	O21-C2	-2.37	1.40	1.46
45	S	201	CDL	OB8-CB7	2.36	1.40	1.33
45	X	201	CDL	OB8-CB7	2.35	1.40	1.33
43	I	304	3PE	O21-C2	-2.35	1.40	1.46
43	E	401	3PE	O31-C31	2.35	1.40	1.33
43	g	102	3PE	O21-C2	-2.35	1.40	1.46
46	2	602	LMN	CBQ-CCM	2.35	1.58	1.54
43	I	304	3PE	O21-C21	2.34	1.40	1.34
43	1	401	3PE	O31-C31	2.34	1.40	1.33
43	4	605	3PE	O31-C31	2.34	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	S	202	PC1	O31-C31	2.34	1.40	1.33
43	5	703	3PE	O31-C31	2.34	1.40	1.33
44	X	202	PC1	O21-C2	-2.33	1.40	1.46
45	g	101	CDL	OB8-CB7	2.33	1.40	1.33
44	X	203	PC1	O31-C31	2.32	1.40	1.33
46	4	603	LMN	OBX-CCF	2.31	1.49	1.44
44	K	302	PC1	O31-C31	2.29	1.40	1.33
45	g	101	CDL	OB8-CB6	-2.29	1.39	1.45
45	D	101	CDL	OA8-CA7	2.28	1.40	1.33
44	X	202	PC1	O31-C3	-2.27	1.40	1.45
43	J	201	3PE	O31-C3	-2.27	1.40	1.45
43	i	102	3PE	O31-C31	2.26	1.39	1.33
44	K	302	PC1	O21-C21	2.25	1.40	1.34
44	5	706	PC1	O31-C3	-2.25	1.40	1.45
43	J	201	3PE	O31-C31	2.25	1.39	1.33
44	X	203	PC1	O21-C21	2.24	1.40	1.34
44	K	302	PC1	O31-C3	-2.24	1.40	1.45
46	4	603	LMN	O5-C5	2.24	1.49	1.44
46	5	705	LMN	OBX-CCF	2.23	1.49	1.44
45	D	101	CDL	OB8-CB6	-2.23	1.40	1.45
45	D	101	CDL	OB8-CB7	2.23	1.39	1.33
44	4	604	PC1	O21-C21	2.23	1.40	1.34
43	W	202	3PE	O31-C3	-2.23	1.40	1.45
43	g	102	3PE	O31-C3	-2.22	1.40	1.45
45	X	201	CDL	OA8-CA7	2.21	1.39	1.33
44	X	202	PC1	O21-C21	2.20	1.40	1.34
45	2	601	CDL	OB8-CB6	-2.20	1.40	1.45
45	S	201	CDL	OB6-CB5	2.20	1.40	1.34
43	I	303	3PE	O31-C31	2.20	1.39	1.33
46	2	602	LMN	OBX-CCF	2.20	1.49	1.44
43	1	401	3PE	O31-C3	-2.20	1.40	1.45
43	4	601	3PE	O31-C3	-2.19	1.40	1.45
45	g	101	CDL	OA8-CA7	2.19	1.39	1.33
44	4	604	PC1	O31-C3	-2.19	1.40	1.45
43	E	401	3PE	O31-C3	-2.19	1.40	1.45
43	I	304	3PE	O31-C3	-2.19	1.40	1.45
43	1	401	3PE	O21-C21	2.19	1.40	1.34
43	n	201	3PE	O21-C21	2.18	1.40	1.34
43	W	201	3PE	O31-C3	-2.18	1.40	1.45
45	g	101	CDL	OA8-CA6	-2.18	1.40	1.45
43	g	102	3PE	O21-C21	2.18	1.40	1.34
45	g	101	CDL	OB6-CB5	2.17	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	402	PC1	O21-C21	2.17	1.40	1.34
46	4	603	LMN	CBQ-CCM	2.17	1.58	1.54
46	2	602	LMN	OCB-CCQ	2.17	1.49	1.43
43	g	102	3PE	O31-C31	2.16	1.39	1.33
43	W	201	3PE	O21-C21	2.16	1.40	1.34
46	5	705	LMN	CBQ-CCM	2.16	1.58	1.54
45	S	201	CDL	OA8-CA6	-2.16	1.40	1.45
44	5	701	PC1	O21-C21	2.15	1.40	1.34
43	4	605	3PE	O31-C3	-2.15	1.40	1.45
44	S	202	PC1	O31-C3	-2.15	1.40	1.45
45	S	201	CDL	OB8-CB6	-2.15	1.40	1.45
43	4	601	3PE	O21-C21	2.15	1.40	1.34
44	S	202	PC1	O21-C21	2.15	1.40	1.34
43	i	102	3PE	O31-C3	-2.14	1.40	1.45
43	5	702	3PE	O31-C3	-2.14	1.40	1.45
46	4	603	LMN	OBX-CCJ	2.14	1.47	1.41
43	i	101	3PE	O31-C3	-2.13	1.40	1.45
43	5	704	3PE	O31-C3	-2.13	1.40	1.45
46	2	602	LMN	C4-C5	-2.13	1.48	1.53
46	5	705	LMN	O5-C5	2.13	1.49	1.44
43	5	704	3PE	O21-C21	2.12	1.40	1.34
43	J	201	3PE	O21-C21	2.12	1.40	1.34
46	4	603	LMN	CBQ-CBK	2.12	1.60	1.52
45	D	101	CDL	OA8-CA6	-2.12	1.40	1.45
45	X	201	CDL	OB8-CB6	-2.11	1.40	1.45
46	5	705	LMN	C3-C4	-2.11	1.46	1.52
44	5	706	PC1	O21-C21	2.11	1.40	1.34
43	4	602	3PE	O21-C21	2.11	1.40	1.34
45	S	201	CDL	OA6-CA4	-2.11	1.41	1.46
44	3	201	PC1	O21-C21	2.11	1.40	1.34
44	X	203	PC1	O31-C3	-2.11	1.40	1.45
43	5	707	3PE	O21-C21	2.10	1.40	1.34
43	W	202	3PE	O31-C31	2.10	1.39	1.33
45	2	601	CDL	OA6-CA5	2.10	1.40	1.34
43	i	101	3PE	O21-C21	2.09	1.40	1.34
43	5	703	3PE	O31-C3	-2.09	1.40	1.45
44	5	701	PC1	O31-C31	2.09	1.39	1.33
44	3	201	PC1	O31-C3	-2.09	1.40	1.45
44	5	701	PC1	C12-N	-2.09	1.44	1.51
43	5	702	3PE	O21-C21	2.09	1.40	1.34
43	E	401	3PE	O21-C21	2.08	1.40	1.34
43	5	707	3PE	O31-C3	-2.08	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	i	102	3PE	O21-C21	2.07	1.40	1.34
45	2	601	CDL	OA8-CA6	-2.07	1.40	1.45
43	W	202	3PE	O21-C21	2.06	1.40	1.34
44	1	402	PC1	O31-C3	-2.04	1.40	1.45
43	n	201	3PE	O31-C3	-2.03	1.40	1.45
43	5	703	3PE	O21-C21	2.02	1.40	1.34
43	4	605	3PE	O21-C21	2.02	1.40	1.34
45	D	101	CDL	OB6-CB5	2.01	1.40	1.34
44	4	604	PC1	O31-C31	2.01	1.39	1.33
43	4	602	3PE	O31-C3	-2.01	1.40	1.45
45	g	101	CDL	OA6-CA4	-2.01	1.41	1.46
45	2	601	CDL	OB6-CB4	-2.00	1.41	1.46
45	D	101	CDL	OA6-CA5	2.00	1.40	1.34

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	4	604	PC1	O21-C21-C22	5.28	122.89	111.50
43	1	401	3PE	O21-C21-C22	4.93	122.12	111.50
44	K	302	PC1	O21-C21-C22	4.67	121.57	111.50
45	2	601	CDL	OB6-CB5-C51	4.63	121.47	111.50
43	4	601	3PE	O21-C21-C22	4.62	121.47	111.50
45	X	201	CDL	OB6-CB5-C51	4.58	121.37	111.50
44	5	701	PC1	O21-C21-C22	4.51	121.22	111.50
43	W	202	3PE	O21-C21-C22	4.46	121.11	111.50
45	X	201	CDL	OA6-CA5-C11	4.46	121.11	111.50
45	D	101	CDL	OB6-CB5-C51	4.42	121.03	111.50
43	5	702	3PE	O21-C21-C22	4.28	120.72	111.50
45	g	101	CDL	OB6-CB5-C51	4.24	120.64	111.50
44	X	202	PC1	O21-C21-C22	4.18	120.51	111.50
43	J	201	3PE	O21-C21-C22	4.18	120.51	111.50
43	g	102	3PE	O21-C21-C22	4.13	120.39	111.50
43	W	201	3PE	O21-C21-C22	4.10	120.33	111.50
44	5	706	PC1	O21-C21-C22	4.07	120.28	111.50
43	5	703	3PE	O21-C21-C22	4.06	120.25	111.50
43	5	704	3PE	O21-C21-C22	4.03	120.18	111.50
45	D	101	CDL	OA6-CA5-C11	4.01	120.15	111.50
43	E	401	3PE	O21-C21-C22	4.01	120.14	111.50
43	I	304	3PE	O21-C21-C22	3.99	120.10	111.50
44	X	203	PC1	O21-C21-C22	3.97	120.06	111.50
43	n	201	3PE	O21-C21-C22	3.94	119.99	111.50
43	4	602	3PE	O21-C21-C22	3.90	119.90	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	402	PC1	O21-C21-C22	3.87	119.85	111.50
45	S	201	CDL	OA6-CA5-C11	3.87	119.83	111.50
43	I	303	3PE	O21-C21-C22	3.83	119.75	111.50
43	i	101	3PE	O21-C21-C22	3.73	119.54	111.50
43	i	102	3PE	O21-C21-C22	3.71	119.49	111.50
43	4	605	3PE	O21-C21-C22	3.67	119.42	111.50
45	2	601	CDL	OA6-CA5-C11	3.65	119.38	111.50
44	S	202	PC1	O21-C21-C22	3.55	119.14	111.50
45	S	201	CDL	OB6-CB5-C51	3.49	119.01	111.50
43	5	707	3PE	O21-C21-C22	3.25	118.51	111.50
44	3	201	PC1	O21-C21-C22	3.17	118.33	111.50
46	2	602	LMN	CCS-OCB-CCQ	-3.08	110.35	117.96
43	W	202	3PE	O31-C31-C32	3.08	121.56	111.91
46	5	705	LMN	CCR-O4-C4	-3.06	110.40	117.96
46	5	705	LMN	CCS-OCB-CCQ	-3.04	110.44	117.96
43	n	201	3PE	O31-C31-C32	2.92	121.06	111.91
46	2	602	LMN	O1-C1-C2	2.91	112.84	108.30
43	4	601	3PE	O31-C31-C32	2.88	120.95	111.91
43	1	401	3PE	O31-C31-C32	2.86	120.89	111.91
44	1	402	PC1	C15-N-C14	2.85	116.29	108.97
46	5	705	LMN	OBX-CCF-CCQ	2.81	115.67	109.75
44	X	202	PC1	O31-C31-C32	2.80	120.68	111.91
43	E	401	3PE	O31-C31-C32	2.76	120.58	111.91
45	g	101	CDL	OA6-CA5-C11	2.75	117.43	111.50
43	5	704	3PE	O31-C31-C32	2.75	120.54	111.91
44	X	203	PC1	O31-C31-C32	2.74	120.50	111.91
45	g	101	CDL	OA8-CA7-C31	2.73	120.48	111.91
44	3	201	PC1	O31-C31-C32	2.72	120.45	111.91
44	3	201	PC1	C11-C12-N	-2.69	106.81	115.78
43	4	605	3PE	O31-C31-C32	2.67	120.28	111.91
44	S	202	PC1	O31-C31-C32	2.64	120.20	111.91
43	I	304	3PE	O31-C31-C32	2.62	120.14	111.91
43	I	303	3PE	O31-C31-C32	2.62	120.14	111.91
43	W	201	3PE	O31-C31-C32	2.61	120.11	111.91
43	4	602	3PE	O31-C31-C32	2.59	120.04	111.91
45	2	601	CDL	OB8-CB7-C71	2.58	120.01	111.91
43	5	707	3PE	O31-C31-C32	2.57	119.97	111.91
45	X	201	CDL	OA8-CA7-C31	2.53	119.84	111.91
43	i	102	3PE	O31-C31-C32	2.53	119.83	111.91
45	D	101	CDL	OA8-CA7-C31	2.52	119.83	111.91
46	5	705	LMN	CBL-CBR-CCM	-2.50	109.12	117.16
46	4	603	LMN	CBL-CBR-CCM	-2.48	109.17	117.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	5	701	PC1	C2-O21-C21	-2.48	111.68	117.79
45	X	201	CDL	OB8-CB7-C71	2.48	119.69	111.91
45	g	101	CDL	CB6-CB4-CB3	-2.47	105.95	111.79
45	2	601	CDL	OA8-CA7-C31	2.47	119.64	111.91
44	5	701	PC1	O31-C31-C32	2.46	119.62	111.91
44	1	402	PC1	O31-C31-C32	2.45	119.60	111.91
45	S	201	CDL	OB8-CB7-C71	2.45	119.59	111.91
43	5	703	3PE	O31-C31-C32	2.43	119.55	111.91
44	5	706	PC1	O31-C31-C32	2.42	119.50	111.91
44	X	203	PC1	C11-C12-N	-2.42	107.70	115.78
44	4	604	PC1	O31-C31-C32	2.41	119.48	111.91
45	S	201	CDL	OA8-CA7-C31	2.40	119.45	111.91
43	5	702	3PE	O31-C31-C32	2.39	119.42	111.91
44	K	302	PC1	O31-C31-C32	2.39	119.41	111.91
44	1	402	PC1	C15-N-C13	-2.37	102.89	108.97
44	4	604	PC1	O21-C21-O22	-2.32	118.09	123.70
46	2	602	LMN	C6-C5-C4	-2.29	107.64	113.00
45	D	101	CDL	OB8-CB7-C71	2.29	119.08	111.91
43	i	101	3PE	O31-C31-C32	2.27	119.03	111.91
46	4	603	LMN	O5-C5-C4	2.26	113.81	109.69
43	g	102	3PE	O31-C31-C32	2.25	118.98	111.91
45	g	101	CDL	CA4-OA6-CA5	2.25	123.32	117.79
43	W	202	3PE	C2-O21-C21	-2.24	112.27	117.79
44	5	706	PC1	C11-C12-N	-2.19	108.47	115.78
43	W	202	3PE	O31-C31-O32	-2.19	118.07	123.59
43	1	401	3PE	C2-O21-C21	-2.18	112.42	117.79
44	X	202	PC1	C11-C12-N	-2.17	108.55	115.78
43	J	201	3PE	O31-C31-C32	2.16	118.67	111.91
49	B	602	FMN	C4-N3-C2	-2.14	121.68	125.64
45	X	201	CDL	OA8-CA7-OA9	-2.10	118.30	123.59
50	E	402	NDP	C5A-C6A-N6A	2.05	123.47	120.35
43	I	303	3PE	C2-O21-C21	-2.04	112.76	117.79
45	X	201	CDL	CA4-OA6-CA5	-2.02	112.81	117.79
46	5	705	LMN	C1-C2-C3	2.01	114.19	110.00
45	g	101	CDL	OB8-CB7-C71	2.01	118.23	111.91
43	g	102	3PE	C33-C32-C31	-2.00	106.34	113.62
50	E	402	NDP	O4D-C1D-C2D	-2.00	102.28	106.64

There are no chirality outliers.

