



wwPDB EM Validation Summary Report ⓘ

Apr 29, 2026 – 04:58 am BST

PDB ID : 9R01 / pdb_00009r01
EMDB ID : EMD-53476
Title : Complex I from Ovis aries in presence of D1 inhibitor, Closed state
Authors : Sazanov, L.; Petrova, O.
Deposited on : 2025-04-24
Resolution : 3.25 Å (reported)
Based on initial model : 6ZKK

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

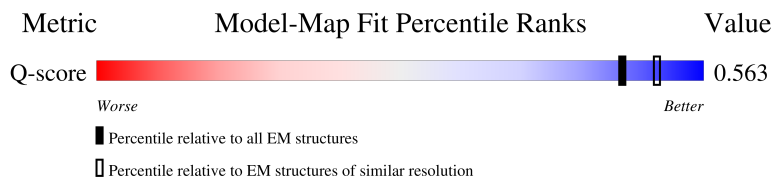
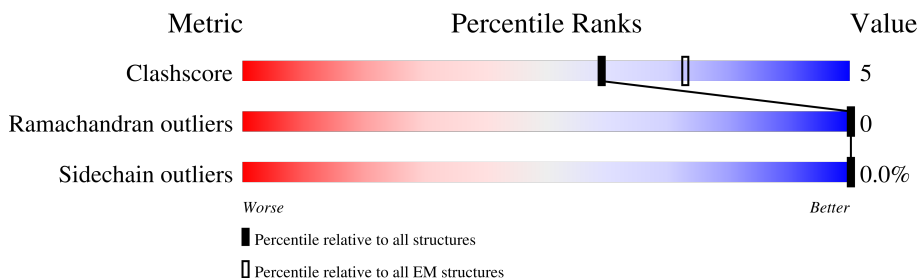
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


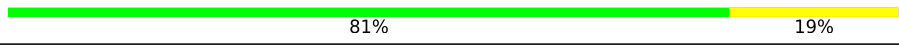
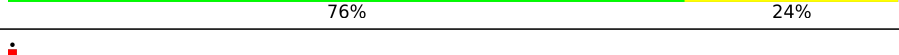

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





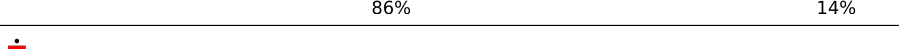
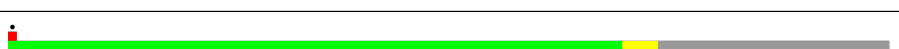



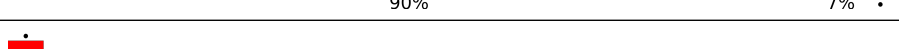



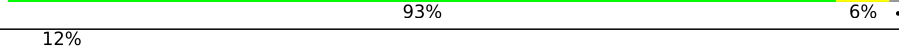

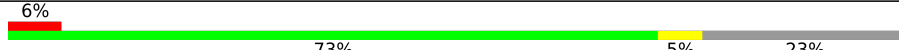


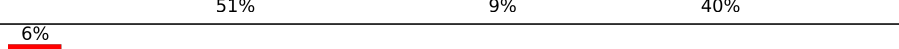







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14599 (2.75 - 3.75)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	115	
2	H	318	
3	J	175	
4	K	98	

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Mol	Chain	Length	Quality of chain
5	L	606	
6	M	459	
7	N	347	
8	V	141	
9	W	189	
10	X	87	
10	j	87	
11	Y	171	
12	Z	175	
13	k	355	
14	l	106	
15	m	84	
16	n	98	
17	o	122	
18	p	130	
19	q	144	
20	r	128	
21	s	137	
22	t	179	
23	u	108	
24	v	186	
25	w	154	
26	x	76	
27	y	58	
28	z	70	

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Mol	Chain	Length	Quality of chain
29	1	464	
30	2	246	
31	3	727	
32	4	463	
33	5	266	
34	6	223	
35	9	217	
36	a	109	
37	b	124	
38	c	170	
39	d	380	
40	e	99	
41	f	116	
42	g	140	
43	h	113	
44	i	145	

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 67257 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	115	Total	C	N	O	S	0	0
			922	621	133	161	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	318	Total	C	N	O	S	0	0
			2528	1704	384	421	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	175	Total	C	N	O	S	0	0
			1344	904	192	235	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	98	Total	C	N	O	S	0	0
			749	490	112	132	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	606	Total	C	N	O	S	0	0
			4807	3188	746	829	44		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	459	Total	C	N	O	S	0	0
			3647	2429	571	607	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	347	Total	C	N	O	S	0	0
			2723	1808	416	459	40		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	141	Total	C	N	O	S	0	0
			1028	656	175	191	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	1	ACE	-	acetylation	UNP A0A8V6VBD6

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	139	Total	C	N	O	S	0	0
			1155	761	194	198	2		

- Molecule 10 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	87	Total	C	N	O	S	0	0
			701	451	103	142	5		
10	j	82	Total	C	N	O	S	0	0
			660	425	98	132	5		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	171	Total	C	N	O	S	0	0
			1403	889	253	251	10		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	171	Total	C	N	O	S	0	0
			1441	905	266	262	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
13	k	320	Total	C	N	O	P	S	0	0
			2596	1659	432	494	1	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	l	105	Total	C	N	O	S	0	0
			874	551	164	153	6		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	m	80	Total	C	N	O	S	0	0
			626	411	103	110	2		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	n	79	Total	C	N	O	S	0	0
			634	415	106	111	2		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	o	120	Total	C	N	O	S	0	0
			1004	652	175	172	5		

- Molecule 18 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	p	128	Total	C	N	O	S	0	0
			1059	675	189	194	1		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-

unit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	q	139	Total	C	N	O	S	0	0
			1142	733	200	200	9		