All (724) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1	401	3PE	C1-O11-P-O12
43	1	401	3PE	C1-O11-P-O14
43	4	601	3PE	C1-O11-P-O12
43	4	601	3PE	C1-O11-P-O14
43	4	601	3PE	C11-O13-P-O12
43	4	601	3PE	C11-O13-P-O14
43	4	602	3PE	C1-O11-P-O12
43	4	602	3PE	C1-O11-P-O14
43	4	602	3PE	C11-O13-P-O11
43	4	602	3PE	C11-O13-P-O14
43	4	602	3PE	O13-C11-C12-N
43	4	602	3PE	O11-C1-C2-O21
43	4	605	3PE	C11-O13-P-O11
43	4	605	3PE	C11-O13-P-O12
43	4	605	3PE	C11-O13-P-O14
43	4	605	3PE	O22-C21-O21-C2
43	4	605	3PE	C22-C21-O21-C2
43	5	702	3PE	C22-C21-O21-C2
43	5	703	3PE	C11-O13-P-O14
43	5	703	3PE	O22-C21-O21-C2
43	5	703	3PE	C22-C21-O21-C2
43	5	704	3PE	C1-O11-P-O14
43	E	401	3PE	C1-O11-P-O14
43	E	401	3PE	C11-O13-P-O12
43	E	401	3PE	C11-O13-P-O14
43	E	401	3PE	O13-C11-C12-N
43	I	303	3PE	C1-O11-P-O14
43	I	303	3PE	C11-O13-P-O12
43	I	303	3PE	O13-C11-C12-N
43	I	304	3PE	C1-O11-P-O12
43	I	304	3PE	C1-O11-P-O13
43	I	304	3PE	O21-C2-C3-O31
43	J	201	3PE	O13-C11-C12-N
43	W	201	3PE	C11-O13-P-O11
43	W	201	3PE	C11-O13-P-O12
43	W	201	3PE	C11-O13-P-O14
43	W	201	3PE	O22-C21-O21-C2
43	W	201	3PE	C22-C21-O21-C2
43	W	202	3PE	C1-O11-P-O12
43	g	102	3PE	C1-O11-P-O12
43	g	102	3PE	C1-O11-P-O13
43	g	102	3PE	C1-O11-P-O14
43	i	101	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
43	i	101	3PE	C12-C11-O13-P
43	i	101	3PE	O13-C11-C12-N
43	i	101	3PE	O21-C2-C3-O31
43	i	101	3PE	O22-C21-O21-C2
43	i	101	3PE	C22-C21-O21-C2
43	i	102	3PE	C1-O11-P-O12
43	i	102	3PE	O13-C11-C12-N
43	i	102	3PE	O11-C1-C2-O21
43	i	102	3PE	O22-C21-O21-C2
43	i	102	3PE	C22-C21-O21-C2
43	n	201	3PE	C1-O11-P-O12
43	n	201	3PE	O22-C21-O21-C2
44	1	402	PC1	C11-O13-P-O12
44	1	402	PC1	C22-C21-O21-C2
44	3	201	PC1	C1-O11-P-O14
44	3	201	PC1	O13-C11-C12-N
44	4	604	PC1	C1-O11-P-O14
44	4	604	PC1	O22-C21-O21-C2
44	5	701	PC1	C1-O11-P-O12
44	5	701	PC1	C1-O11-P-O14
44	5	701	PC1	C1-O11-P-O13
44	5	701	PC1	C22-C21-O21-C2
44	5	706	PC1	C22-C21-O21-C2
44	K	302	PC1	C11-O13-P-O12
44	K	302	PC1	O22-C21-O21-C2
44	K	302	PC1	C22-C21-O21-C2
44	S	202	PC1	C1-O11-P-O12
44	S	202	PC1	C1-O11-P-O14
44	X	202	PC1	O22-C21-O21-C2
44	X	202	PC1	C22-C21-O21-C2
44	X	203	PC1	C11-O13-P-O12
44	X	203	PC1	C11-O13-P-O11
44	X	203	PC1	C1-O11-P-O12
44	X	203	PC1	O13-C11-C12-N
45	2	601	CDL	OA5-CA3-CA4-OA6
45	2	601	CDL	CB3-OB5-PB2-OB3
45	2	601	CDL	C51-CB5-OB6-CB4
45	D	101	CDL	CA3-OA5-PA1-OA4
45	D	101	CDL	CB3-OB5-PB2-OB4
45	S	201	CDL	CA3-CA4-OA6-CA5
45	S	201	CDL	C11-CA5-OA6-CA4
45	S	201	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
45	X	201	CDL	CA3-OA5-PA1-OA2
45	X	201	CDL	CA3-OA5-PA1-OA3
45	X	201	CDL	CB3-OB5-PB2-OB3
45	X	201	CDL	CB3-OB5-PB2-OB4
45	X	201	CDL	C51-CB5-OB6-CB4
45	g	101	CDL	CA2-OA2-PA1-OA4
45	g	101	CDL	CA3-OA5-PA1-OA4
45	g	101	CDL	CB2-OB2-PB2-OB3
45	g	101	CDL	CB2-OB2-PB2-OB4
45	g	101	CDL	OB7-CB5-OB6-CB4
46	2	602	LMN	CBK-CBQ-CCM-CBR
46	2	602	LMN	CBK-CBQ-CCM-CBS
46	2	602	LMN	CBK-CBQ-CCM-CBT
46	2	602	LMN	CBL-CBR-CCM-CBQ
46	2	602	LMN	CBL-CBR-CCM-CBS
46	2	602	LMN	CBL-CBR-CCM-CBT
46	4	603	LMN	O5-C1-O1-CBS
46	4	603	LMN	CBK-CBQ-CCM-CBR
46	4	603	LMN	CBK-CBQ-CCM-CBS
46	4	603	LMN	CBK-CBQ-CCM-CBT
46	4	603	LMN	CBL-CBR-CCM-CBQ
46	4	603	LMN	CBL-CBR-CCM-CBS
46	4	603	LMN	CBL-CBR-CCM-CBT
46	4	603	LMN	O1-CBS-CCM-CBQ
46	4	603	LMN	O1-CBS-CCM-CBR
46	4	603	LMN	OBV-CBT-CCM-CBQ
46	4	603	LMN	OBV-CBT-CCM-CBR
46	5	705	LMN	CBK-CBQ-CCM-CBR
46	5	705	LMN	CBK-CBQ-CCM-CBS
46	5	705	LMN	CBK-CBQ-CCM-CBT
46	5	705	LMN	CBL-CBR-CCM-CBQ
46	5	705	LMN	CBL-CBR-CCM-CBS
46	5	705	LMN	CBL-CBR-CCM-CBT
46	5	705	LMN	O1-CBS-CCM-CBQ
46	5	705	LMN	O1-CBS-CCM-CBR
46	5	705	LMN	OBV-CBT-CCM-CBQ
46	5	705	LMN	OBV-CBT-CCM-CBR
49	B	602	FMN	N10-C1'-C2'-C3'
52	O	201	ZMP	O4-C17-C18-C21
52	O	201	ZMP	C16-C17-C18-C21
52	O	201	ZMP	O4-C17-C18-C19
52	O	201	ZMP	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
52	O	201	ZMP	O4-C17-C18-C20
52	O	201	ZMP	C16-C17-C18-C20
52	O	201	ZMP	O3-C16-C17-C18
52	O	201	ZMP	N2-C16-C17-C18
52	O	201	ZMP	C13-C14-C15-N2
52	O	201	ZMP	C14-C13-N1-C12
52	O	201	ZMP	C7-C8-C9-C10
52	Q	201	ZMP	N2-C16-C17-O4
52	Q	201	ZMP	C17-C16-N2-C15
52	Q	201	ZMP	O3-C16-N2-C15
52	Q	201	ZMP	O1-C10-S1-C11
52	Q	201	ZMP	C9-C10-S1-C11
46	2	602	LMN	OBZ-CCS-OCB-CCQ
46	5	705	LMN	OBY-CCR-O4-C4
43	4	602	3PE	C32-C31-O31-C3
52	O	201	ZMP	O2-C13-N1-C12
43	4	602	3PE	O32-C31-O31-C3
43	5	704	3PE	O32-C31-O31-C3
43	E	401	3PE	O32-C31-O31-C3
45	2	601	CDL	OA9-CA7-OA8-CA6
43	5	702	3PE	O22-C21-O21-C2
44	1	402	PC1	O22-C21-O21-C2
44	5	706	PC1	O22-C21-O21-C2
45	2	601	CDL	OB7-CB5-OB6-CB4
45	S	201	CDL	OA7-CA5-OA6-CA4
45	S	201	CDL	OB7-CB5-OB6-CB4
44	4	604	PC1	O32-C31-O31-C3
43	5	704	3PE	C32-C31-O31-C3
43	E	401	3PE	C32-C31-O31-C3
45	X	201	CDL	C71-CB7-OB8-CB6
43	n	201	3PE	C22-C21-O21-C2
44	4	604	PC1	C22-C21-O21-C2
45	g	101	CDL	C51-CB5-OB6-CB4
44	4	604	PC1	C32-C31-O31-C3
44	X	202	PC1	C32-C31-O31-C3
45	2	601	CDL	C31-CA7-OA8-CA6
45	S	201	CDL	C31-CA7-OA8-CA6
46	4	603	LMN	OBV-CBT-CCM-CBS
46	2	602	LMN	CBA-CBC-CBE-CBG
43	W	202	3PE	O22-C21-O21-C2
44	5	701	PC1	O22-C21-O21-C2
45	X	201	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
45	X	201	CDL	OB9-CB7-OB8-CB6
44	1	402	PC1	C11-C12-N-C14
46	5	705	LMN	CBA-CBC-CBE-CBG
45	X	201	CDL	O1-C1-CB2-OB2
45	g	101	CDL	O1-C1-CB2-OB2
44	X	202	PC1	O32-C31-O31-C3
45	S	201	CDL	OA9-CA7-OA8-CA6
43	4	602	3PE	C22-C21-O21-C2
43	W	202	3PE	C22-C21-O21-C2
45	2	601	CDL	C11-CA5-OA6-CA4
46	2	602	LMN	CBB-CBD-CBF-CBH
45	2	601	CDL	OA7-CA5-OA6-CA4
46	2	602	LMN	OAL-CBP-CCF-OBX
43	J	201	3PE	C32-C33-C34-C35
43	1	401	3PE	C32-C31-O31-C3
44	S	202	PC1	C25-C26-C27-C28
46	5	705	LMN	OAJ-CBN-CCD-OBZ
46	4	603	LMN	OAL-CBP-CCF-CCQ
44	S	202	PC1	C23-C24-C25-C26
46	5	705	LMN	OAJ-CBN-CCD-CCO
44	3	201	PC1	C32-C31-O31-C3
50	E	402	NDP	O4D-C1D-N1N-C6N
45	S	201	CDL	CA5-C11-C12-C13
44	5	706	PC1	O11-C1-C2-O21
43	5	703	3PE	C32-C33-C34-C35
46	2	602	LMN	OAL-CBP-CCF-CCQ
43	I	303	3PE	C21-C22-C23-C24
46	4	603	LMN	CBE-CBG-CBI-CBK
43	W	202	3PE	C31-C32-C33-C34
44	X	202	PC1	C21-C22-C23-C24
45	X	201	CDL	CA5-C11-C12-C13
44	3	201	PC1	O32-C31-O31-C3
46	5	705	LMN	OBV-CBT-CCM-CBS
46	5	705	LMN	CBI-CBK-CBQ-CCM
43	4	602	3PE	O22-C21-O21-C2
43	4	601	3PE	C37-C38-C39-C3A
44	S	202	PC1	C11-C12-N-C15
45	D	101	CDL	C11-CA5-OA6-CA4
46	4	603	LMN	OAL-CBP-CCF-OBX
46	5	705	LMN	O5-C1-O1-CBS
46	4	603	LMN	CAW-CAY-CBA-CBC
43	1	401	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
43	4	602	3PE	C32-C33-C34-C35
43	1	401	3PE	C1-O11-P-O13
43	4	601	3PE	C1-O11-P-O13
43	4	601	3PE	C11-O13-P-O11
43	4	602	3PE	C1-O11-P-O13
43	5	702	3PE	C1-O11-P-O13
43	5	704	3PE	C1-O11-P-O13
43	E	401	3PE	C1-O11-P-O13
43	E	401	3PE	C11-O13-P-O11
43	I	303	3PE	C1-O11-P-O13
43	I	303	3PE	C11-O13-P-O11
43	W	202	3PE	C1-O11-P-O13
43	i	101	3PE	C1-O11-P-O13
43	i	101	3PE	C11-O13-P-O11
43	i	102	3PE	C1-O11-P-O13
43	n	201	3PE	C1-O11-P-O13
44	1	402	PC1	C11-O13-P-O11
44	3	201	PC1	C11-O13-P-O11
44	K	302	PC1	C11-O13-P-O11
44	S	202	PC1	C11-O13-P-O11
44	S	202	PC1	C1-O11-P-O13
44	X	203	PC1	C1-O11-P-O13
45	2	601	CDL	CB3-OB5-PB2-OB2
45	D	101	CDL	CA3-OA5-PA1-OA2
45	D	101	CDL	CB3-OB5-PB2-OB2
45	X	201	CDL	CB3-OB5-PB2-OB2
45	g	101	CDL	CA3-OA5-PA1-OA2
45	g	101	CDL	CB2-OB2-PB2-OB5
46	5	705	LMN	CBE-CBG-CBI-CBK
45	g	101	CDL	CA2-C1-CB2-OB2
45	D	101	CDL	OA7-CA5-OA6-CA4
44	1	402	PC1	C11-C12-N-C13
44	S	202	PC1	C11-C12-N-C14
44	K	302	PC1	C3A-C3B-C3C-C3D
46	5	705	LMN	O1-CBS-CCM-CBT
45	S	201	CDL	C11-C12-C13-C14
43	I	304	3PE	C38-C39-C3A-C3B
45	X	201	CDL	C11-CA5-OA6-CA4
43	4	605	3PE	C26-C27-C28-C29
45	g	101	CDL	C74-C75-C76-C77
46	4	603	LMN	CBD-CBF-CBH-CBJ
45	X	201	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
43	5	704	3PE	C2B-C2C-C2D-C2E
45	D	101	CDL	C14-C15-C16-C17
45	g	101	CDL	C51-C52-C53-C54
44	4	604	PC1	C3A-C3B-C3C-C3D
46	5	705	LMN	C2-C1-O1-CBS
43	g	102	3PE	C2A-C2B-C2C-C2D
44	S	202	PC1	C3D-C3E-C3F-C3G
45	2	601	CDL	C72-C73-C74-C75
45	X	201	CDL	C74-C75-C76-C77
43	E	401	3PE	C33-C34-C35-C36
43	i	102	3PE	C32-C33-C34-C35
45	g	101	CDL	C52-C53-C54-C55
43	E	401	3PE	C22-C21-O21-C2
46	4	603	LMN	CBA-CBC-CBE-CBG
44	1	402	PC1	C21-C22-C23-C24
43	i	101	3PE	C3A-C3B-C3C-C3D
44	X	203	PC1	C22-C23-C24-C25
46	4	603	LMN	CAZ-CBB-CBD-CBF
46	4	603	LMN	CBH-CBJ-CBL-CBR
44	1	402	PC1	C11-C12-N-C15
43	5	703	3PE	O13-C11-C12-N
43	5	707	3PE	O13-C11-C12-N
45	D	101	CDL	CA5-C11-C12-C13
45	D	101	CDL	CA7-C31-C32-C33
43	5	702	3PE	C32-C31-O31-C3
45	D	101	CDL	C51-C52-C53-C54
43	n	201	3PE	C34-C35-C36-C37
46	2	602	LMN	CBH-CBJ-CBL-CBR
46	4	603	LMN	O1-CBS-CCM-CBT
45	X	201	CDL	C16-C17-C18-C19
46	5	705	LMN	CAY-CBA-CBC-CBE
45	X	201	CDL	CA2-C1-CB2-OB2
43	E	401	3PE	O22-C21-O21-C2
46	4	603	LMN	CBC-CBE-CBG-CBI
46	5	705	LMN	CBC-CBE-CBG-CBI
43	I	304	3PE	C32-C33-C34-C35
43	g	102	3PE	C22-C21-O21-C2
44	4	604	PC1	C32-C33-C34-C35
44	X	202	PC1	C25-C26-C27-C28
43	n	201	3PE	C37-C38-C39-C3A
46	2	602	LMN	O5-C5-C6-O6
44	3	201	PC1	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
44	5	701	PC1	C3B-C3C-C3D-C3E
45	2	601	CDL	C74-C75-C76-C77
46	2	602	LMN	CBF-CBH-CBJ-CBL
44	1	402	PC1	C32-C31-O31-C3
43	5	704	3PE	C22-C21-O21-C2
43	I	304	3PE	C22-C21-O21-C2
45	D	101	CDL	OB5-CB3-CB4-OB6
45	S	201	CDL	C74-C75-C76-C77
43	5	702	3PE	O21-C2-C3-O31
43	W	202	3PE	O21-C2-C3-O31
43	5	702	3PE	O32-C31-O31-C3
44	S	202	PC1	C11-C12-N-C13
44	X	202	PC1	C35-C36-C37-C38
52	O	201	ZMP	C1-C2-C3-C4
46	5	705	LMN	O5-C5-C6-O6
44	S	202	PC1	C32-C33-C34-C35
45	X	201	CDL	C18-C19-C20-C21
45	X	201	CDL	C22-C23-C24-C25
45	2	601	CDL	C76-C77-C78-C79
49	B	602	FMN	O2'-C2'-C3'-C4'
43	5	703	3PE	C11-O13-P-O11
43	W	202	3PE	C11-O13-P-O11
44	4	604	PC1	C1-O11-P-O13
44	5	706	PC1	C1-O11-P-O13
45	2	601	CDL	CB2-OB2-PB2-OB5
45	g	101	CDL	CA2-OA2-PA1-OA5
43	4	601	3PE	C32-C33-C34-C35
45	g	101	CDL	C31-C32-C33-C34
43	4	602	3PE	O11-C1-C2-C3
44	4	604	PC1	O11-C1-C2-C3
44	5	706	PC1	O11-C1-C2-C3
44	X	203	PC1	O11-C1-C2-C3
45	X	201	CDL	OA5-CA3-CA4-CA6
45	2	601	CDL	C14-C15-C16-C17
45	X	201	CDL	C34-C35-C36-C37
43	W	201	3PE	C21-C22-C23-C24
44	5	701	PC1	C31-C32-C33-C34
43	g	102	3PE	O22-C21-O21-C2
46	2	602	LMN	CBC-CBE-CBG-CBI
43	4	605	3PE	C35-C36-C37-C38
43	5	703	3PE	C34-C35-C36-C37
43	1	401	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
43	5	702	3PE	C1-C2-C3-O31
43	5	704	3PE	C1-C2-C3-O31
43	E	401	3PE	C1-C2-C3-O31
43	I	303	3PE	C1-C2-C3-O31
43	I	304	3PE	C1-C2-C3-O31
43	n	201	3PE	C1-C2-C3-O31
44	5	706	PC1	C32-C33-C34-C35
45	D	101	CDL	CB3-CB4-CB6-OB8
45	X	201	CDL	C15-C16-C17-C18
45	X	201	CDL	CB3-CB4-CB6-OB8
46	2	602	LMN	CAA-CAW-CAY-CBA
46	2	602	LMN	CAX-CAZ-CBB-CBD
43	1	401	3PE	O21-C21-C22-C23
52	Q	201	ZMP	O3-C16-C17-O4
45	2	601	CDL	CA6-CA4-OA6-CA5
45	2	601	CDL	CB3-CB4-OB6-CB5
45	S	201	CDL	CB3-CB4-OB6-CB5
45	2	601	CDL	C52-C53-C54-C55
45	2	601	CDL	O1-C1-CA2-OA2
45	X	201	CDL	O1-C1-CA2-OA2
44	1	402	PC1	O32-C31-O31-C3
46	4	603	LMN	CAY-CBA-CBC-CBE
45	S	201	CDL	C76-C77-C78-C79
46	2	602	LMN	CBE-CBG-CBI-CBK
52	Q	201	ZMP	C22-C23-C24-C25
43	i	102	3PE	C21-C22-C23-C24
43	4	605	3PE	C33-C34-C35-C36
45	S	201	CDL	C71-C72-C73-C74
52	Q	201	ZMP	O2-C13-C14-C15
43	i	102	3PE	C38-C39-C3A-C3B
43	W	202	3PE	C32-C33-C34-C35
52	Q	201	ZMP	N1-C13-C14-C15
43	g	102	3PE	O11-C1-C2-C3
44	5	701	PC1	O11-C1-C2-C3
45	D	101	CDL	OB5-CB3-CB4-CB6
45	X	201	CDL	OB5-CB3-CB4-CB6
43	4	605	3PE	O13-C11-C12-N
43	I	304	3PE	O13-C11-C12-N
43	W	202	3PE	O13-C11-C12-N
43	n	201	3PE	C31-C32-C33-C34
43	I	304	3PE	O22-C21-O21-C2
43	5	702	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
45	S	201	CDL	CA4-CA3-OA5-PA1
43	i	101	3PE	C36-C37-C38-C39
44	1	402	PC1	C39-C3A-C3B-C3C
45	S	201	CDL	C78-C79-C80-C81
43	4	601	3PE	C29-C2A-C2B-C2C
43	4	601	3PE	C1-C2-C3-O31
43	W	202	3PE	C1-C2-C3-O31
45	2	601	CDL	CA3-CA4-CA6-OA8
45	X	201	CDL	CA3-CA4-CA6-OA8
43	5	704	3PE	O22-C21-O21-C2
45	g	101	CDL	C16-C17-C18-C19
43	I	303	3PE	C34-C35-C36-C37
45	S	201	CDL	C12-C13-C14-C15
43	1	401	3PE	O11-C1-C2-O21
43	g	102	3PE	O11-C1-C2-O21
44	5	701	PC1	O11-C1-C2-O21
44	X	202	PC1	O11-C1-C2-O21
43	5	704	3PE	O21-C2-C3-O31
43	g	102	3PE	O21-C2-C3-O31
45	2	601	CDL	OA6-CA4-CA6-OA8
45	X	201	CDL	OA6-CA4-CA6-OA8
46	4	603	LMN	CAA-CAW-CAY-CBA
46	5	705	LMN	CAZ-CBB-CBD-CBF
43	4	601	3PE	C24-C25-C26-C27
43	I	304	3PE	C33-C34-C35-C36
43	g	102	3PE	C33-C34-C35-C36
46	5	705	LMN	CBH-CBJ-CBL-CBR
45	2	601	CDL	C59-C60-C61-C62
45	g	101	CDL	C1-CB2-OB2-PB2
49	B	602	FMN	C4'-C5'-O5'-P
46	2	602	LMN	CAY-CBA-CBC-CBE
52	O	201	ZMP	C2-C3-C4-C5
43	I	303	3PE	C25-C26-C27-C28
43	1	401	3PE	C22-C21-O21-C2
44	3	201	PC1	C22-C23-C24-C25
52	Q	201	ZMP	S1-C10-C9-C8
52	Q	201	ZMP	O1-C10-C9-C8
46	2	602	LMN	CAB-CAX-CAZ-CBB
43	E	401	3PE	O11-C1-C2-C3
43	i	102	3PE	O11-C1-C2-C3
45	2	601	CDL	OA5-CA3-CA4-CA6
45	S	201	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
44	4	604	PC1	C26-C27-C28-C29
44	X	203	PC1	C25-C26-C27-C28
44	X	203	PC1	C23-C24-C25-C26
52	O	201	ZMP	N2-C16-C17-O4
45	X	201	CDL	C31-CA7-OA8-CA6
43	4	602	3PE	C33-C34-C35-C36
45	2	601	CDL	C71-C72-C73-C74
45	X	201	CDL	C13-C14-C15-C16
45	g	101	CDL	C76-C77-C78-C79
43	I	303	3PE	C28-C29-C2A-C2B
43	4	605	3PE	C1-C2-C3-O31
43	g	102	3PE	C1-C2-C3-O31
43	i	101	3PE	C1-C2-C3-O31
44	1	402	PC1	C1-C2-C3-O31
44	4	604	PC1	C2-C1-O11-P
43	4	605	3PE	O11-C1-C2-O21
43	E	401	3PE	O11-C1-C2-O21
43	I	304	3PE	O11-C1-C2-O21
44	4	604	PC1	O11-C1-C2-O21
44	X	203	PC1	O11-C1-C2-O21
45	g	101	CDL	OB5-CB3-CB4-OB6
45	X	201	CDL	CB2-C1-CA2-OA2
52	Q	201	ZMP	C16-C17-C18-C20
45	D	101	CDL	C20-C21-C22-C23
43	5	702	3PE	C33-C34-C35-C36
43	n	201	3PE	C26-C27-C28-C29
43	4	601	3PE	O21-C2-C3-O31
43	4	605	3PE	O21-C2-C3-O31
43	I	303	3PE	O21-C2-C3-O31
45	2	601	CDL	OB6-CB4-CB6-OB8
45	D	101	CDL	OB6-CB4-CB6-OB8
46	2	602	LMN	O1-CBS-CCM-CBR
46	2	602	LMN	OBV-CBT-CCM-CBQ
46	2	602	LMN	OBV-CBT-CCM-CBR
45	g	101	CDL	C57-C58-C59-C60
43	5	703	3PE	C32-C31-O31-C3
45	X	201	CDL	C72-C73-C74-C75
50	E	402	NDP	O4B-C4B-C5B-O5B
44	3	201	PC1	C23-C24-C25-C26
43	i	102	3PE	C3C-C3D-C3E-C3F
43	5	707	3PE	C11-O13-P-O11
43	I	304	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
43	i	102	3PE	C11-O13-P-O11
43	n	201	3PE	C11-O13-P-O11
43	i	101	3PE	C32-C33-C34-C35
44	4	604	PC1	C23-C24-C25-C26
45	g	101	CDL	O1-C1-CA2-OA2
43	I	303	3PE	C3D-C3E-C3F-C3G
43	g	102	3PE	O21-C21-C22-C23
45	D	101	CDL	CB4-CB3-OB5-PB2
45	X	201	CDL	C1-CB2-OB2-PB2
45	g	101	CDL	C1-CA2-OA2-PA1
43	4	602	3PE	C11-O13-P-O12
43	5	702	3PE	C1-O11-P-O14
43	5	703	3PE	C11-O13-P-O12
43	E	401	3PE	C1-O11-P-O12
43	I	303	3PE	C1-O11-P-O12
43	I	303	3PE	C11-O13-P-O14
43	I	304	3PE	C1-O11-P-O14
43	W	202	3PE	C1-O11-P-O14
43	W	202	3PE	C11-O13-P-O12
43	i	101	3PE	C11-O13-P-O14
43	i	102	3PE	C1-O11-P-O14
43	n	201	3PE	C1-O11-P-O14
43	n	201	3PE	C11-O13-P-O14
44	1	402	PC1	C11-O13-P-O14
44	3	201	PC1	C11-O13-P-O14
44	4	604	PC1	C1-O11-P-O12
44	5	706	PC1	C1-O11-P-O12
44	S	202	PC1	C11-O13-P-O12
44	S	202	PC1	C11-O13-P-O14
44	X	203	PC1	C11-O13-P-O14
44	X	203	PC1	C1-O11-P-O14
45	2	601	CDL	CB2-OB2-PB2-OB4
45	2	601	CDL	CB3-OB5-PB2-OB4
45	D	101	CDL	CB2-OB2-PB2-OB4
45	D	101	CDL	CB3-OB5-PB2-OB3
45	g	101	CDL	CA2-OA2-PA1-OA3
45	g	101	CDL	CA3-OA5-PA1-OA3
45	g	101	CDL	CB3-OB5-PB2-OB4
45	D	101	CDL	C71-CB7-OB8-CB6
43	1	401	3PE	O11-C1-C2-C3
43	I	304	3PE	O11-C1-C2-C3
45	g	101	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
44	5	701	PC1	C12-C11-O13-P
44	S	202	PC1	C12-C11-O13-P
44	X	203	PC1	C12-C11-O13-P
45	D	101	CDL	C33-C34-C35-C36
45	g	101	CDL	CB2-C1-CA2-OA2
43	4	605	3PE	C31-C32-C33-C34
43	n	201	3PE	O11-C1-C2-O21
45	S	201	CDL	OA5-CA3-CA4-OA6
45	X	201	CDL	OA5-CA3-CA4-OA6
49	B	602	FMN	N10-C1'-C2'-O2'
52	Q	201	ZMP	C16-C17-C18-C21
44	3	201	PC1	C26-C27-C28-C29
43	I	303	3PE	C33-C34-C35-C36
43	I	303	3PE	C26-C27-C28-C29
44	5	701	PC1	C11-C12-N-C15
44	1	402	PC1	C22-C23-C24-C25
44	4	604	PC1	O13-C11-C12-N
44	5	706	PC1	O13-C11-C12-N
44	K	302	PC1	O13-C11-C12-N
44	X	202	PC1	O13-C11-C12-N
43	1	401	3PE	O22-C21-O21-C2
43	1	401	3PE	O21-C2-C3-O31
43	E	401	3PE	O21-C2-C3-O31
43	W	201	3PE	O21-C2-C3-O31
45	X	201	CDL	CB7-C71-C72-C73
45	X	201	CDL	OA9-CA7-OA8-CA6
43	i	102	3PE	C33-C34-C35-C36
45	2	601	CDL	C15-C16-C17-C18
43	5	703	3PE	O32-C31-O31-C3
43	g	102	3PE	C23-C24-C25-C26
44	K	302	PC1	C24-C25-C26-C27
45	S	201	CDL	C77-C78-C79-C80
45	D	101	CDL	OB9-CB7-OB8-CB6
44	5	701	PC1	C11-C12-N-C14
43	5	704	3PE	O21-C21-C22-C23
46	2	602	LMN	CBG-CBI-CBK-CBQ
43	4	605	3PE	O11-C1-C2-C3
43	i	101	3PE	C2E-C2F-C2G-C2H
46	5	705	LMN	CAW-CAY-CBA-CBC
49	B	602	FMN	C2'-C3'-C4'-O4'
45	S	201	CDL	C51-C52-C53-C54
43	4	602	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
45	g	101	CDL	CA4-CA3-OA5-PA1
44	K	302	PC1	C38-C39-C3A-C3B
44	5	701	PC1	C11-C12-N-C13
49	B	602	FMN	C2'-C3'-C4'-C5'
44	4	604	PC1	C27-C28-C29-C2A
43	5	703	3PE	C21-C22-C23-C24
43	i	102	3PE	O31-C31-C32-C33
43	n	201	3PE	O21-C2-C3-O31
43	W	202	3PE	C34-C35-C36-C37
43	5	703	3PE	C1-O11-P-O13
43	W	201	3PE	C1-O11-P-O13
43	g	102	3PE	C11-O13-P-O11
44	5	701	PC1	C11-O13-P-O11
44	5	706	PC1	C11-O13-P-O11
44	X	202	PC1	C11-O13-P-O11
45	2	601	CDL	CA2-OA2-PA1-OA5
45	S	201	CDL	CA3-OA5-PA1-OA2
45	D	101	CDL	C72-C73-C74-C75
45	2	601	CDL	CB3-CB4-CB6-OB8
44	5	701	PC1	C21-C22-C23-C24
43	1	401	3PE	C2-C1-O11-P
43	4	605	3PE	C2-C1-O11-P
45	X	201	CDL	C1-CA2-OA2-PA1
45	g	101	CDL	C53-C54-C55-C56
45	X	201	CDL	C11-C12-C13-C14
45	2	601	CDL	CB2-C1-CA2-OA2
43	4	601	3PE	C31-C32-C33-C34
43	1	401	3PE	C32-C33-C34-C35
44	5	701	PC1	C2E-C2F-C2G-C2H
43	W	202	3PE	C33-C34-C35-C36
44	X	203	PC1	O32-C31-O31-C3
44	4	604	PC1	C3B-C3C-C3D-C3E
44	X	203	PC1	C32-C31-O31-C3
43	5	707	3PE	C2-C1-O11-P
43	i	101	3PE	C2-C1-O11-P
49	B	602	FMN	O2'-C2'-C3'-O3'
43	J	201	3PE	C33-C34-C35-C36
46	5	705	LMN	CAA-CAW-CAY-CBA
52	Q	201	ZMP	C11-C12-N1-C13
43	W	201	3PE	C1-C2-C3-O31
43	1	401	3PE	O22-C21-C22-C23
44	4	604	PC1	C3-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
45	D	101	CDL	CA6-CA4-OA6-CA5
45	g	101	CDL	CA6-CA4-OA6-CA5
43	n	201	3PE	C33-C34-C35-C36
44	3	201	PC1	C1-O11-P-O13
45	D	101	CDL	CB2-OB2-PB2-OB5
43	g	102	3PE	C26-C27-C28-C29
43	I	304	3PE	O31-C31-C32-C33
45	X	201	CDL	C31-C32-C33-C34
43	n	201	3PE	O11-C1-C2-C3
45	2	601	CDL	OB5-CB3-CB4-CB6
44	3	201	PC1	C28-C29-C2A-C2B
43	I	303	3PE	C31-C32-C33-C34
44	S	202	PC1	C3E-C3F-C3G-C3H
43	g	102	3PE	C29-C2A-C2B-C2C
45	S	201	CDL	C55-C56-C57-C58
52	O	201	ZMP	C12-C11-S1-C10
44	1	402	PC1	O21-C2-C3-O31
45	S	201	CDL	OB6-CB4-CB6-OB8
45	g	101	CDL	C71-CB7-OB8-CB6
43	E	401	3PE	C31-C32-C33-C34
44	5	701	PC1	C37-C38-C39-C3A
43	i	102	3PE	C37-C38-C39-C3A
43	n	201	3PE	C3A-C3B-C3C-C3D
50	E	402	NDP	PN-O3-PA-O1A
50	E	402	NDP	PN-O3-PA-O2A
44	5	706	PC1	O31-C31-C32-C33
45	2	601	CDL	O1-C1-CB2-OB2
43	4	601	3PE	C22-C23-C24-C25
50	E	402	NDP	O4D-C4D-C5D-O5D
44	X	202	PC1	O11-C1-C2-C3
43	g	102	3PE	O31-C31-C32-C33
45	X	201	CDL	C55-C56-C57-C58
45	D	101	CDL	C38-C39-C40-C41
46	5	705	LMN	CAX-CAZ-CBB-CBD
45	X	201	CDL	OB6-CB4-CB6-OB8
44	3	201	PC1	C24-C25-C26-C27
43	J	201	3PE	C32-C31-O31-C3
44	3	201	PC1	C36-C37-C38-C39
45	S	201	CDL	C31-C32-C33-C34
49	B	602	FMN	C5'-O5'-P-O3P
43	5	707	3PE	C23-C24-C25-C26
43	5	707	3PE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
44	X	202	PC1	C37-C38-C39-C3A
45	X	201	CDL	CB3-CB4-OB6-CB5
45	X	201	CDL	CB6-CB4-OB6-CB5
43	i	101	3PE	C25-C26-C27-C28
43	5	702	3PE	O31-C31-C32-C33
45	D	101	CDL	C52-C51-CB5-OB6
52	Q	201	ZMP	C2-C1-C22-C23
46	5	705	LMN	CBG-CBI-CBK-CBQ
43	5	703	3PE	O31-C31-C32-C33
43	W	201	3PE	O21-C21-C22-C23
44	3	201	PC1	O21-C21-C22-C23
44	K	302	PC1	C25-C26-C27-C28
43	I	303	3PE	O11-C1-C2-O21
44	K	302	PC1	O31-C31-C32-C33
45	S	201	CDL	C32-C31-CA7-OA8
43	I	304	3PE	O21-C21-C22-C23
43	E	401	3PE	C34-C35-C36-C37
52	Q	201	ZMP	C16-C17-C18-C19
43	I	303	3PE	C22-C23-C24-C25
43	J	201	3PE	O21-C21-C22-C23
44	X	202	PC1	O31-C31-C32-C33
45	g	101	CDL	OA6-CA4-CA6-OA8
45	2	601	CDL	CB5-C51-C52-C53
43	4	601	3PE	C2F-C2G-C2H-C2I
43	4	605	3PE	O31-C31-C32-C33
43	4	601	3PE	C3B-C3C-C3D-C3E
45	S	201	CDL	C73-C74-C75-C76
46	2	602	LMN	O1-CBS-CCM-CBQ
50	E	402	NDP	C5D-O5D-PN-O3
43	I	304	3PE	C23-C24-C25-C26
43	4	601	3PE	C28-C29-C2A-C2B
43	W	202	3PE	C3C-C3D-C3E-C3F
43	I	303	3PE	C3B-C3C-C3D-C3E
49	B	602	FMN	O3'-C3'-C4'-C5'
45	D	101	CDL	C34-C35-C36-C37
44	3	201	PC1	O22-C21-C22-C23
45	S	201	CDL	C32-C31-CA7-OA9
43	5	702	3PE	O32-C31-C32-C33
44	5	701	PC1	O31-C31-C32-C33
43	4	605	3PE	C32-C33-C34-C35
44	K	302	PC1	O32-C31-C32-C33
44	S	202	PC1	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
43	5	703	3PE	O32-C31-C32-C33
45	D	101	CDL	C52-C51-CB5-OB7
43	I	304	3PE	C2A-C2B-C2C-C2D
45	g	101	CDL	CB7-C71-C72-C73
43	W	201	3PE	O22-C21-C22-C23
45	2	601	CDL	C1-CA2-OA2-PA1
43	I	304	3PE	O22-C21-C22-C23
43	5	702	3PE	C1-O11-P-O12
43	5	703	3PE	C1-O11-P-O14
43	J	201	3PE	C1-O11-P-O12
43	W	201	3PE	C1-O11-P-O14
43	i	102	3PE	C11-O13-P-O14
43	n	201	3PE	C11-O13-P-O12
44	5	701	PC1	C11-O13-P-O14
44	5	706	PC1	C1-O11-P-O14
45	2	601	CDL	CB2-OB2-PB2-OB3
43	W	202	3PE	C38-C39-C3A-C3B
43	n	201	3PE	C38-C39-C3A-C3B
44	1	402	PC1	C28-C29-C2A-C2B
46	4	603	LMN	CAB-CAX-CAZ-CBB
43	5	702	3PE	O13-C11-C12-N
45	g	101	CDL	OB9-CB7-OB8-CB6
43	4	605	3PE	O32-C31-C32-C33
44	S	202	PC1	C3B-C3C-C3D-C3E
43	I	304	3PE	C12-C11-O13-P
43	W	201	3PE	C12-C11-O13-P
43	W	202	3PE	C12-C11-O13-P
45	S	201	CDL	C72-C71-CB7-OB8
45	X	201	CDL	C20-C21-C22-C23
43	4	601	3PE	C33-C34-C35-C36
43	4	601	3PE	O31-C31-C32-C33
45	g	101	CDL	C12-C11-CA5-OA6
45	2	601	CDL	C12-C13-C14-C15
45	g	101	CDL	C72-C73-C74-C75
43	4	602	3PE	O31-C31-C32-C33
44	S	202	PC1	C37-C38-C39-C3A
44	3	201	PC1	C21-C22-C23-C24
52	Q	201	ZMP	C2-C3-C4-C5
43	g	102	3PE	O22-C21-C22-C23
45	D	101	CDL	C31-C32-C33-C34
43	W	201	3PE	O31-C31-C32-C33
43	W	202	3PE	O21-C21-C22-C23

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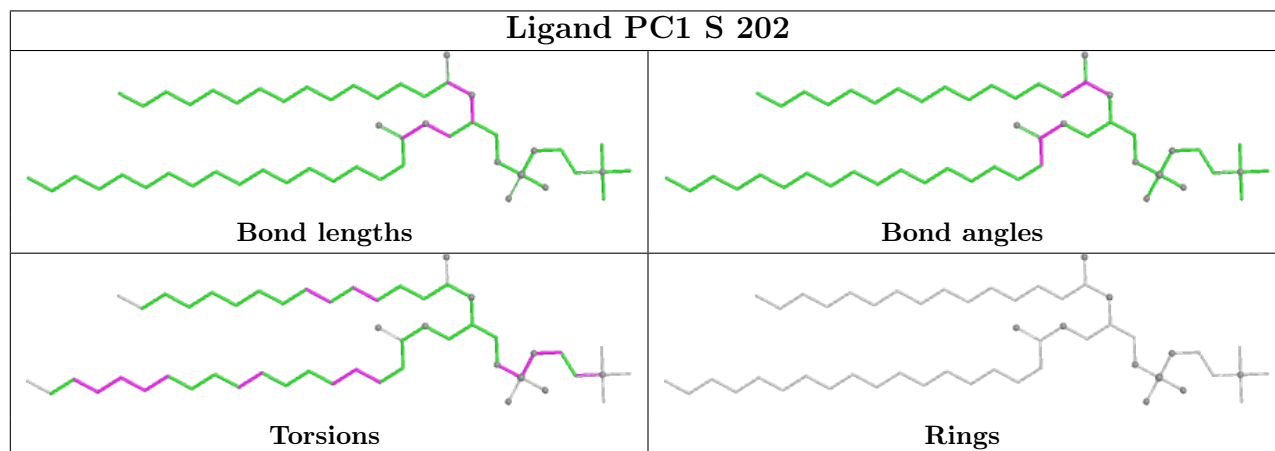
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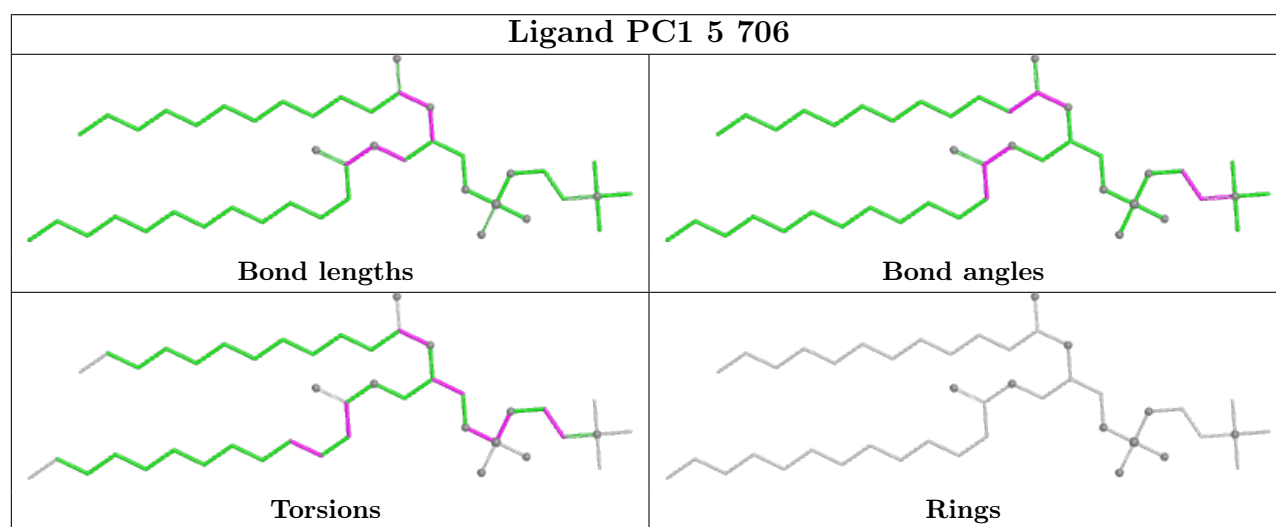
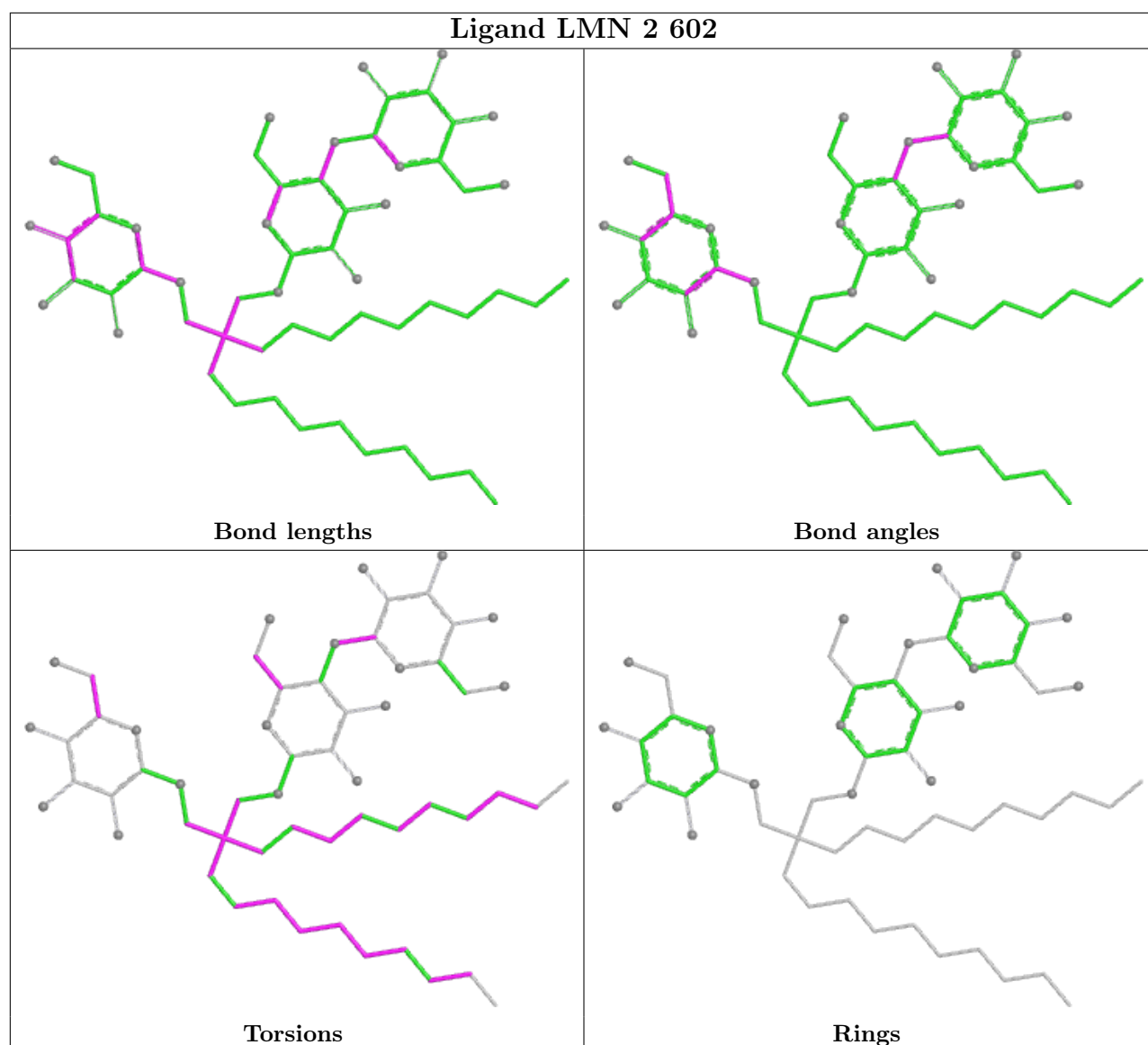
Mol	Chain	Res	Type	Atoms
45	D	101	CDL	C32-C31-CA7-OA8
44	5	701	PC1	O32-C31-C32-C33
44	X	202	PC1	O32-C31-C32-C33
45	D	101	CDL	C71-C72-C73-C74
44	S	202	PC1	C33-C34-C35-C36
45	S	201	CDL	C72-C71-CB7-OB9
45	X	201	CDL	C52-C53-C54-C55
45	S	201	CDL	C82-C83-C84-C85
45	X	201	CDL	C32-C31-CA7-OA8

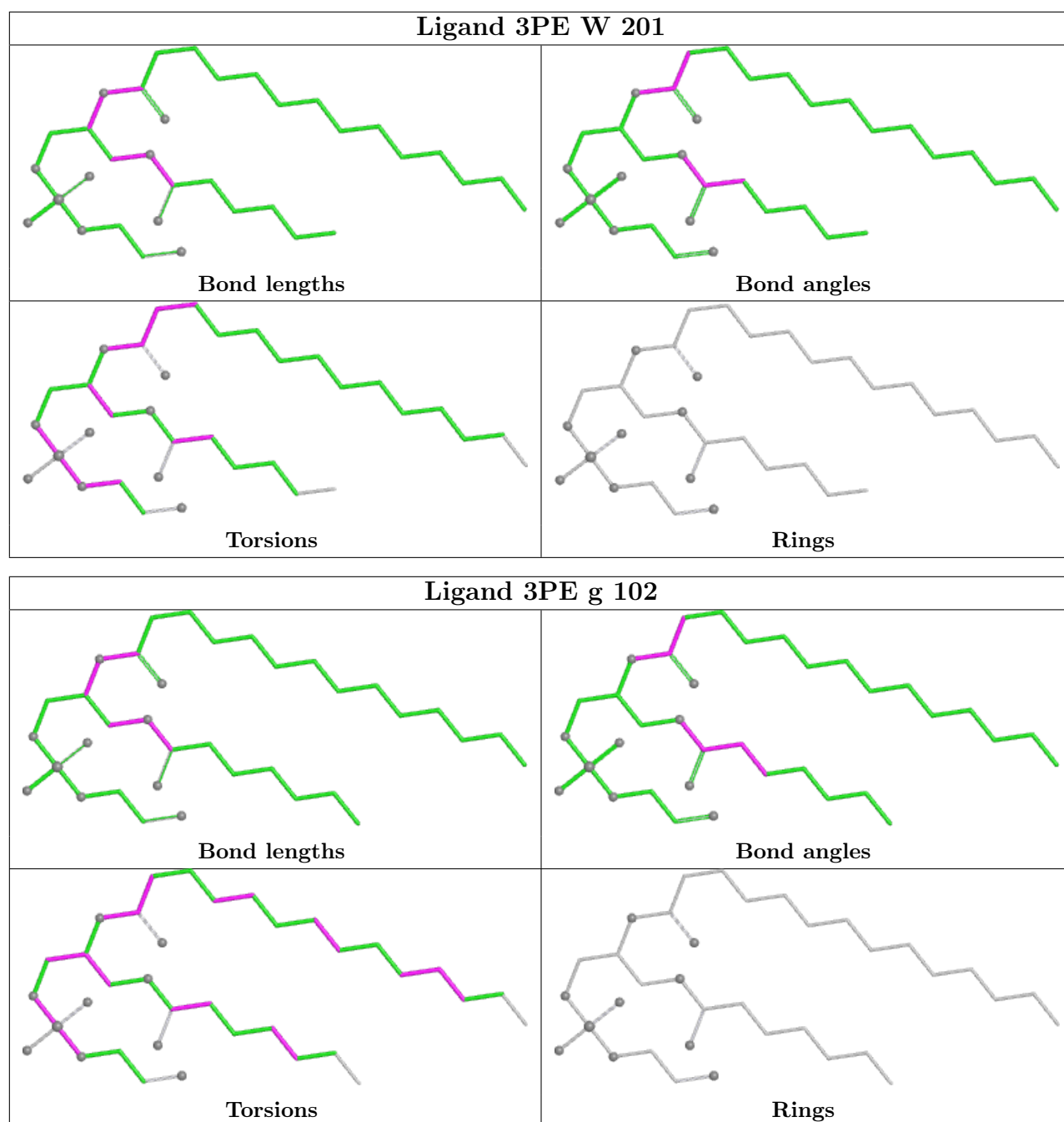
There are no ring outliers.