- Molecule 20 is a protein called Mitochondrial complex I, B17 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	r	99	Total	C	N	O	S	0	0
			846	554	149	142	1		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	s	122	Total	C	N	O	S	0	0
			1047	653	199	186	9		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	t	177	Total	C	N	O	S	0	0
			1520	973	279	262	6		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	u	65	Total	C	N	O	S	0	0
			563	372	93	97	1		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	v	155	Total	C	N	O	S	0	0
			1307	846	213	239	9		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	w	101	Total	C	N	O	S	0	0
			846	542	140	160	4		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	x	49	Total	C	N	O		0	0
			412	271	70	71			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	y	50	Total	C	N	O		0	0
			436	287	77	72			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	z	70	Total	C	N	O	S	0	0
			576	369	106	96	5		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	1	430	Total	C	N	O	S	0	0
			3312	2086	593	613	20		

- Molecule 30 is a protein called Mitochondrial complex I, 24 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	2	213	Total	C	N	O	S	0	0
			1655	1058	278	309	10		

- Molecule 31 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	3	688	Total	C	N	O	S	0	0
			5275	3301	922	1011	41		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	4	430	Total	C	N	O	S	0	0
			3457	2207	594	631	25		

- Molecule 33 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	5	208	Total	C	N	O	S	0	0
			1726	1112	296	315	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	6	156	Total	C	N	O	S	0	0
			1247	795	225	213	14		

- Molecule 35 is a protein called Complex I-23kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	a	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	b	95	Total	C	N	O	S	0	0
			737	451	139	144	3		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	c	126	Total	C	N	O	S	0	0
			1024	646	182	193	3		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	d	340	Total	C	N	O	S	0	0
			2748	1775	489	478	6		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	e	86	Total	C	N	O	S	0	0
			691	434	129	126	2		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	f	113	Total	C	N	O	S	0	0
			917	595	153	167	2		

- Molecule 42 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	g	114	Total	C	N	O	S	0	0
			969	619	180	166	4		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	h	97	Total	C	N	O	S	0	0
			769	480	146	140	3		

There is a discrepancy between the modelled and reference sequences:

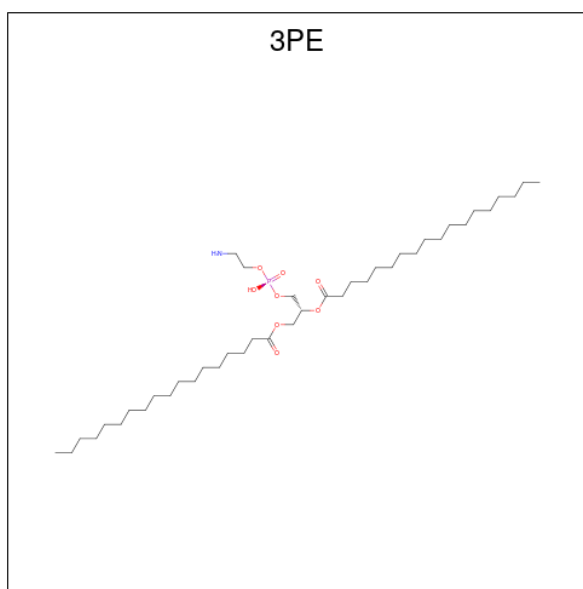
Chain	Residue	Modelled	Actual	Comment	Reference
h	1	ACE	-	acetylation	UNP A0A6P3E9B7

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-

unit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	i	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



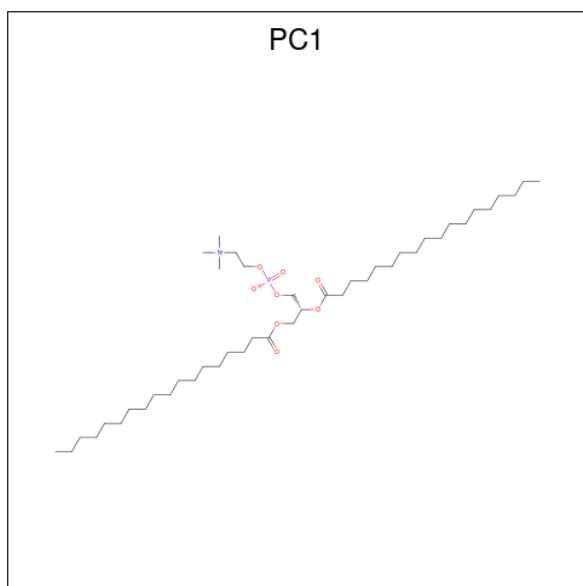
Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	J	1	Total	C	N	O	P	0
			40	30	1	8	1	
45	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	L	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	M	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	V	1	Total	C	O	P		0
			27	18	8	1		
45	V	1	Total	C	N	O	P	0
			37	27	1	8	1	

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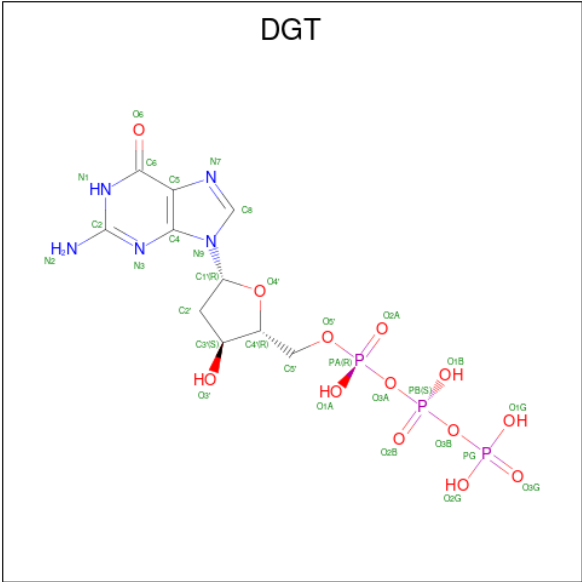
Mol	Chain	Residues	Atoms					AltConf
45	o	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	4	1	Total	C	N	O	P	0
			40	30	1	8	1	
45	6	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	i	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
46	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	6	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	9	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 47 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

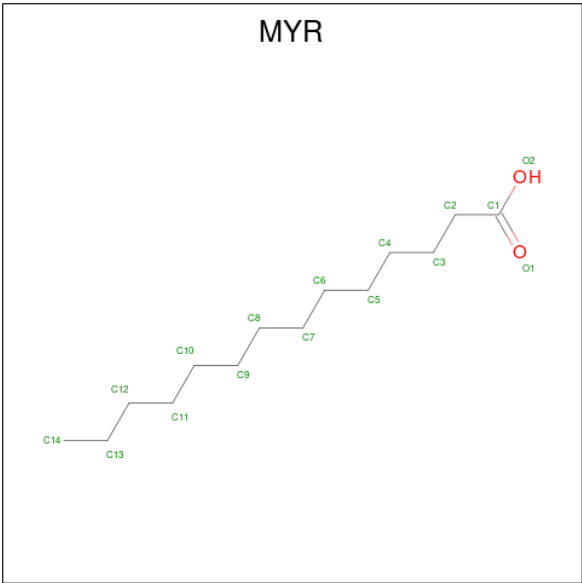


Mol	Chain	Residues	Atoms					AltConf
47	k	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 48 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

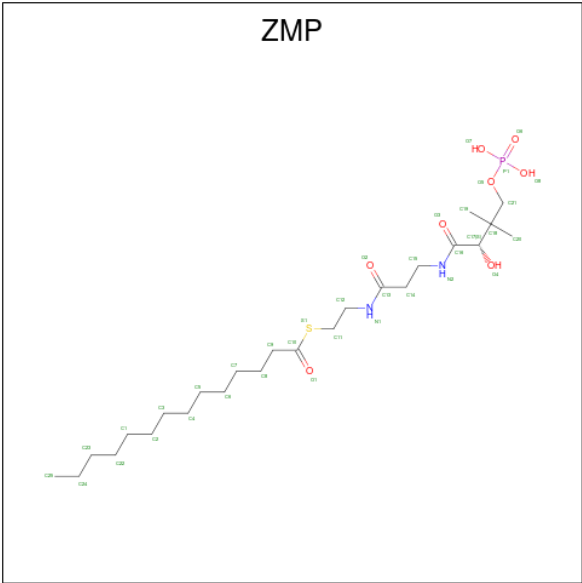
Mol	Chain	Residues	Atoms		AltConf
48	k	1	Total	Mg	0
			1	1	

- Molecule 49 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).



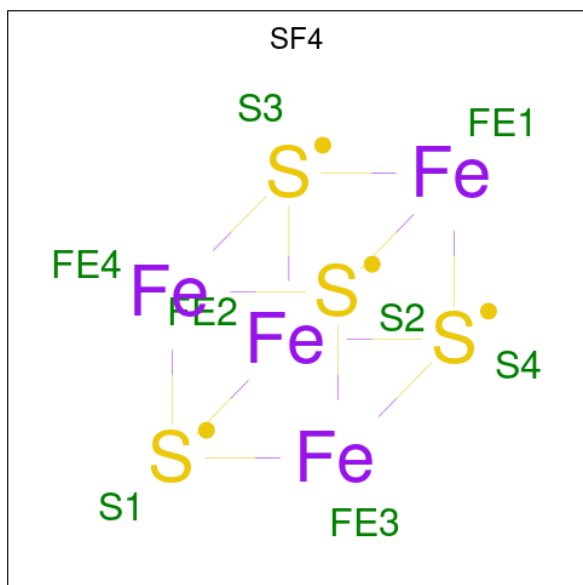
Mol	Chain	Residues	Atoms			AltConf
49	s	1	Total	C	O	0
			15	14	1	

- Molecule 50 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



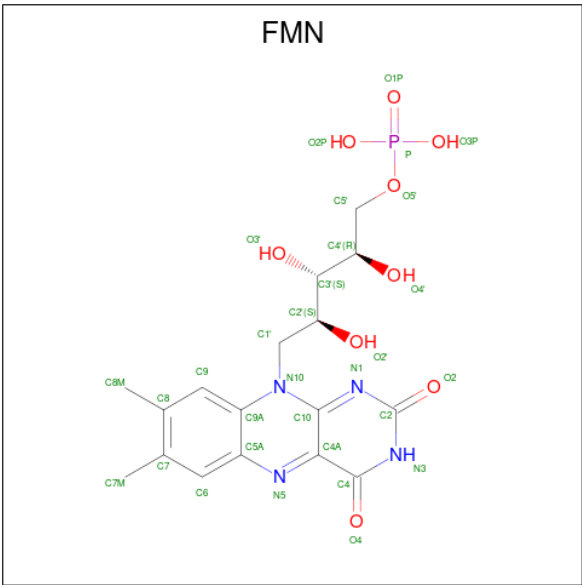
Mol	Chain	Residues	Atoms						AltConf
50	t	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	
50	j	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	

- Molecule 51 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



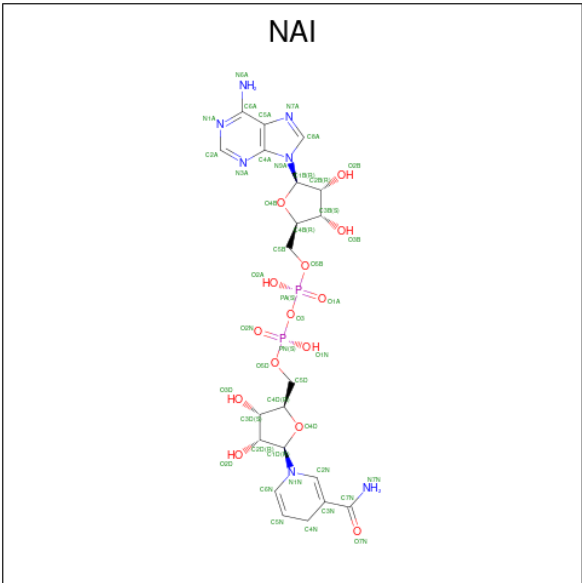
Mol	Chain	Residues	Atoms			AltConf
51	1	1	Total	Fe	S	0
			8	4	4	
51	3	1	Total	Fe	S	0
			8	4	4	
51	3	1	Total	Fe	S	0
			8	4	4	
51	6	1	Total	Fe	S	0
			8	4	4	
51	9	1	Total	Fe	S	0
			8	4	4	
51	9	1	Total	Fe	S	0
			8	4	4	