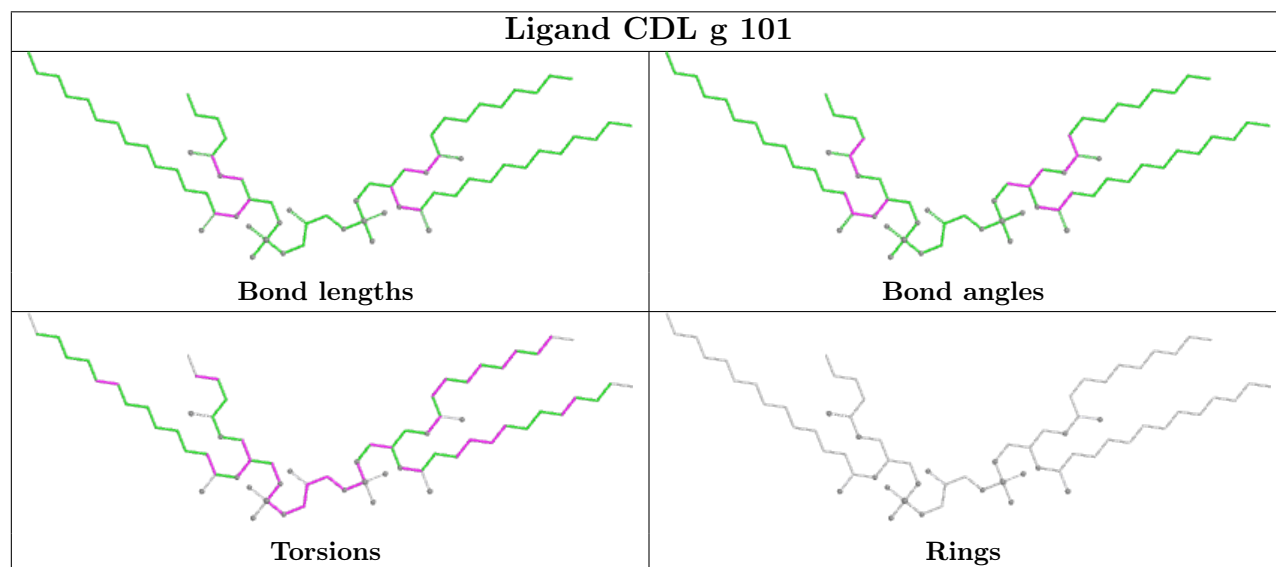
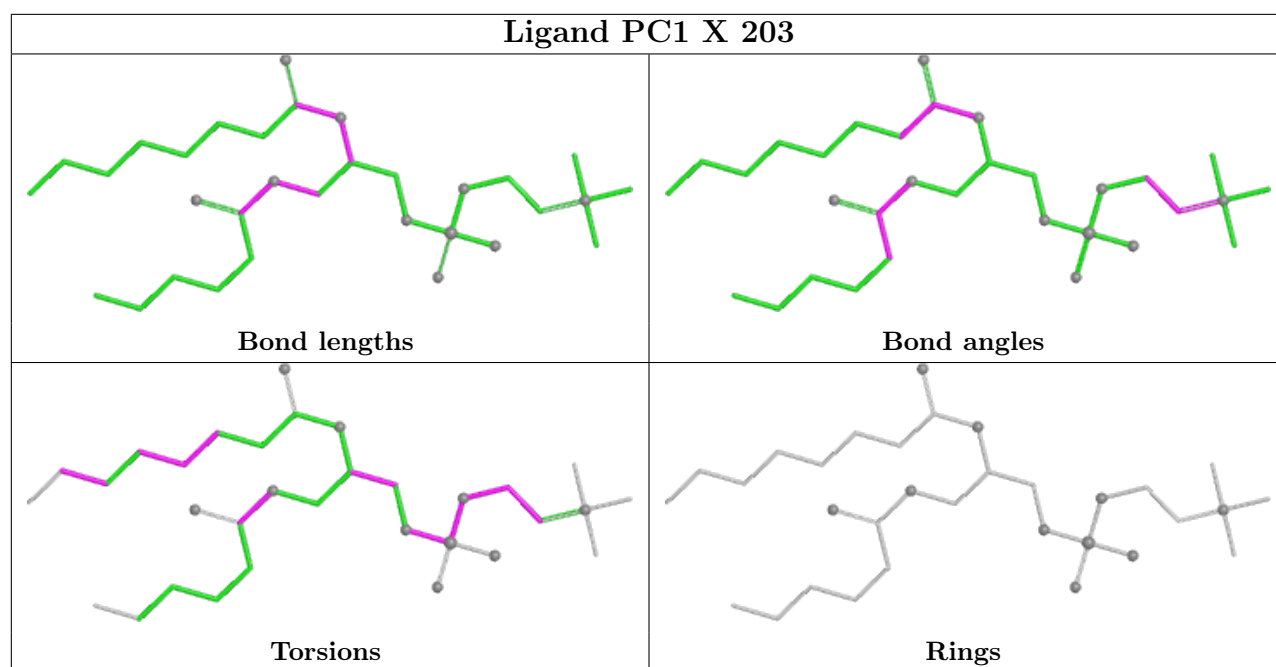
No monomer is involved in short contacts.

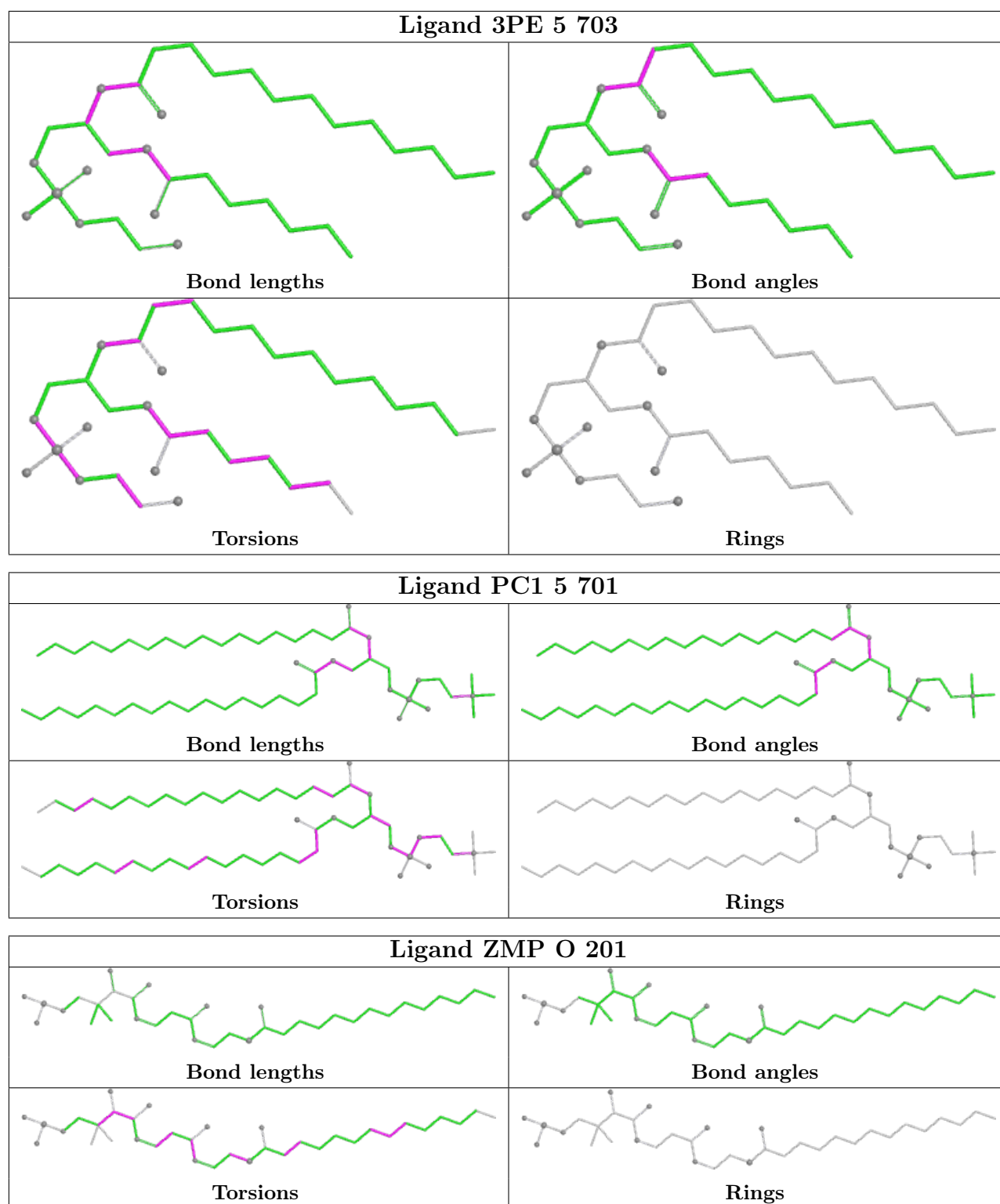
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

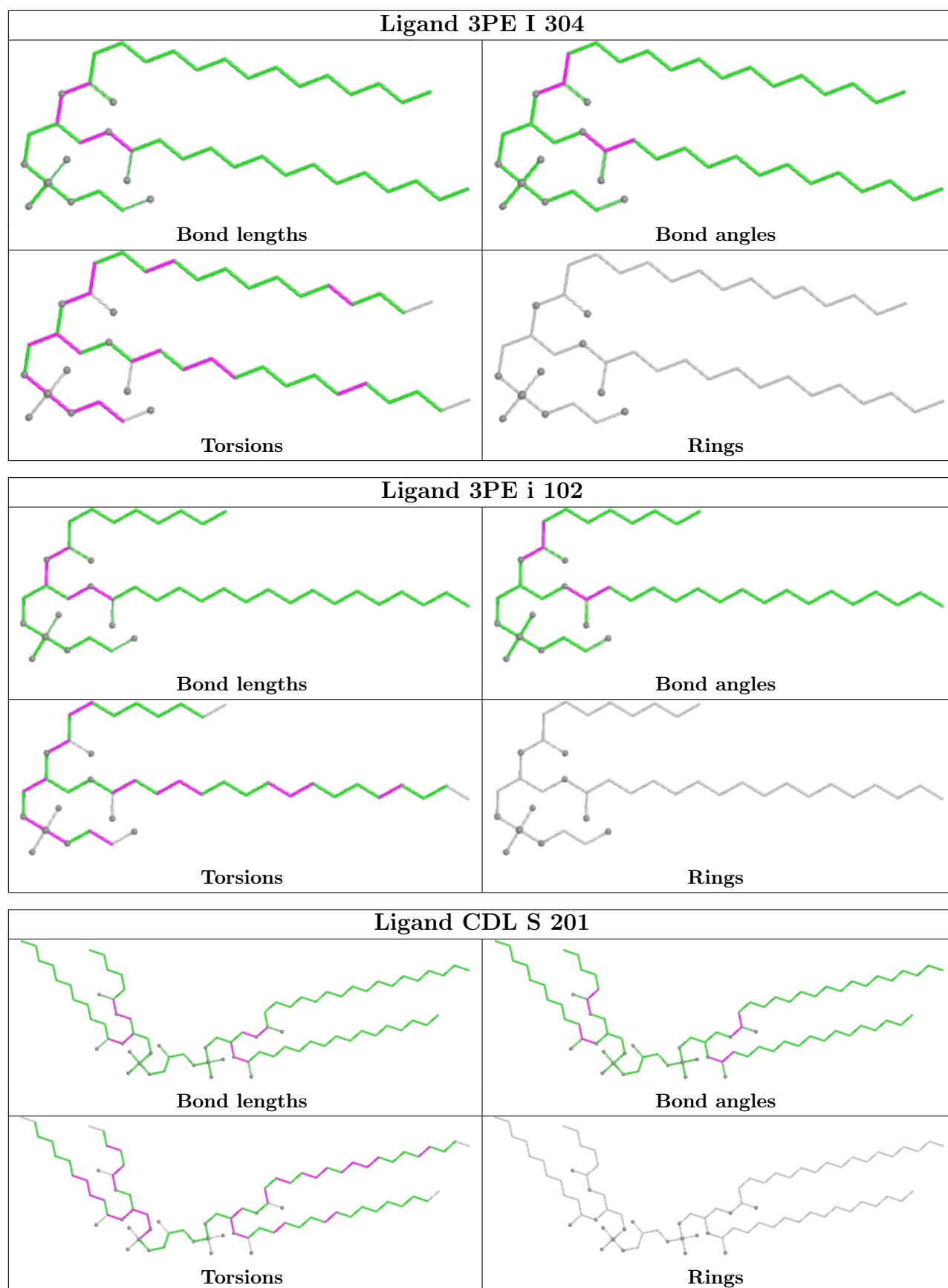


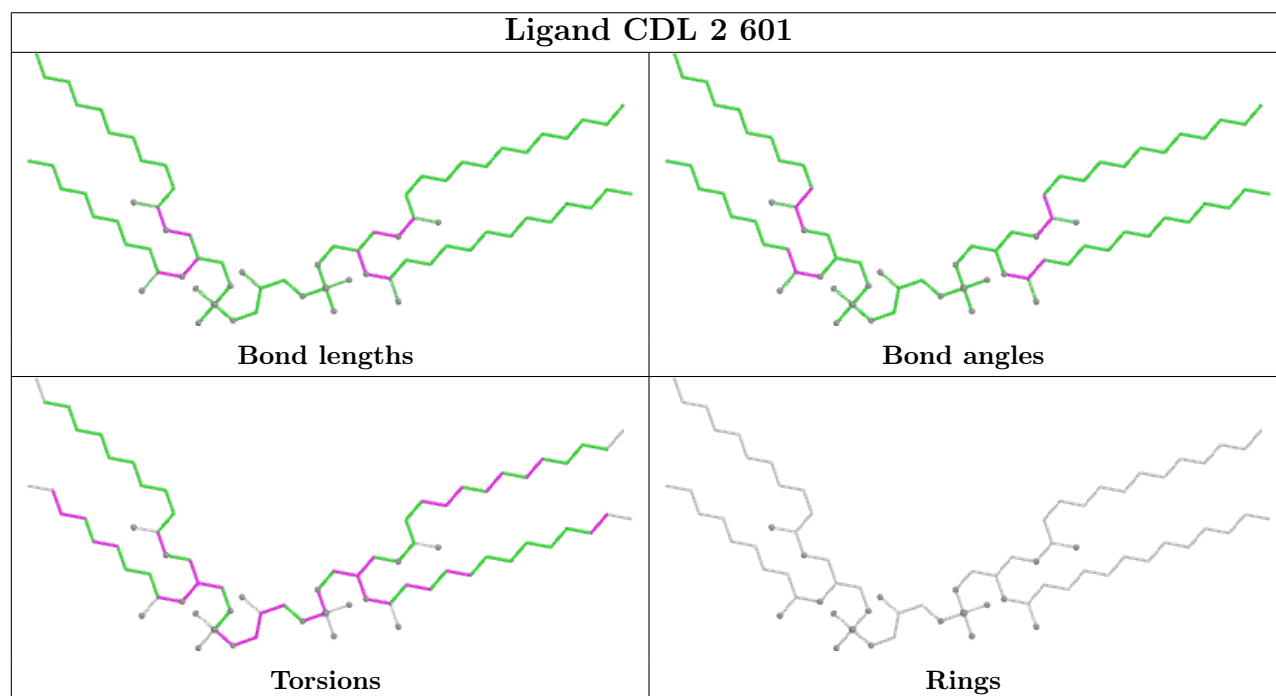
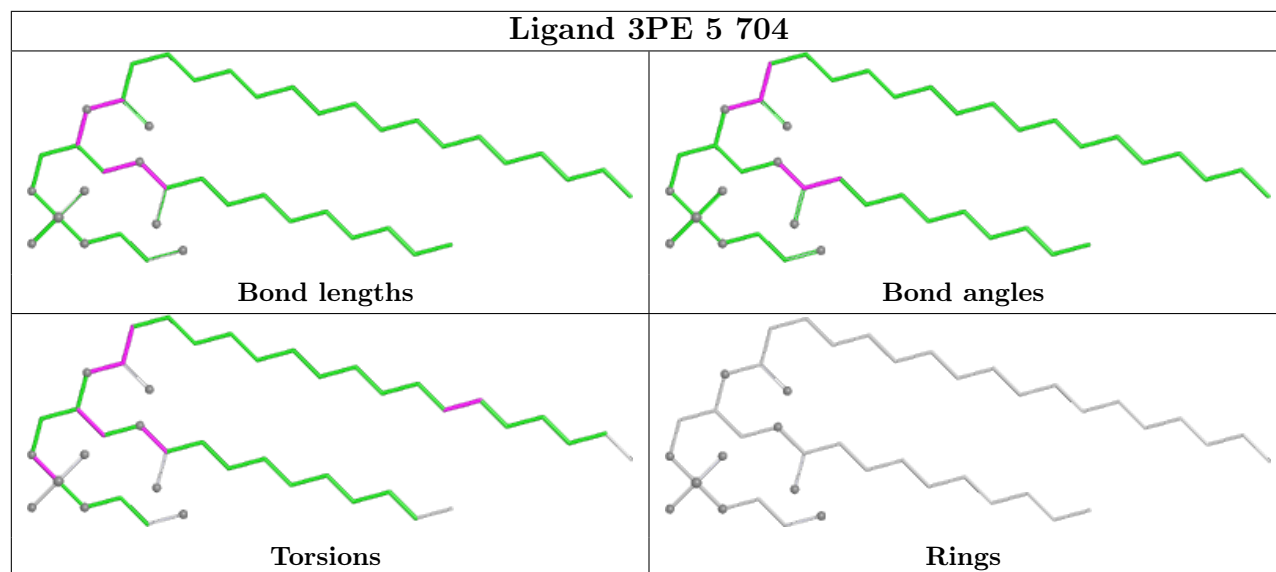