- Molecule 52 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
52	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 53 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf
53	1	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
54	2	1	Total	Fe	S	0
			4	2	2	
54	3	1	Total	Fe	S	0
			4	2	2	

- Molecule 55 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
55	3	1	Total	K	0
			1	1	

- Molecule 56 is (7 {S})-7-[(2 {S})-1-(6-azanylpurin-3-yl)propan-2-yl]-3-methyl-6,7,8,9-tetrahydro-5 {a} {H}-pyrano[4,3-b]chromen-1-one (CCD ID: A1JBT) (formula: C₂₁H₂₃N₅O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltCon
56	4	1	Total	C	N	O	0
			29	21	5	3	

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltCon
57	b	1	Total Zn 1 1	0

- Molecule 58 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).

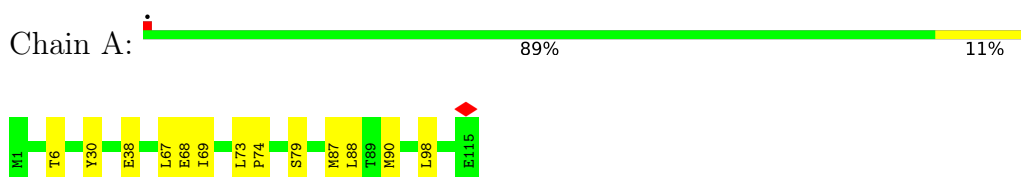


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	d	1	48	21	7	17	3	0

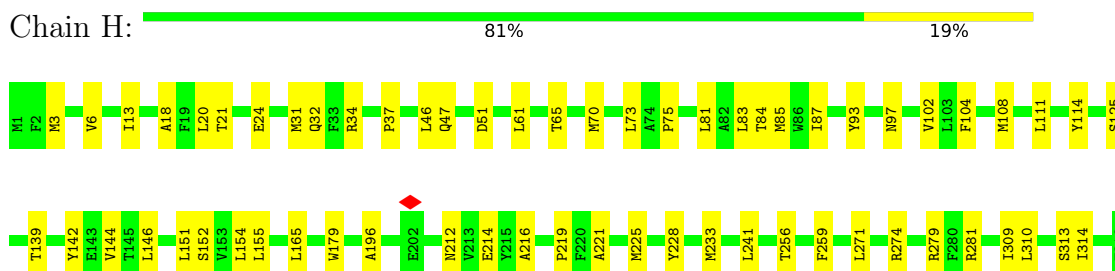
3 Residue-property plots

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

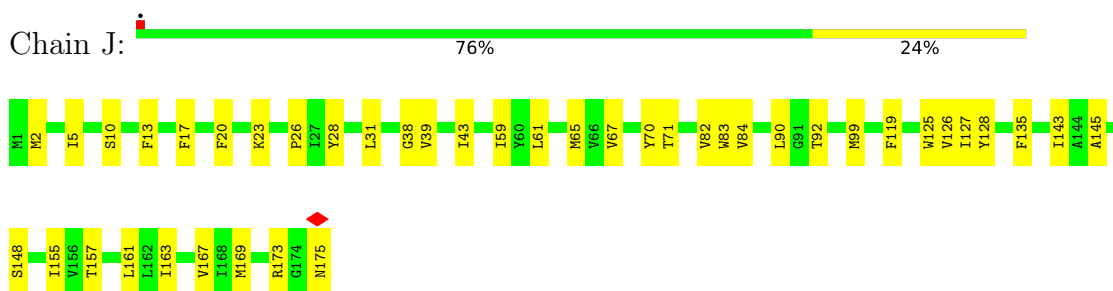
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



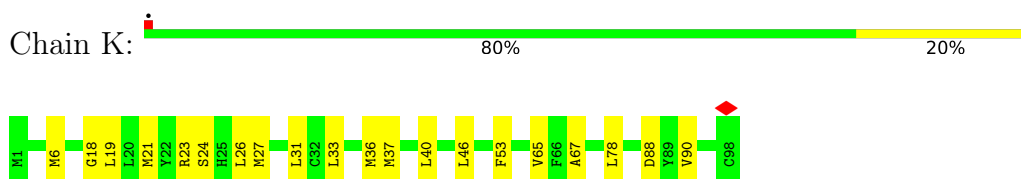
- Molecule 2: NADH-ubiquinone oxidoreductase chain 1



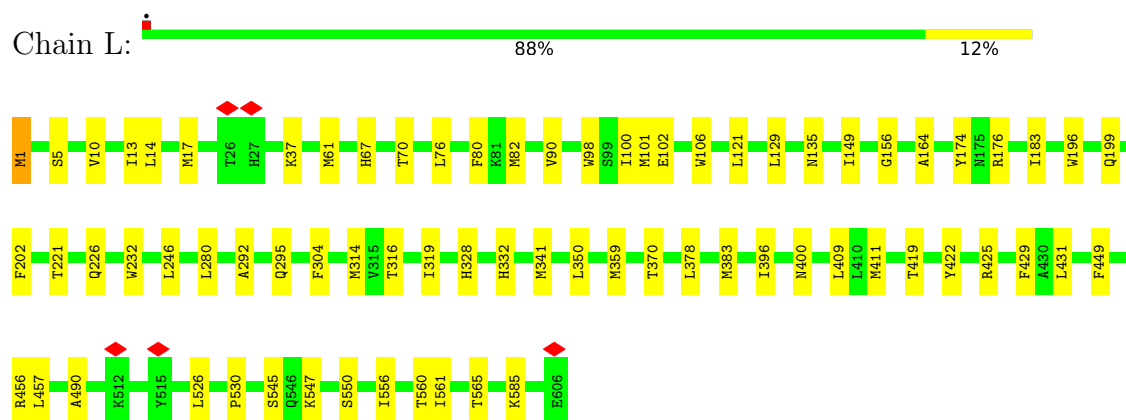
- Molecule 3: NADH-ubiquinone oxidoreductase chain 6



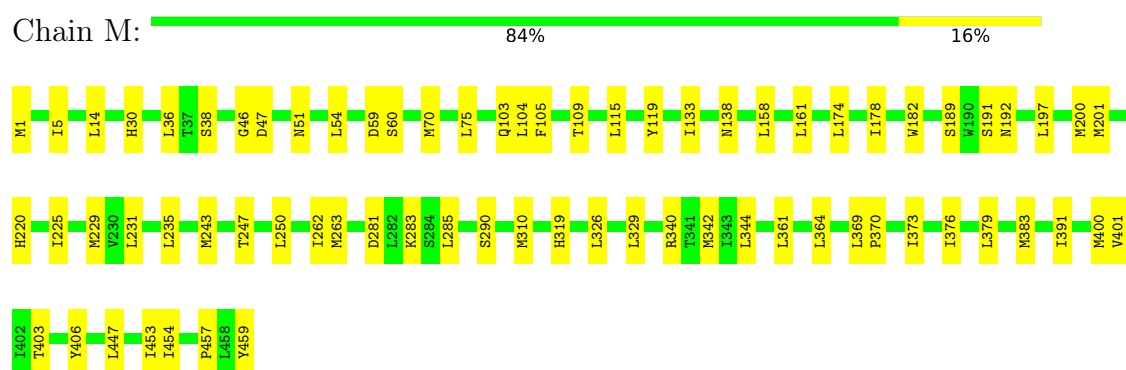
- Molecule 4: NADH-ubiquinone oxidoreductase chain 4L



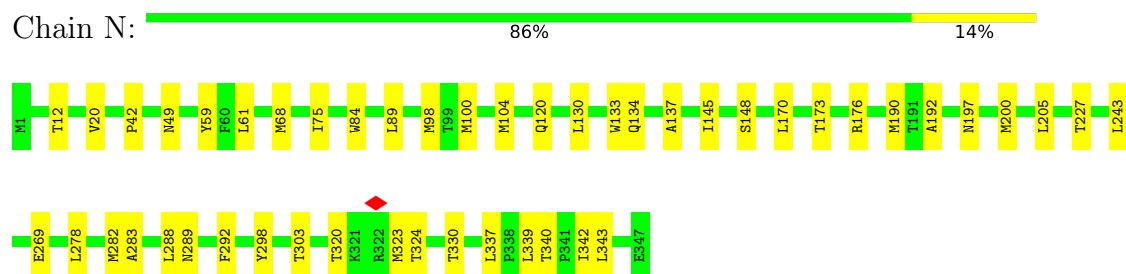
- Molecule 5: NADH-ubiquinone oxidoreductase chain 5



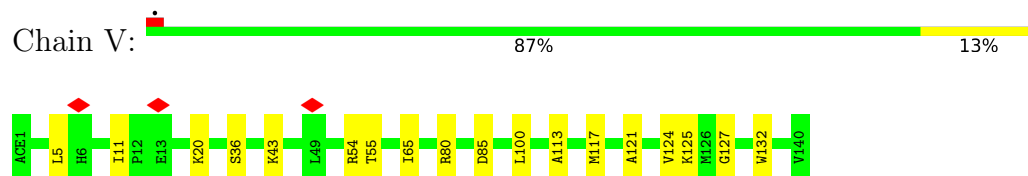
- Molecule 6: NADH-ubiquinone oxidoreductase chain 4



- Molecule 7: NADH-ubiquinone oxidoreductase chain 2

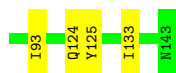
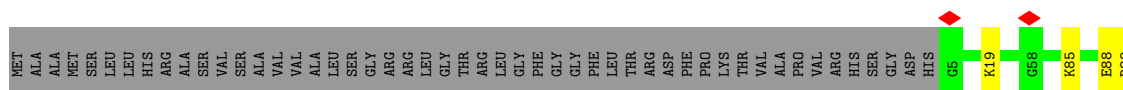


- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

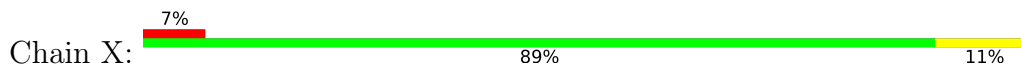


- Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

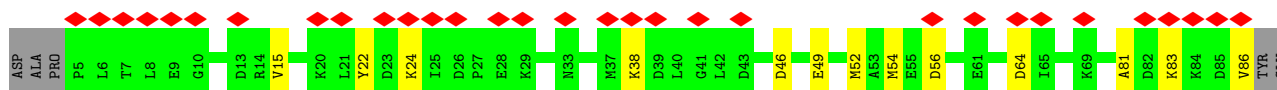
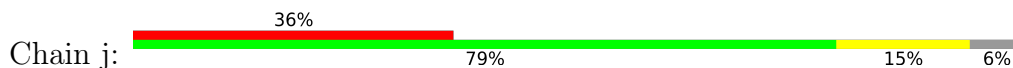




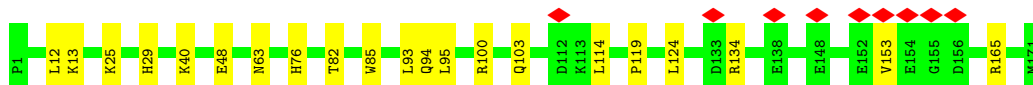
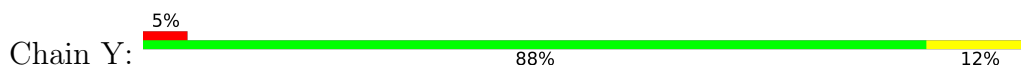
- Molecule 10: Acyl carrier protein