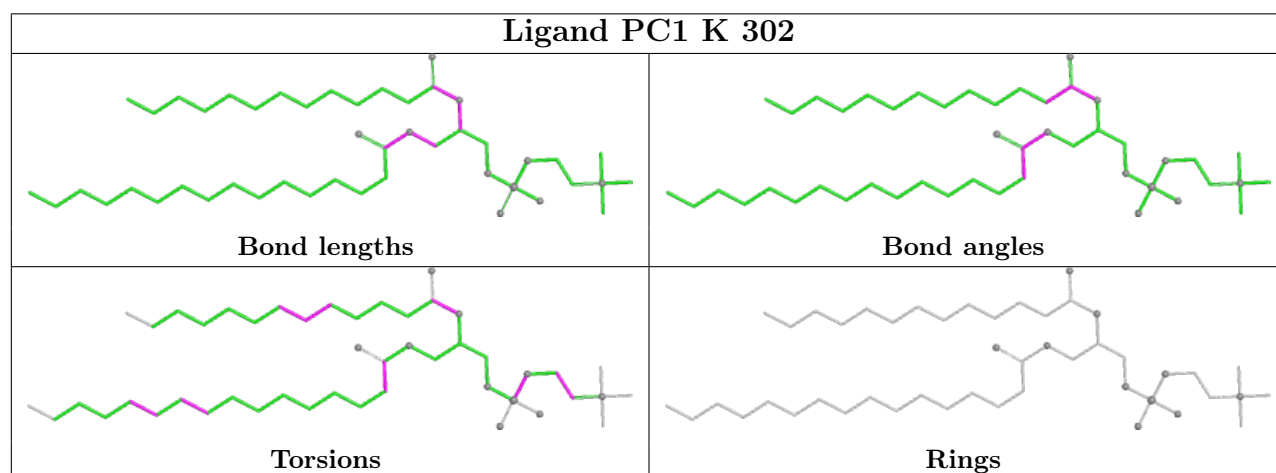
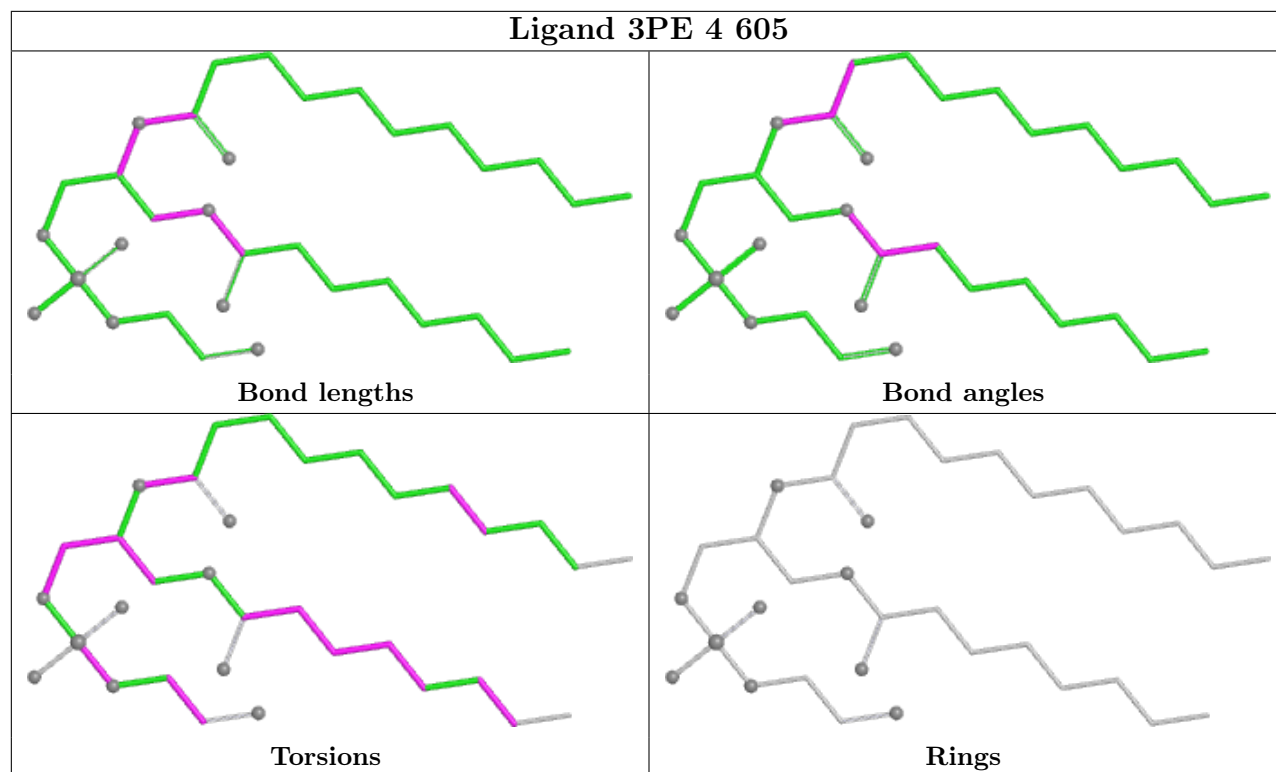


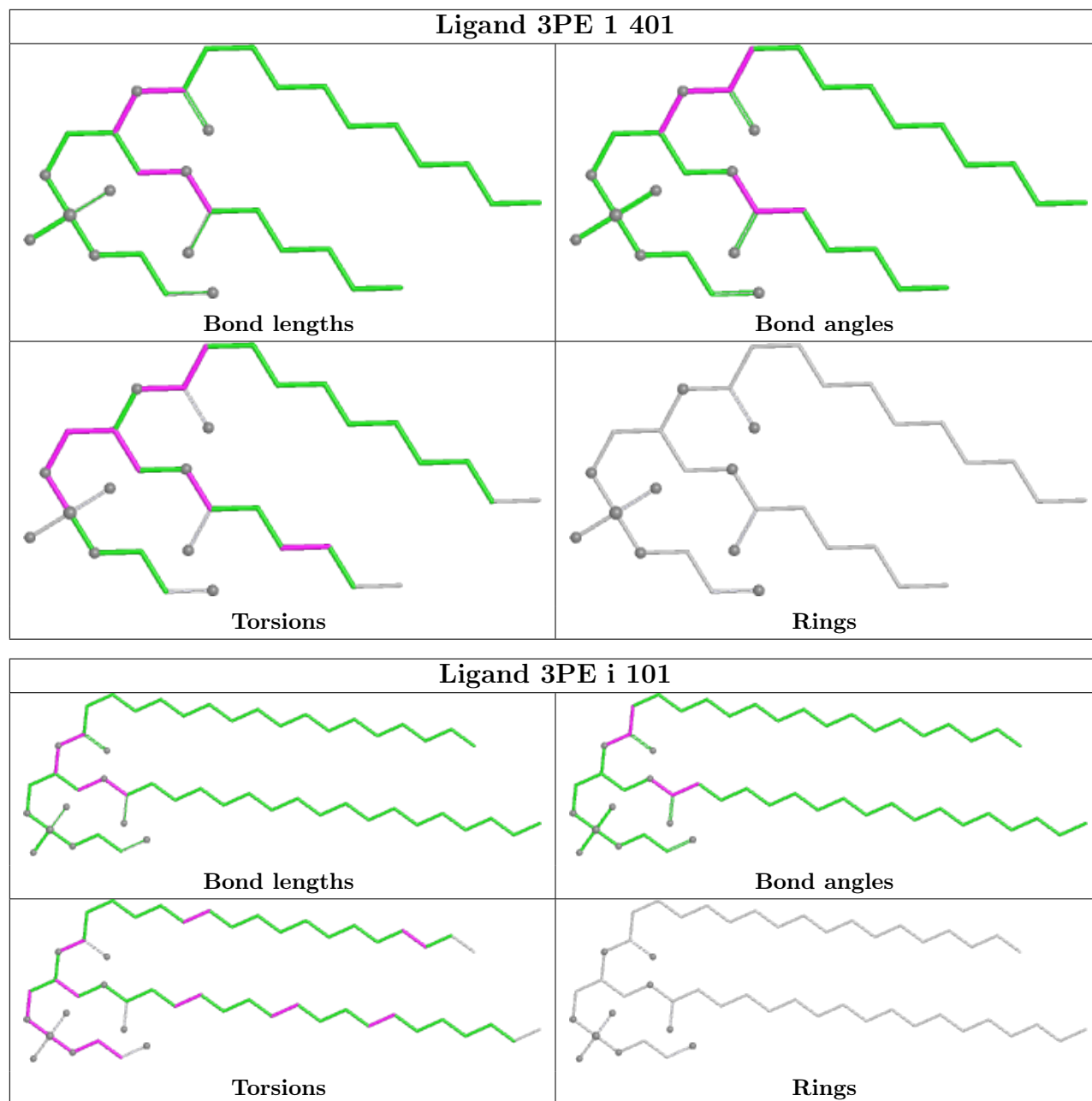


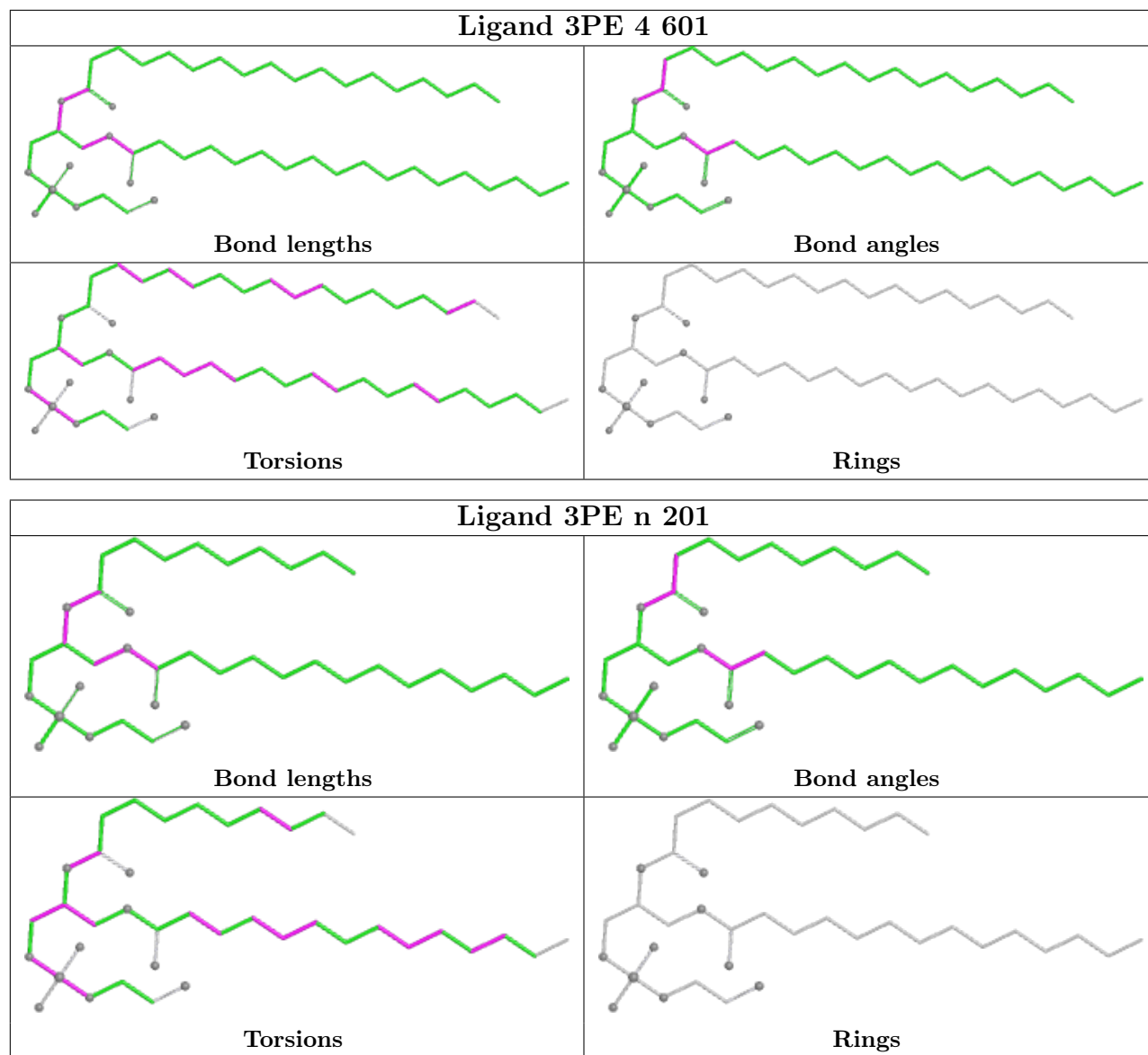


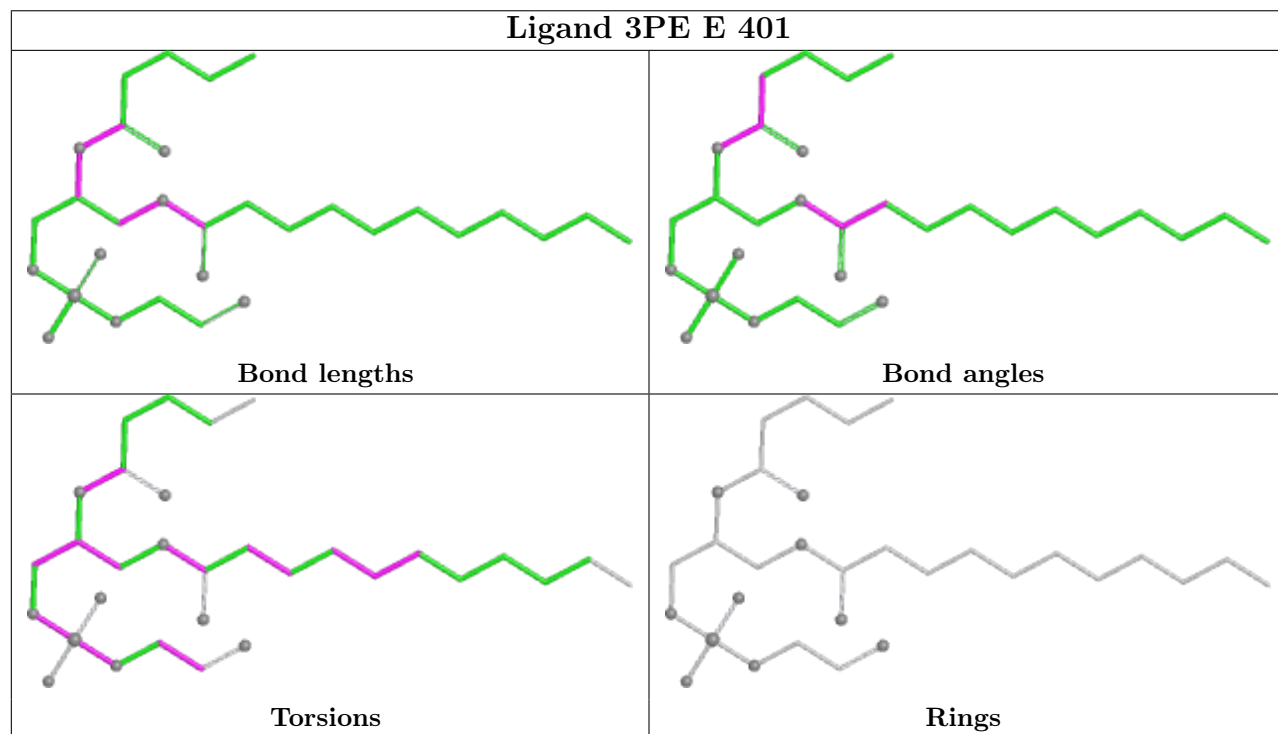
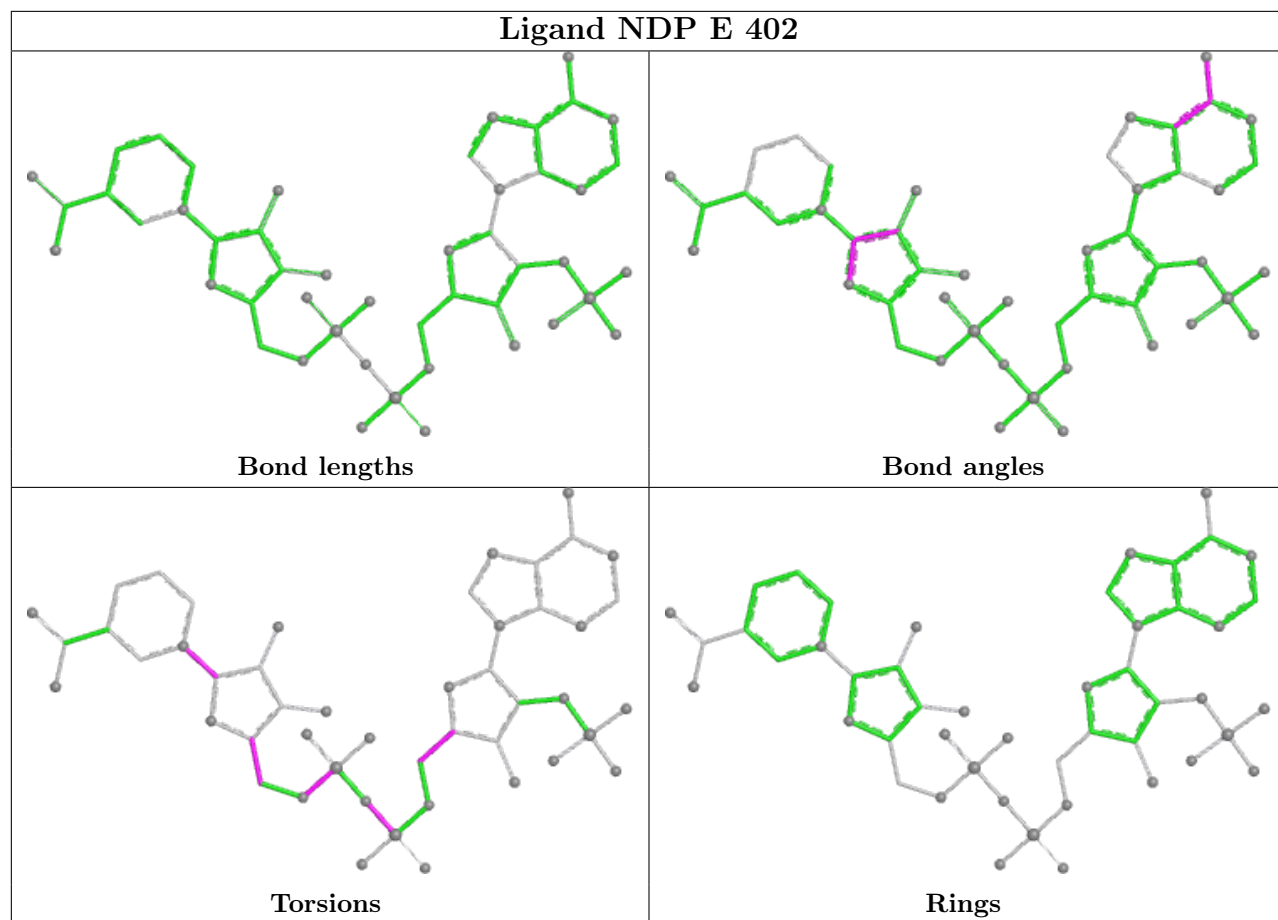