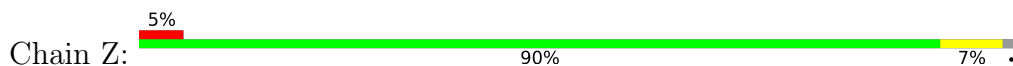
- Molecule 10: Acyl carrier protein



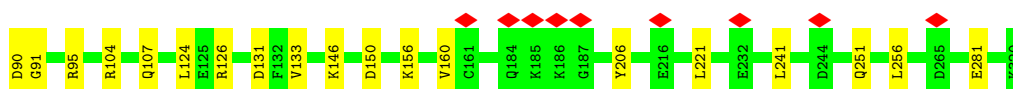
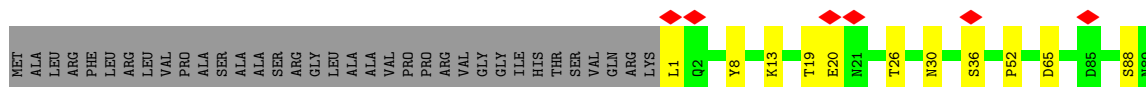
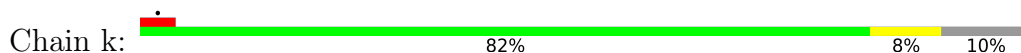
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



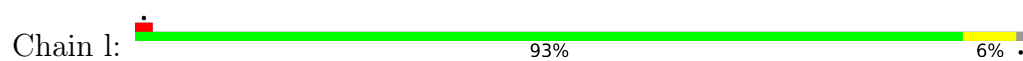
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



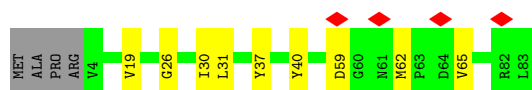
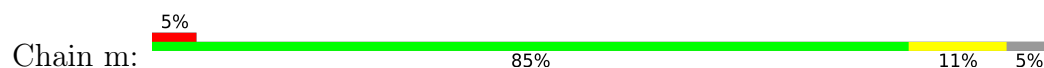
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



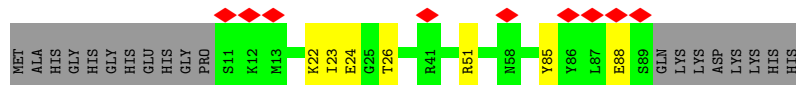
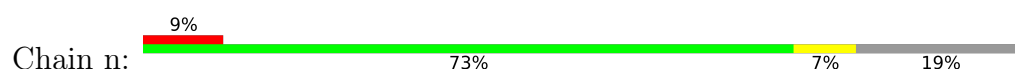
- Molecule 14: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



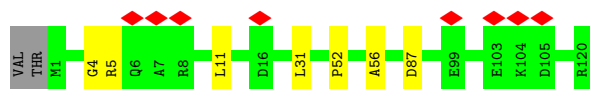
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



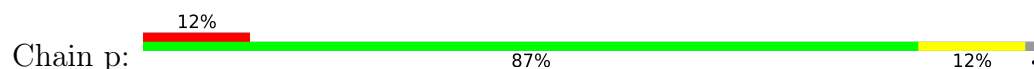
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



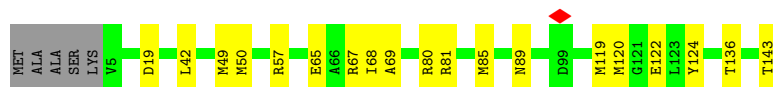
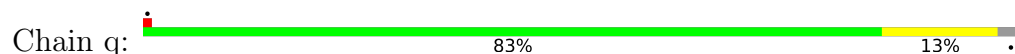
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 subunit C2



- Molecule 18: NADH:ubiquinone oxidoreductase subunit B4

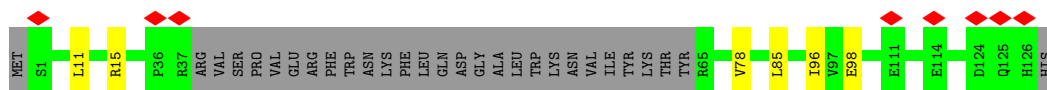


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

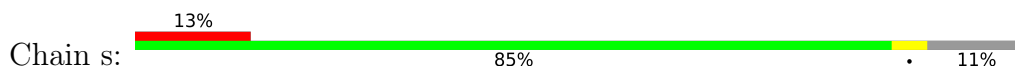


- Molecule 20: Mitochondrial complex I, B17 subunit

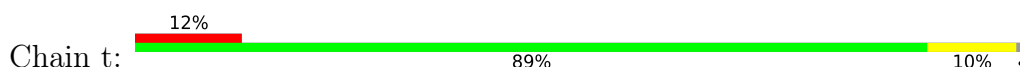




- Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



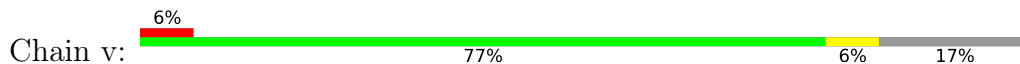
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