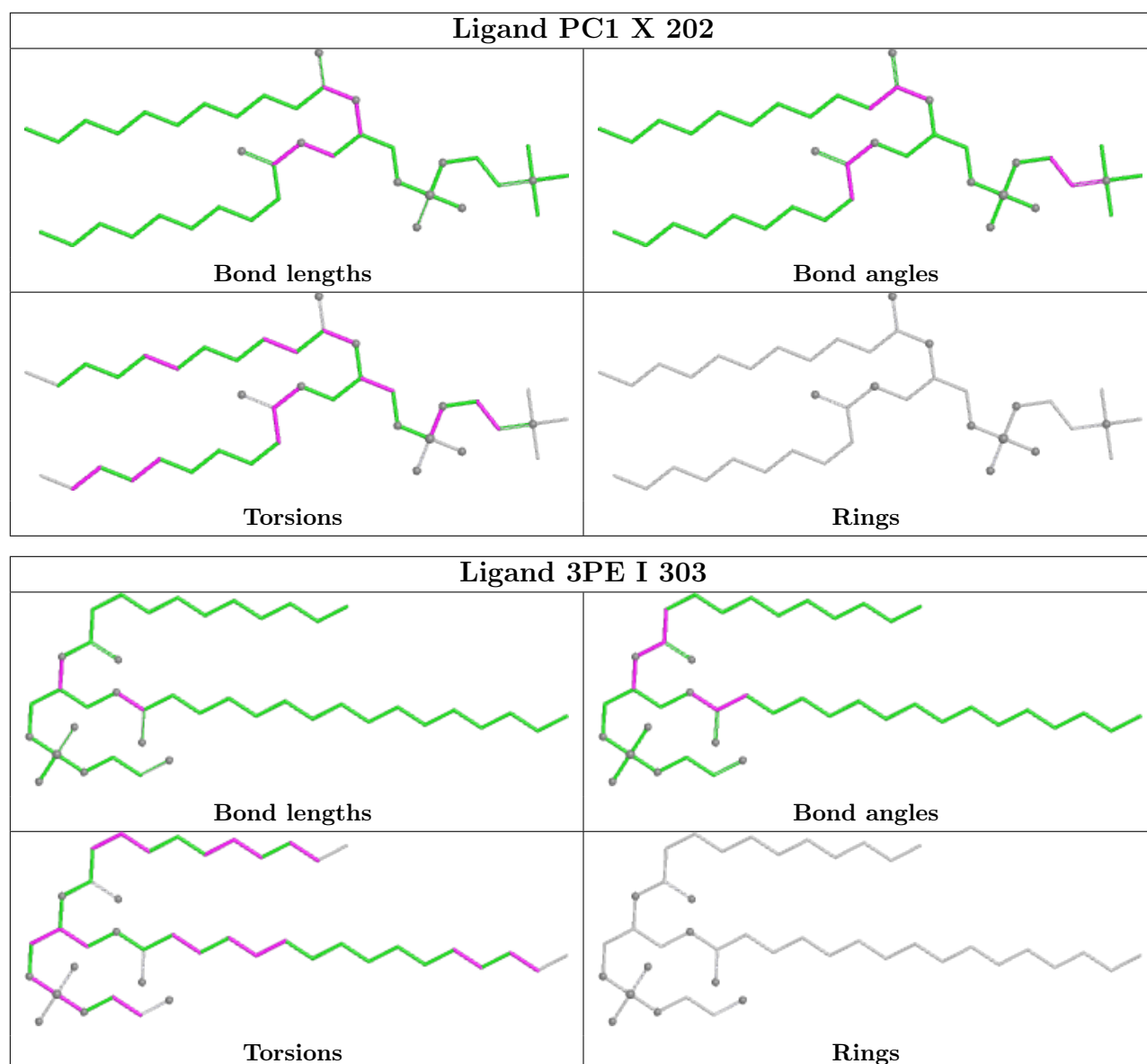


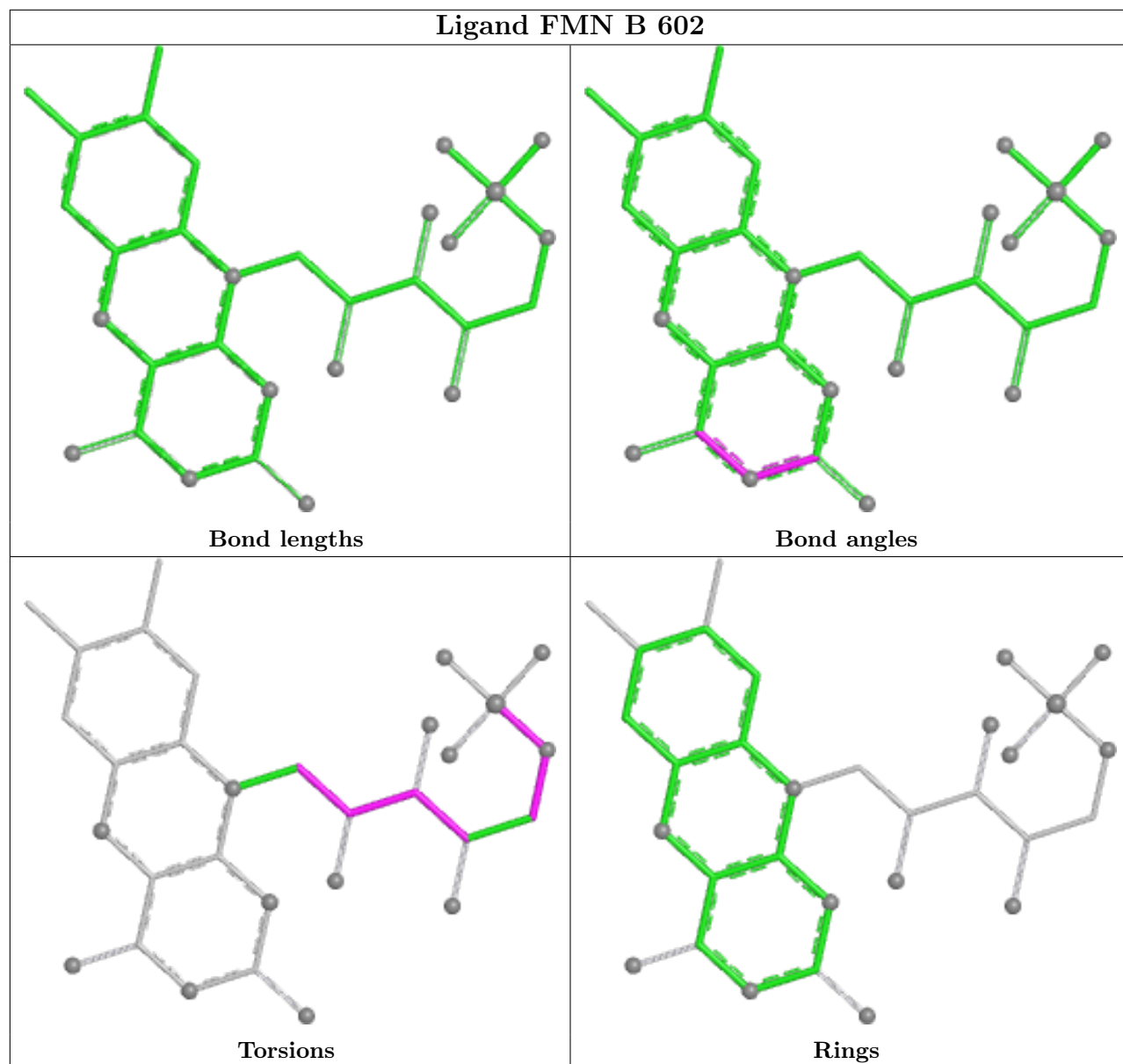


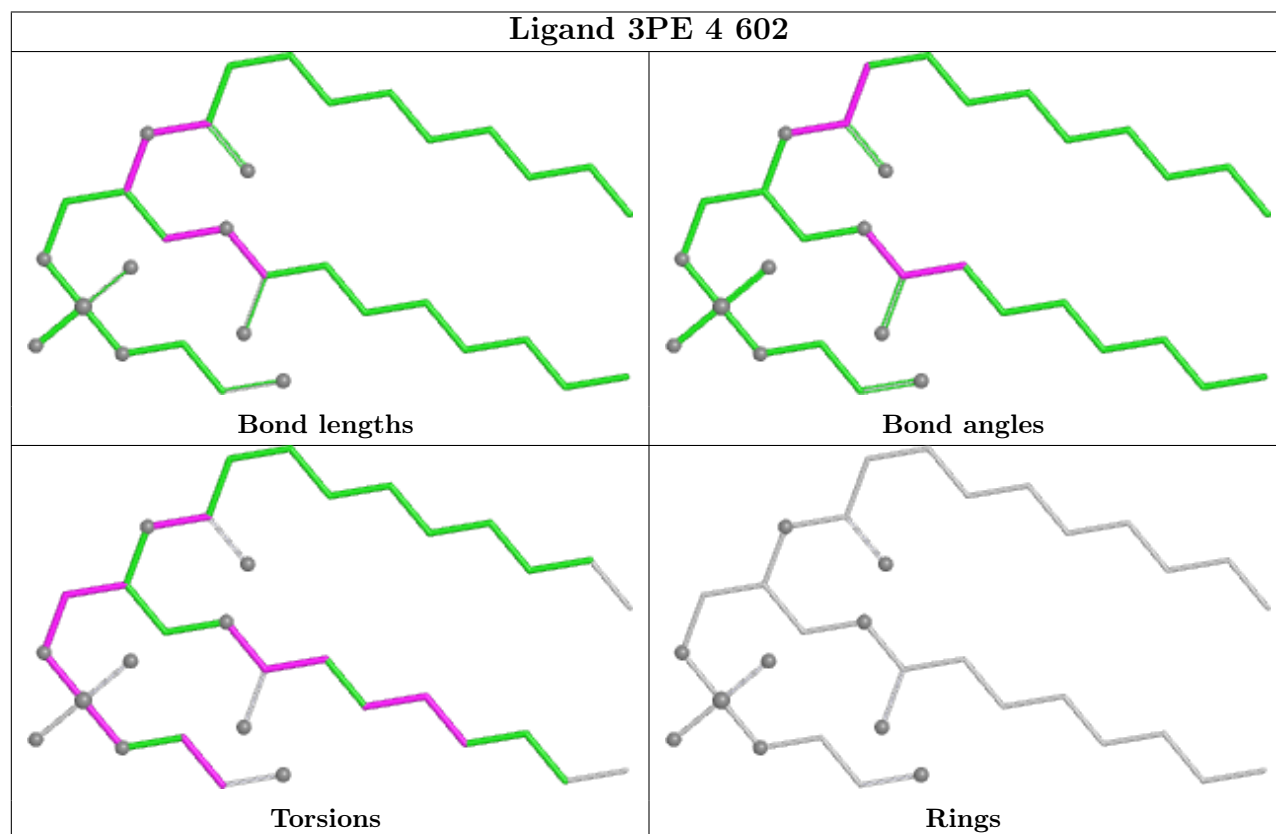
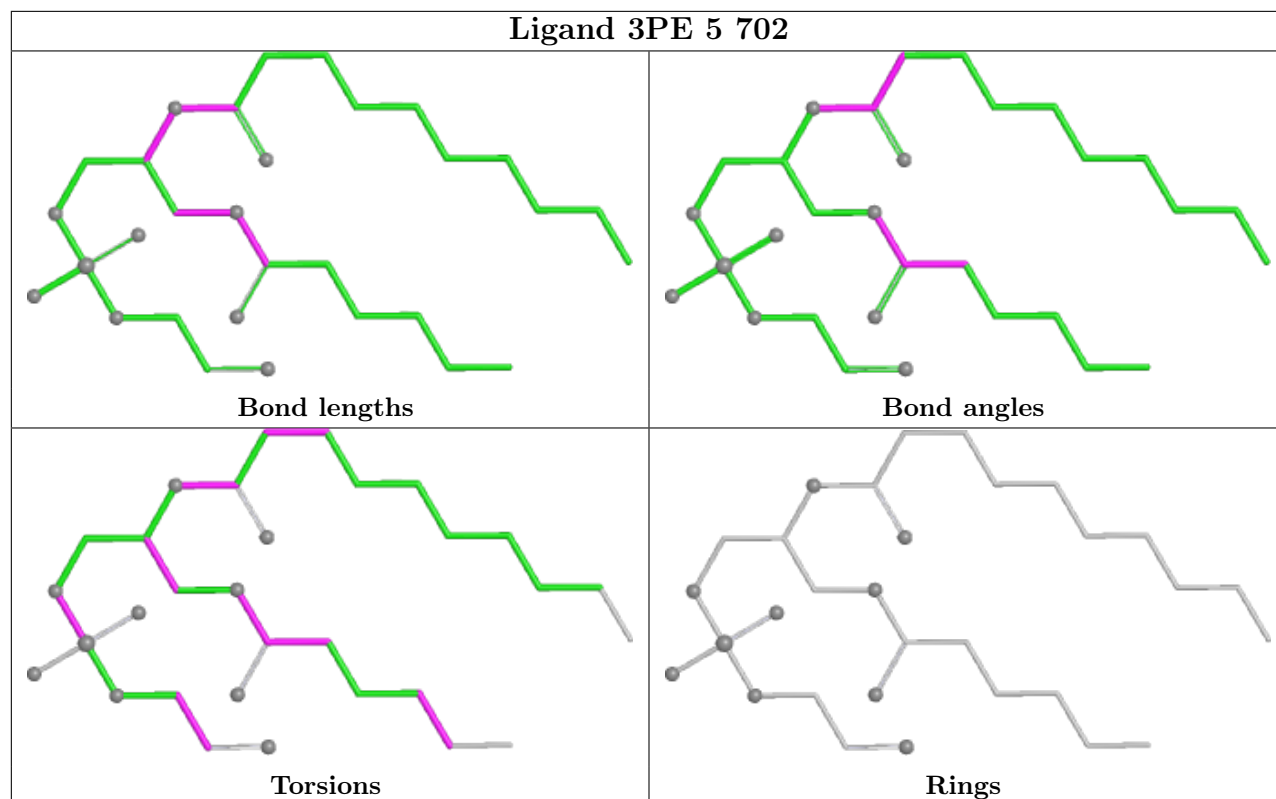


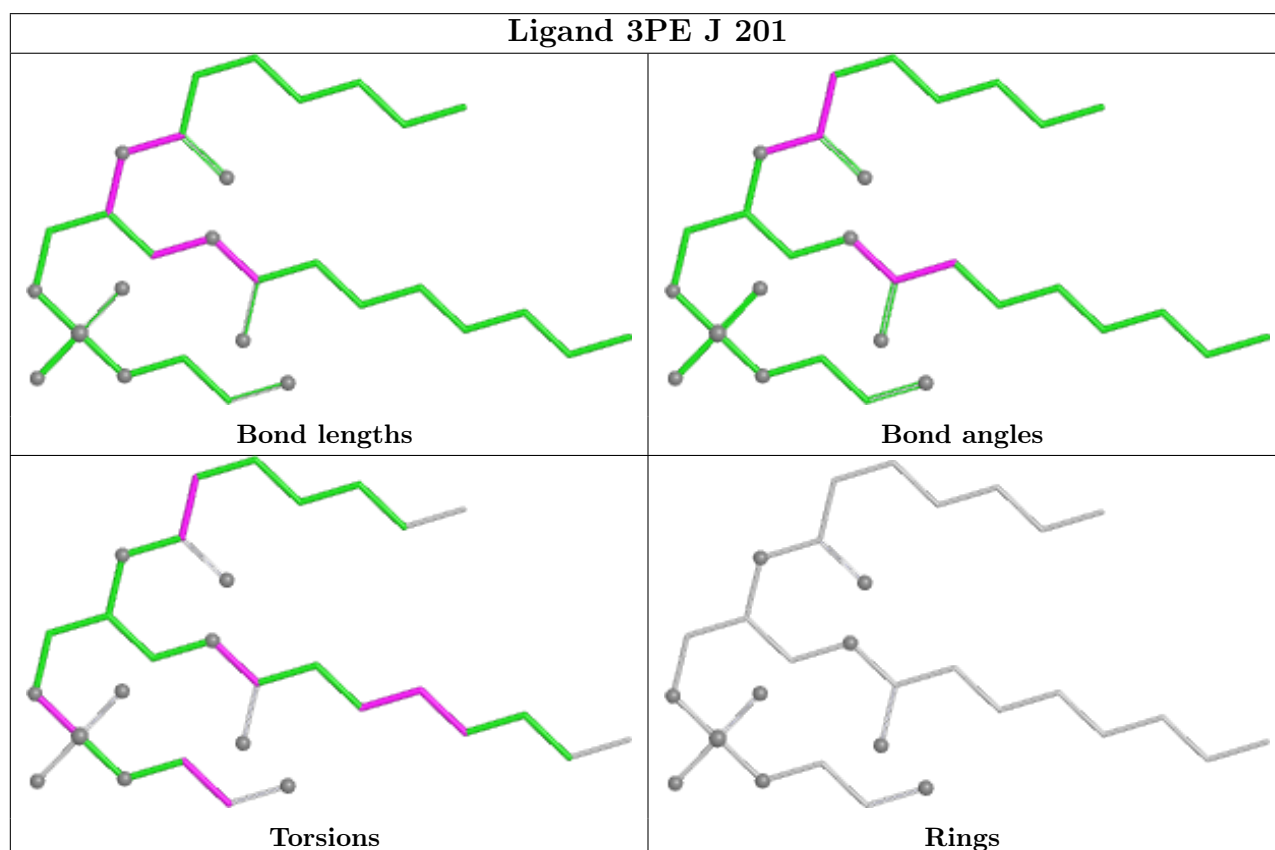
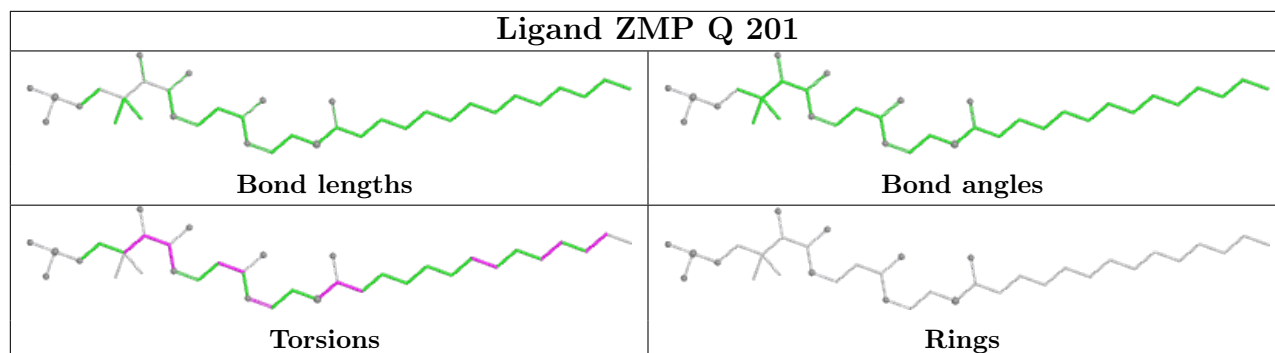


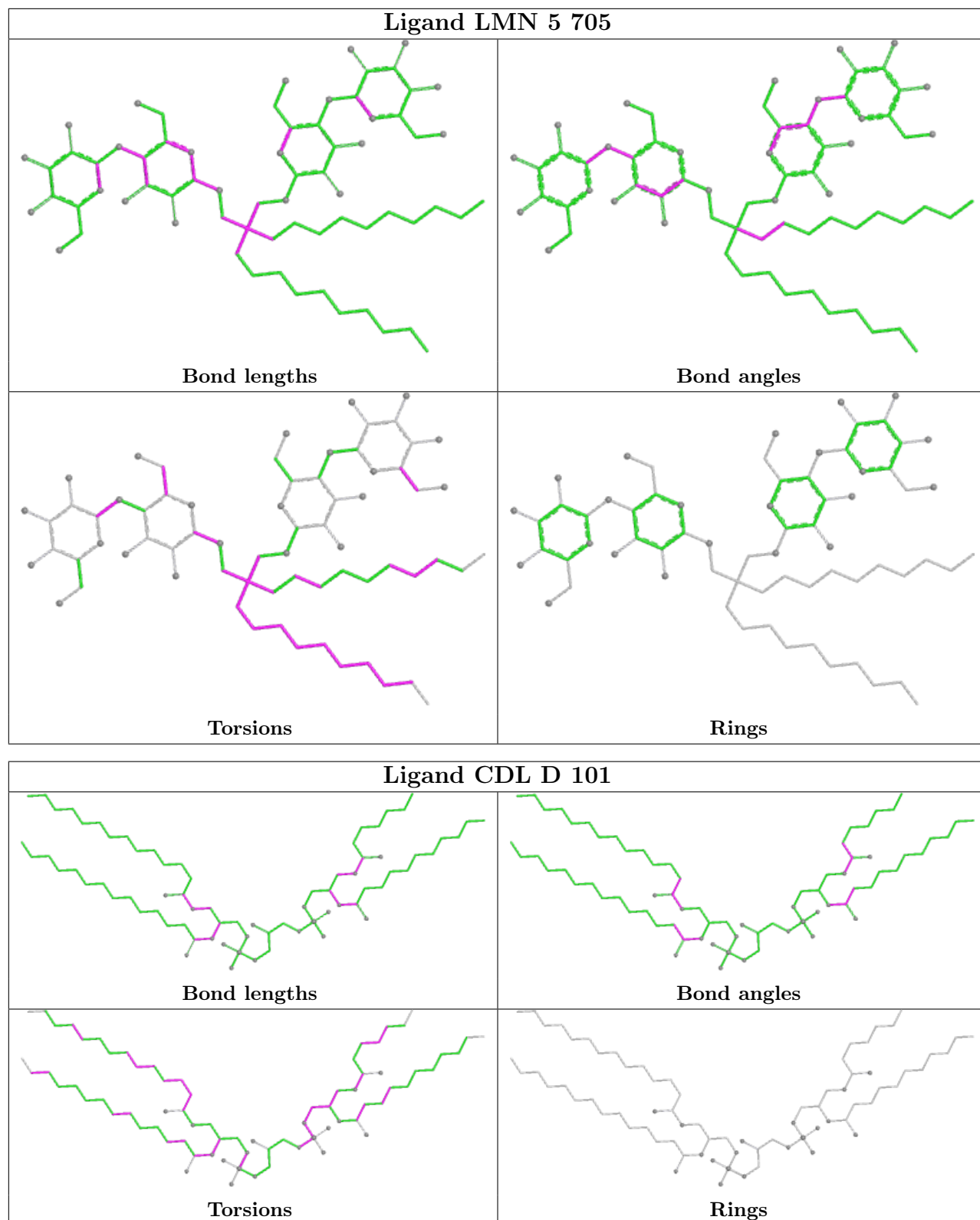


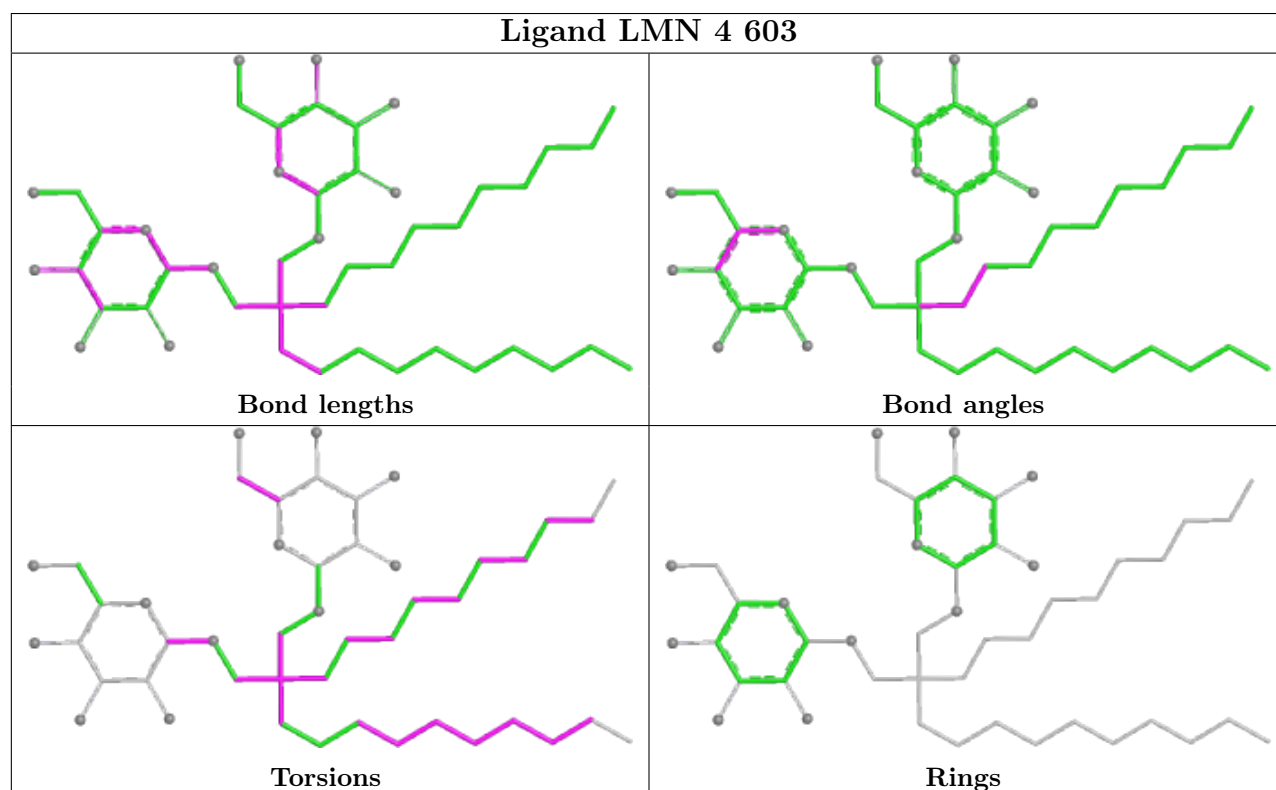
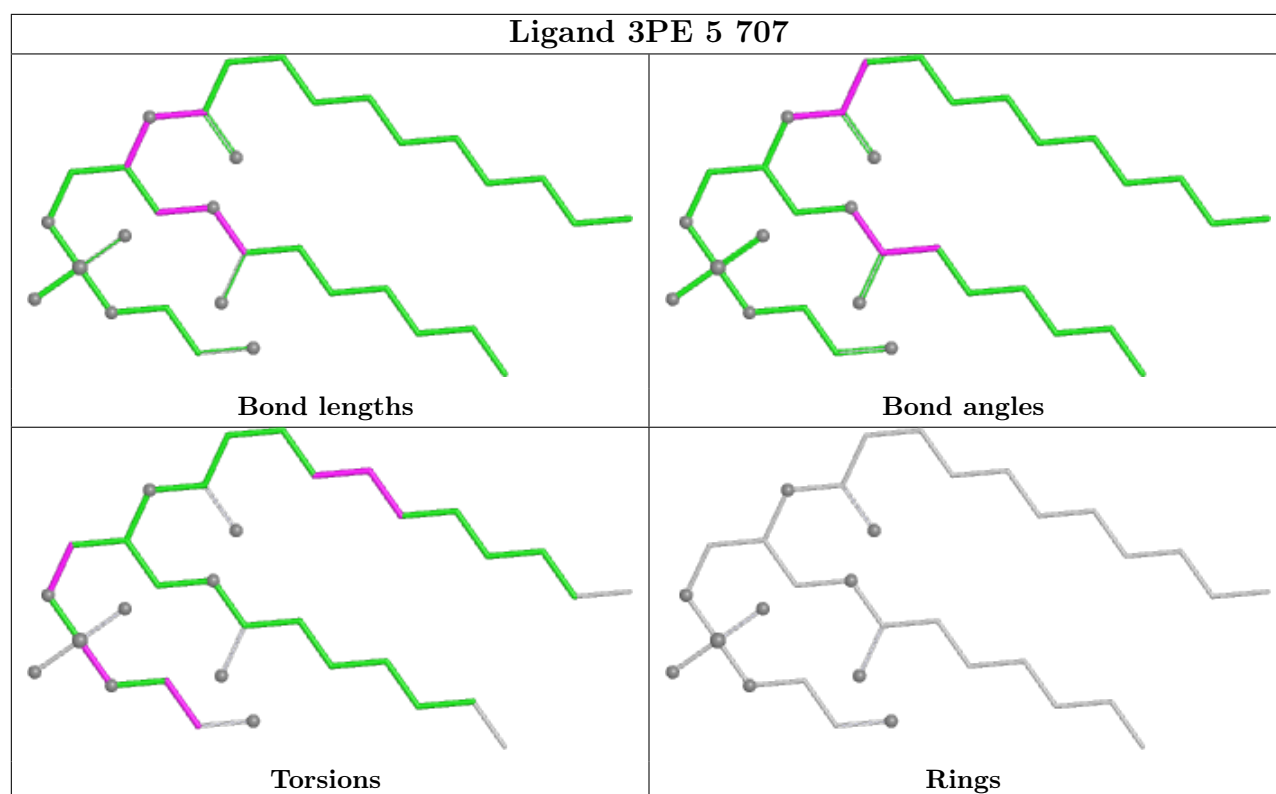


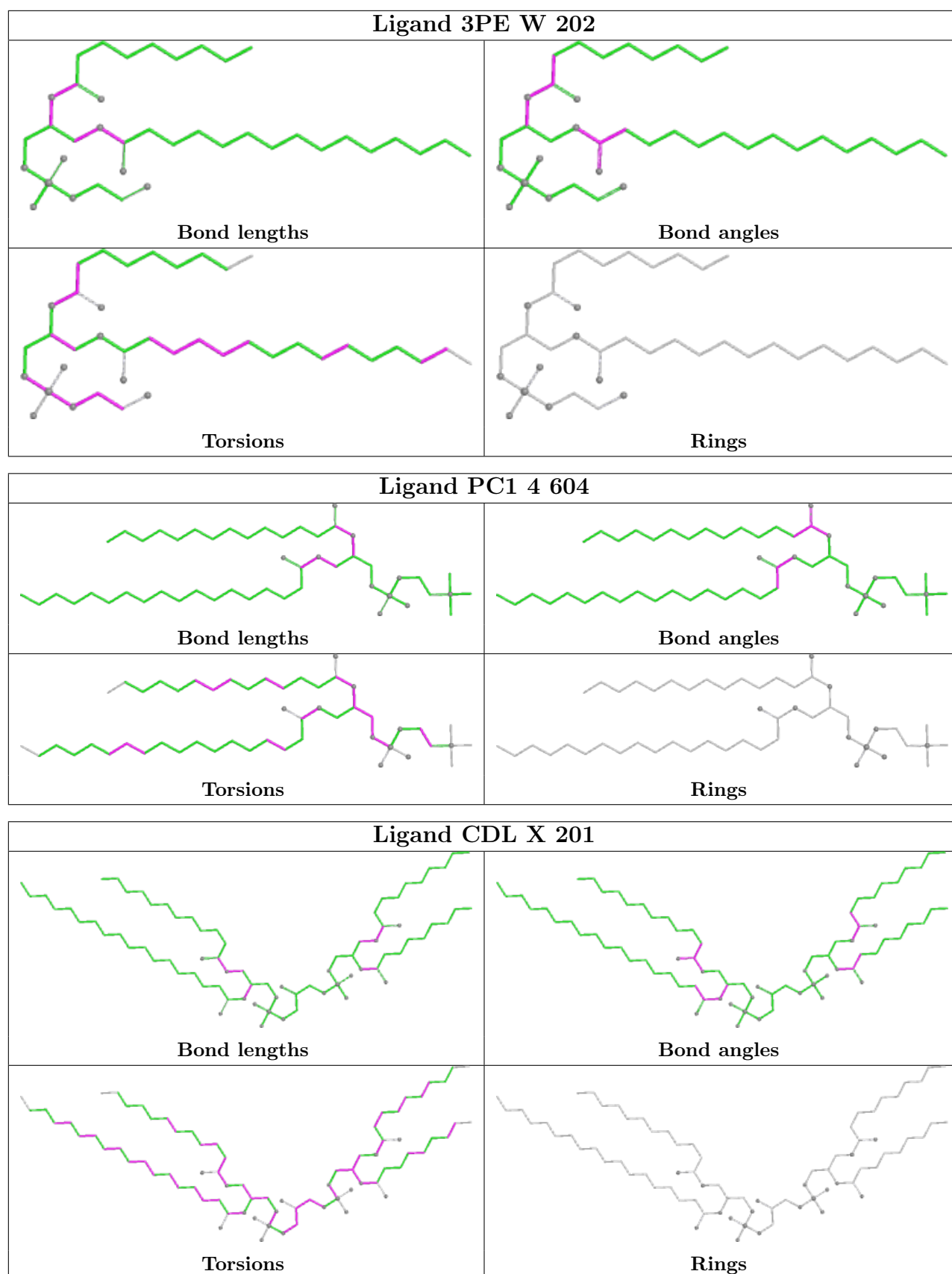


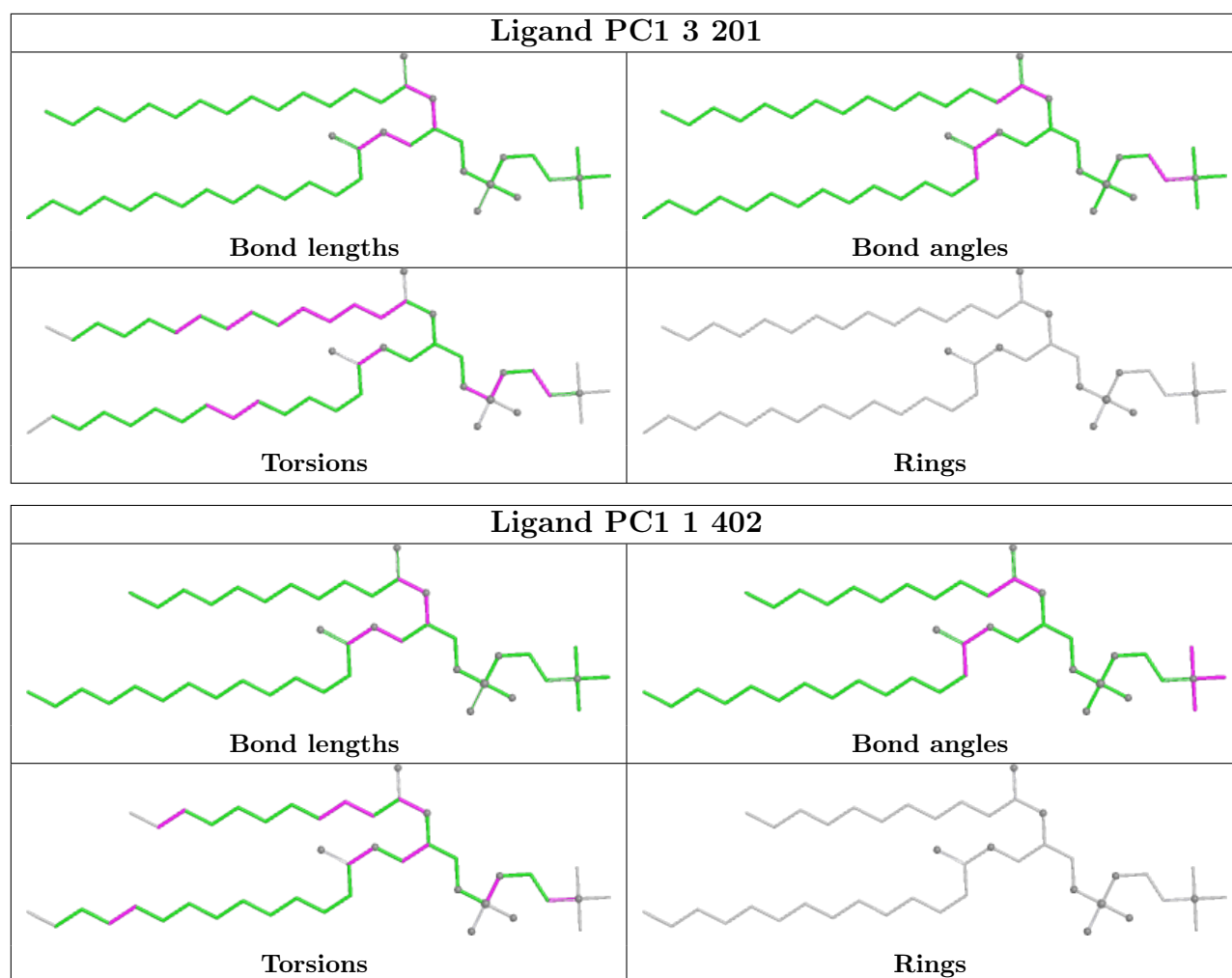












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

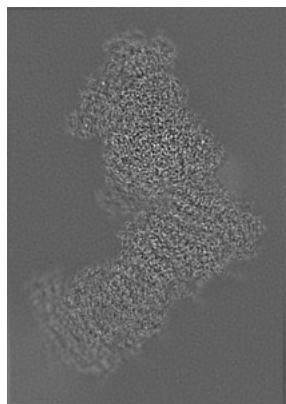
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14797. These allow visual inspection of the internal detail of the map and identification of artifacts.

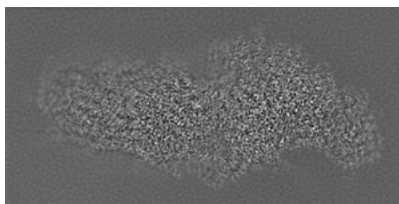
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

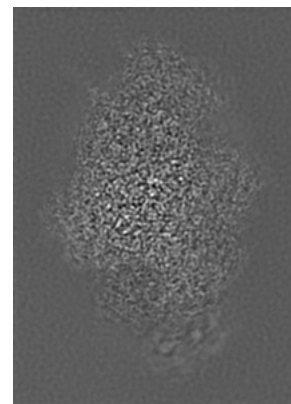
6.1.1 Primary map



X

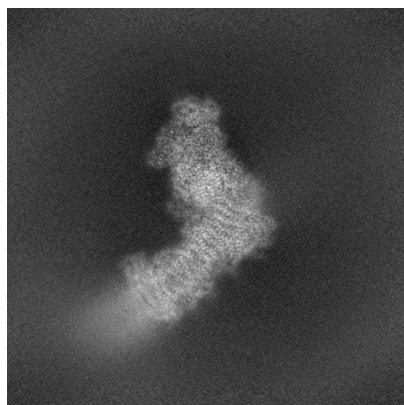


Y

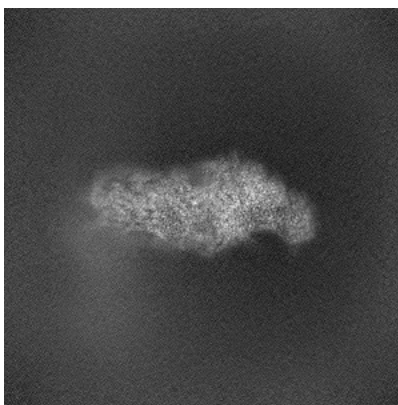


Z

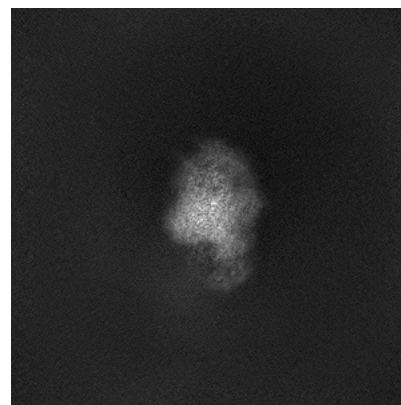
6.1.2 Raw map



X



Y

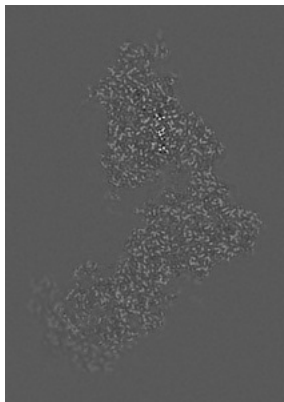


Z

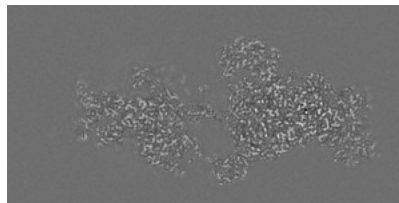
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

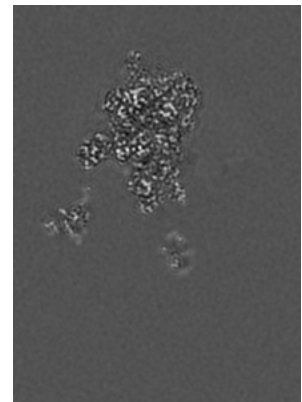
6.2.1 Primary map



X Index: 95

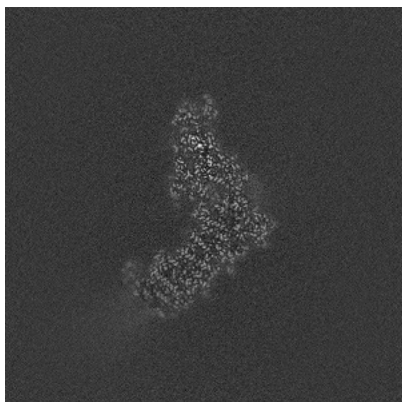


Y Index: 132

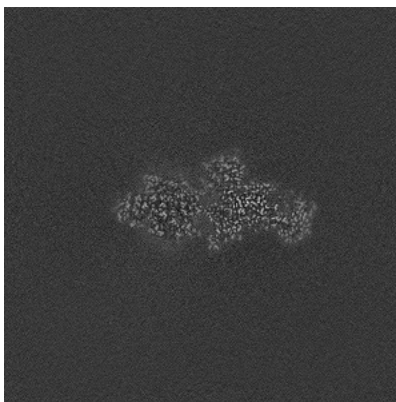


Z Index: 191

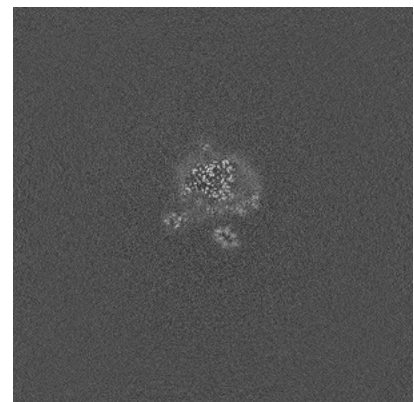
6.2.2 Raw map



X Index: 294



Y Index: 294

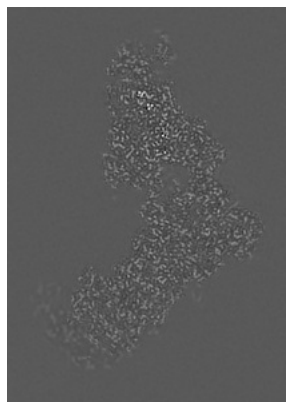


Z Index: 294

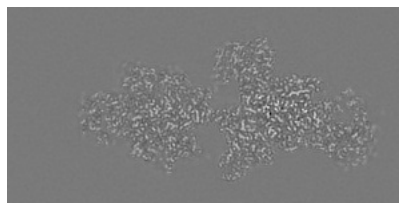
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

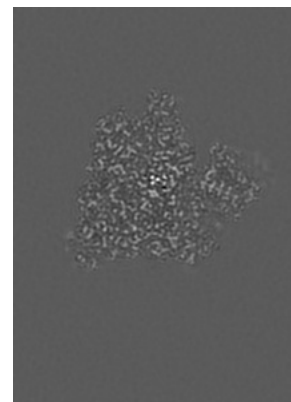
6.3.1 Primary map



X Index: 90

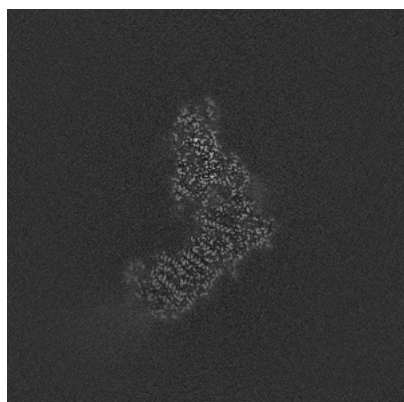


Y Index: 140

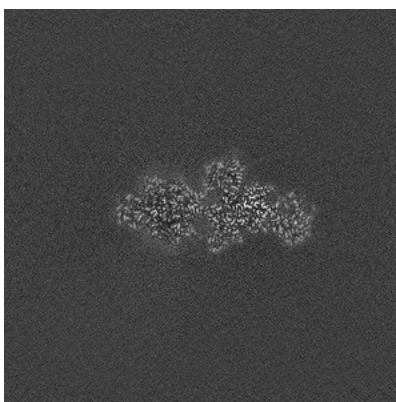


Z Index: 245

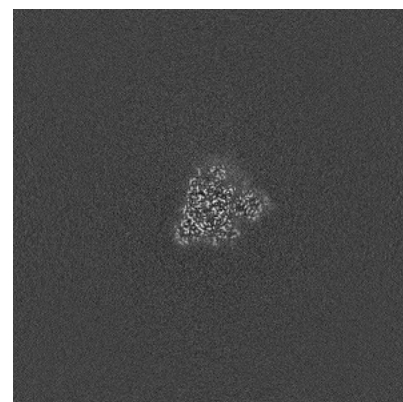
6.3.2 Raw map



X Index: 296



Y Index: 292



Z Index: 337

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

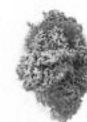
6.4.2 Raw map



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.