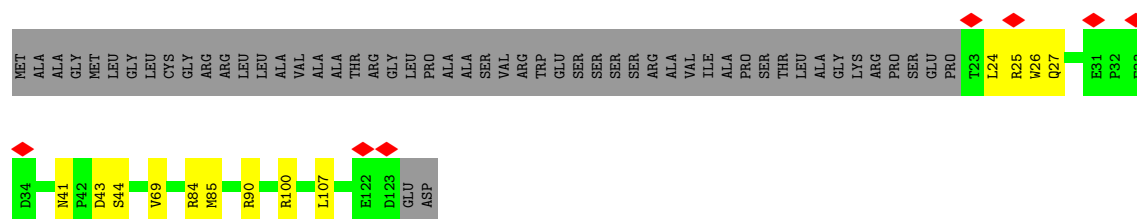


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

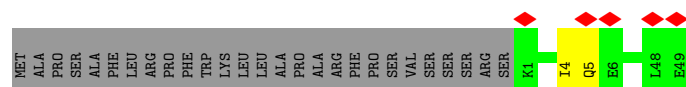


- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

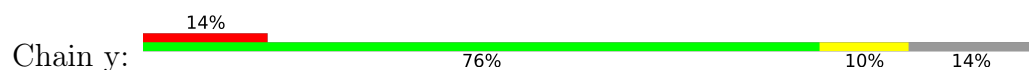




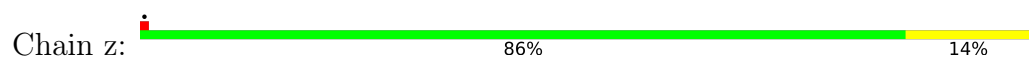
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



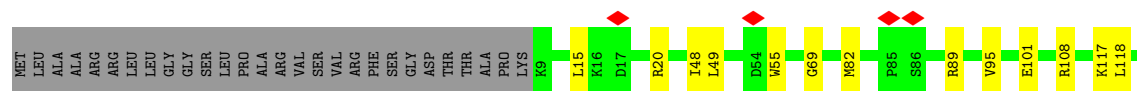
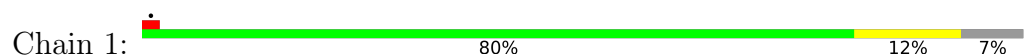
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



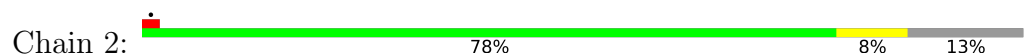
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

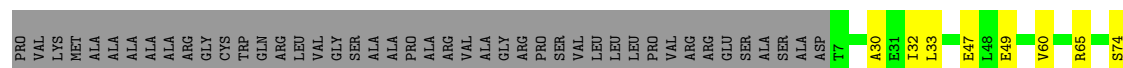


- Molecule 29: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



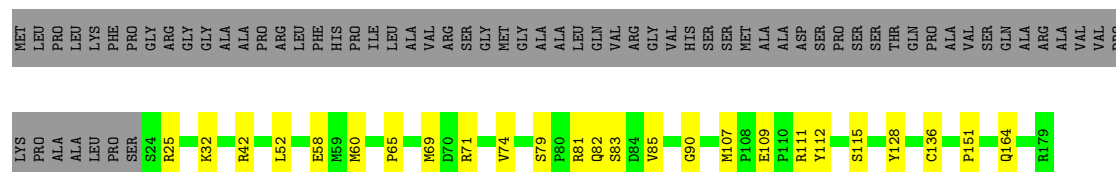
- Molecule 30: Mitochondrial complex I, 24 kDa subunit



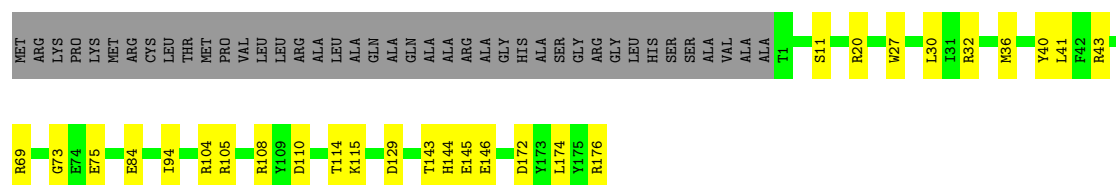




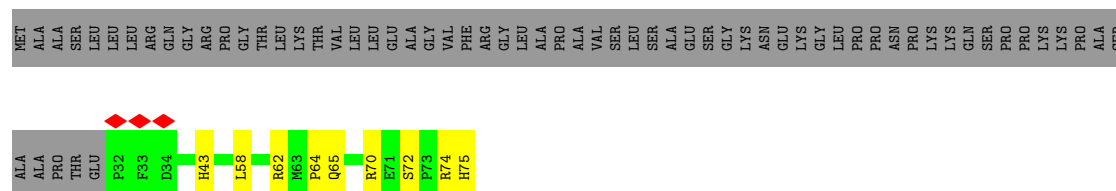
- Molecule 34: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



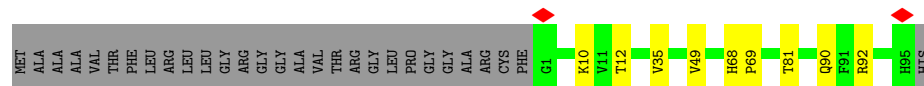
- Molecule 35: Complex I-23kD



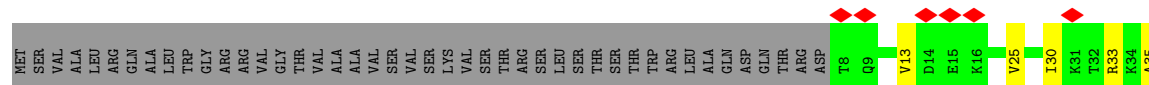
- Molecule 36: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



- Molecule 37: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

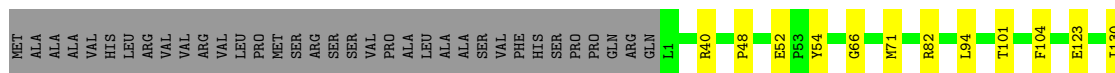
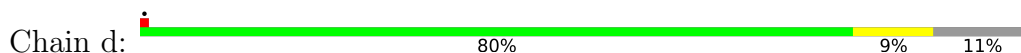