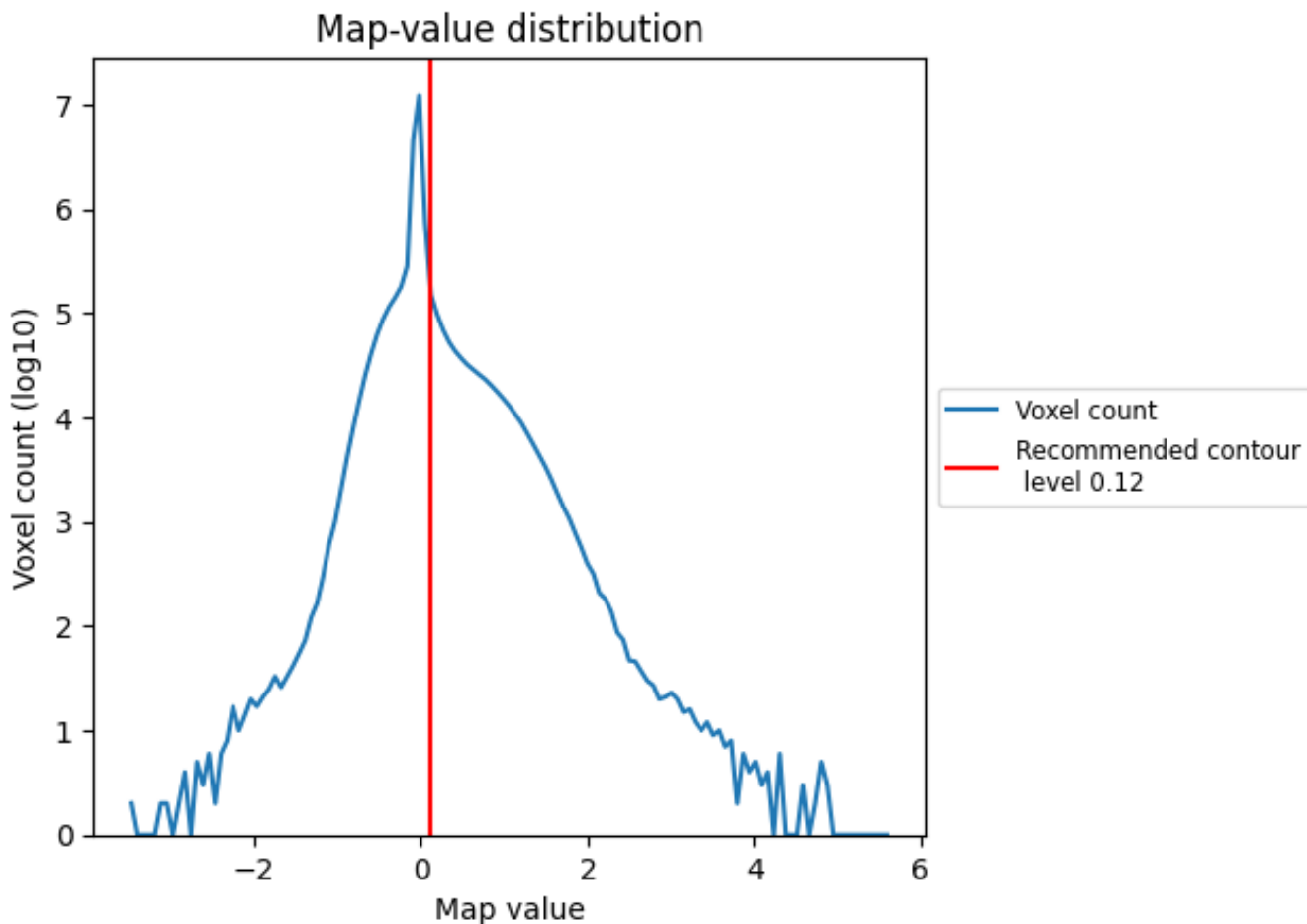
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

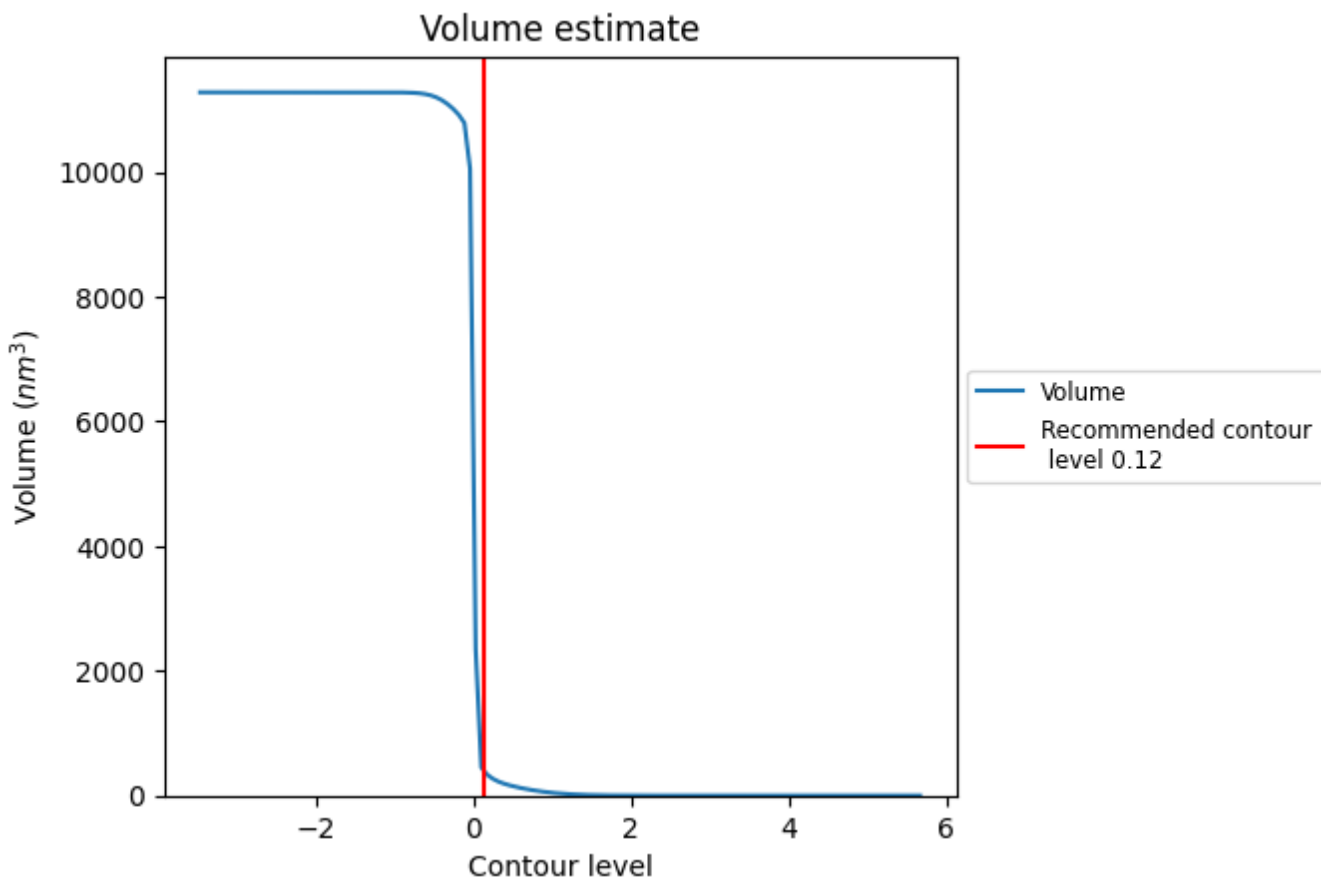
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 410 nm³; this corresponds to an approximate mass of 370 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.

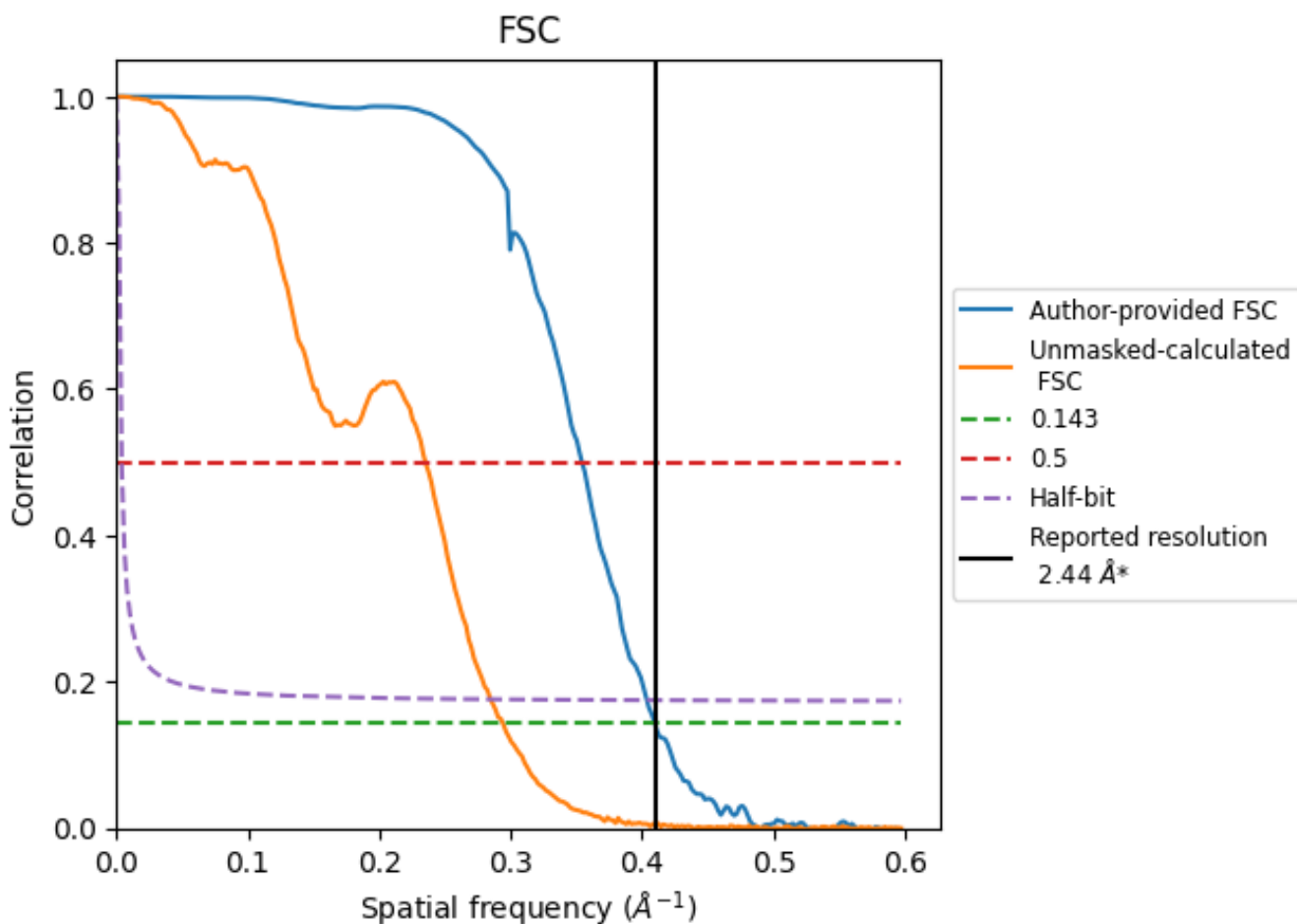
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.410 Å⁻¹

8.2 Resolution estimates [i](#)

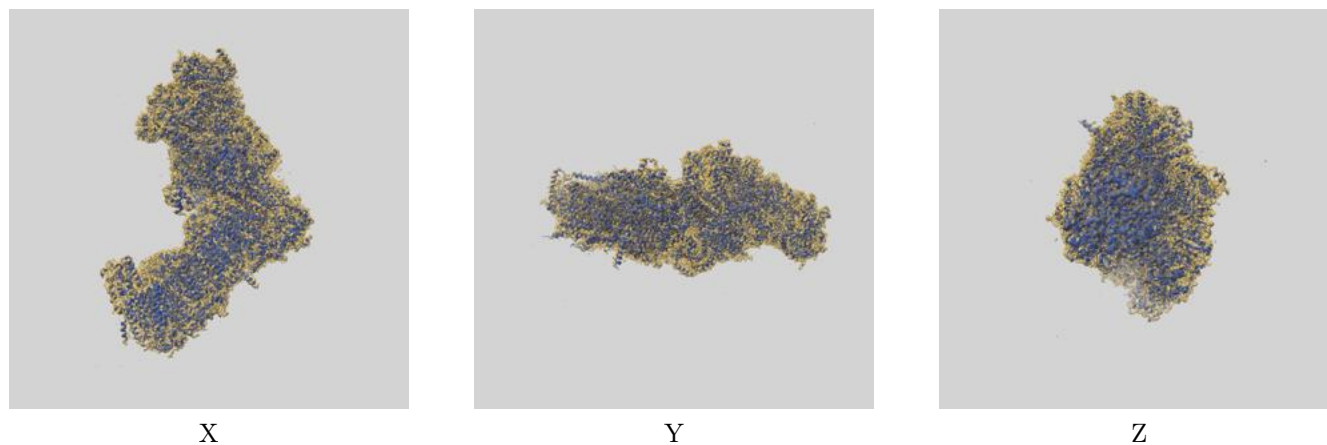
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.44	-	-
Author-provided FSC curve	2.44	2.82	2.48
Unmasked-calculated*	3.40	4.25	3.51

*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 3.40 differs from the reported value 2.44 by more than 10 %

9 Map-model fit [i](#)

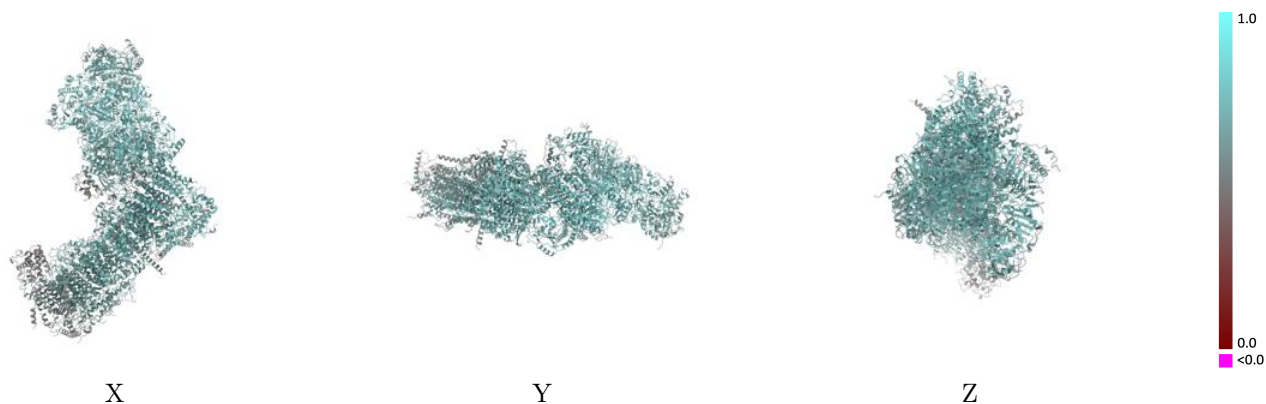
This section contains information regarding the fit between EMDB map EMD-14797 and PDB model 7ZMG. Per-residue inclusion information can be found in section [3](#) on page [25](#).

9.1 Map-model overlay [i](#)



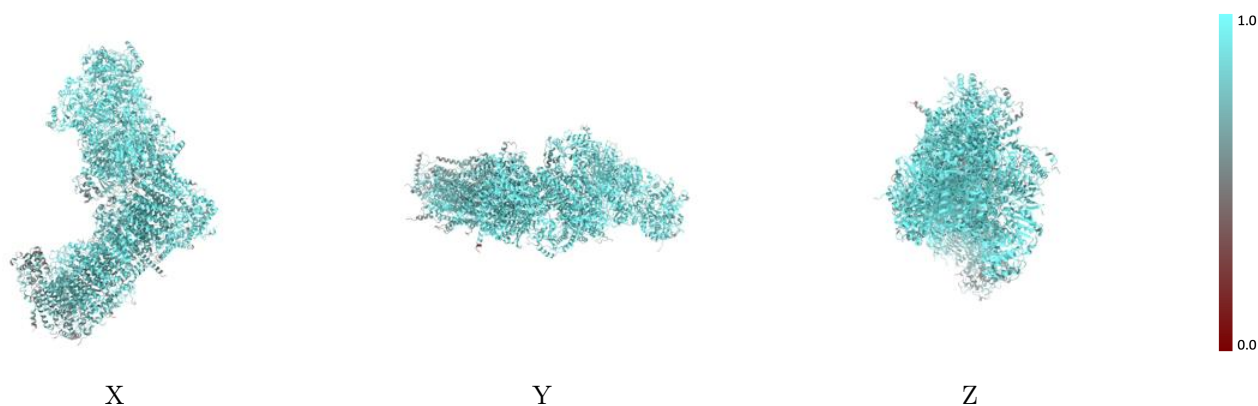
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



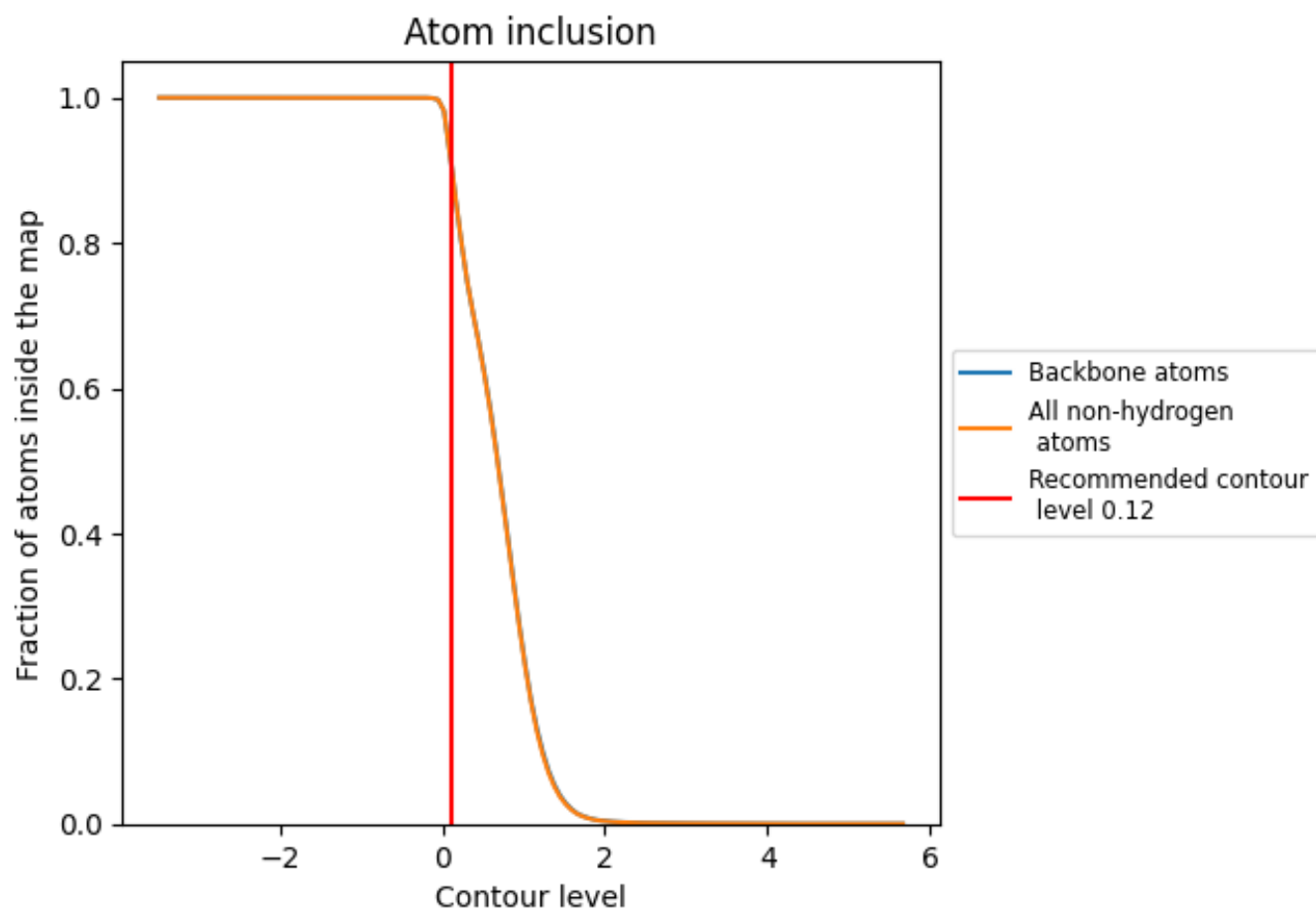
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary



















The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9017	 0.6670
1	 0.9502	 0.7140
2	 0.9653	 0.7240
3	 0.8970	 0.6640
4	 0.9532	 0.6980
5	 0.8446	 0.6060
6	 0.9264	 0.6900
8	 0.6789	 0.5170
9	 0.8466	 0.6410
A	 0.9610	 0.7110
B	 0.9353	 0.6570
C	 0.9669	 0.7340
D	 0.9714	 0.7020
E	 0.9106	 0.6510
F	 0.9127	 0.6660
G	 0.9698	 0.7350
H	 0.9055	 0.6400
I	 0.9702	 0.7340
J	 0.8118	 0.5910
K	 0.9368	 0.7070
L	 0.9729	 0.7200
M	 0.9560	 0.7060
O	 0.6742	 0.4750
P	 0.9059	 0.6630
Q	 0.5661	 0.4730
R	 0.7136	 0.5290
S	 0.8147	 0.5980
U	 0.9427	 0.6880
W	 0.9244	 0.6870
X	 0.9205	 0.6840
Y	 0.9563	 0.7180
Z	 0.9246	 0.6810
a	 0.7967	 0.5770
b	 0.8862	 0.6620
c	 0.6502	 0.5040



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Chain	Atom inclusion	Q-score
d	 0.8575	 0.6290
e	 0.6656	 0.5240
f	 0.8835	 0.6270
g	 0.9283	 0.6630
h	 0.9480	 0.7030
i	 0.7407	 0.5790
j	 0.9122	 0.6570
n	 0.7910	 0.6120
o	 0.8049	 0.5670