- Molecule 38: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

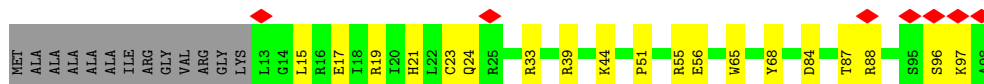




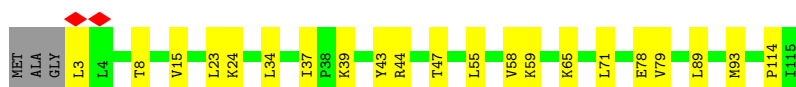
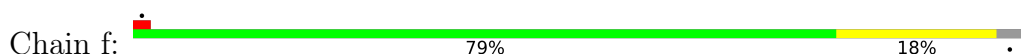
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



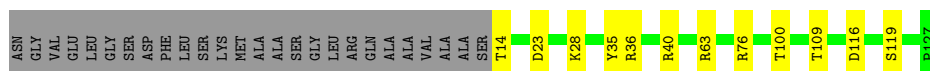
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



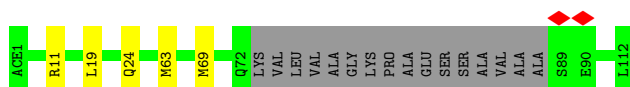
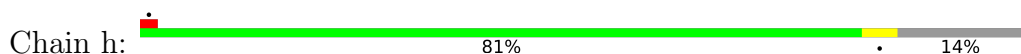
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



- Molecule 42: NADH:ubiquinone oxidoreductase subunit A6



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50108	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	90	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.706	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.1	Depositor
Map size (\AA)	173.24, 191.54001, 289.14	wwPDB
Map dimensions	237, 157, 142	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.22, 1.22, 1.22	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAI, ZMP, ACE, FME, FES, NDP, SF4, K, A1JBT, ZN, 3PE, 2MR, MYR, DGT, FMN, MG, PC1, SEP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/947	0.50	0/1296
2	H	0.25	0/2603	0.51	0/3561
3	J	0.23	0/1378	0.51	0/1868
4	K	0.23	0/749	0.50	0/1014
5	L	0.20	0/4925	0.43	0/6700
6	M	0.23	0/3731	0.46	0/5085
7	N	0.23	0/2787	0.45	0/3795
8	V	0.16	0/1047	0.33	0/1421
9	W	0.17	0/1188	0.34	0/1607
10	X	0.16	0/713	0.38	0/963
10	j	0.17	0/670	0.44	0/902
11	Y	0.18	0/1440	0.38	0/1942
12	Z	0.18	0/1475	0.34	0/1989
13	k	0.16	0/2646	0.31	0/3579
14	l	0.18	0/896	0.38	0/1200
15	m	0.20	0/647	0.45	0/890
16	n	0.16	0/653	0.38	0/882
17	o	0.18	0/1035	0.33	0/1398
18	p	0.16	0/1085	0.32	0/1467
19	q	0.21	0/1171	0.38	0/1579
20	r	0.16	0/874	0.37	0/1188
21	s	0.15	0/1072	0.36	0/1436
22	t	0.15	0/1573	0.33	0/2130
23	u	0.17	0/590	0.36	0/810
24	v	0.16	0/1361	0.37	0/1861
25	w	0.24	0/872	0.47	0/1185
26	x	0.14	0/425	0.32	0/576
27	y	0.17	0/449	0.39	0/605
28	z	0.20	0/591	0.39	0/795
29	1	0.21	0/3386	0.41	0/4575
30	2	0.19	0/1695	0.43	0/2306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	3	0.19	0/5362	0.36	0/7266
32	4	0.22	0/3535	0.39	0/4791
33	5	0.20	0/1776	0.40	0/2417
34	6	0.23	0/1278	0.43	0/1728
35	9	0.22	0/1445	0.41	0/1956
36	a	0.14	0/383	0.30	0/518
37	b	0.15	0/749	0.30	0/1009
38	c	0.17	0/1047	0.33	0/1415
39	d	0.18	0/2824	0.35	0/3830
40	e	0.16	0/702	0.39	0/945
41	f	0.18	0/937	0.33	0/1271
42	g	0.19	0/993	0.34	0/1336
43	h	0.17	0/785	0.32	0/1062
44	i	0.17	0/1250	0.32	0/1698
All	All	0.20	0/67740	0.40	0/91847

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
25	w	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	w	25	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	922	0	953	13	0
2	H	2528	0	2641	50	0
3	J	1344	0	1364	36	0
4	K	749	0	793	18	0
5	L	4807	0	4949	48	0
6	M	3647	0	3849	53	0
7	N	2723	0	2930	33	0
8	V	1028	0	1036	12	0
9	W	1155	0	1177	8	0
10	X	701	0	693	7	0
10	j	660	0	663	10	0
11	Y	1403	0	1392	14	0
12	Z	1441	0	1419	10	0
13	k	2596	0	2559	18	0
14	l	874	0	869	6	0
15	m	626	0	635	6	0
16	n	634	0	616	4	0
17	o	1004	0	995	6	0
18	p	1059	0	1062	14	0
19	q	1142	0	1137	16	0
20	r	846	0	864	4	0
21	s	1047	0	1013	5	0
22	t	1520	0	1477	13	0
23	u	563	0	509	6	0
24	v	1307	0	1207	11	0
25	w	846	0	792	9	0
26	x	412	0	411	1	0
27	y	436	0	437	5	0
28	z	576	0	570	7	0
29	1	3312	0	3267	39	0
30	2	1655	0	1668	14	0
31	3	5275	0	5300	65	0
32	4	3457	0	3397	47	0
33	5	1726	0	1676	20	0
34	6	1247	0	1256	21	0
35	9	1414	0	1371	22	0
36	a	371	0	344	8	0
37	b	737	0	710	5	0
38	c	1024	0	1023	13	0
39	d	2748	0	2763	22	0
40	e	691	0	706	11	0
41	f	917	0	958	15	0
42	g	969	0	980	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	h	769	0	780	6	0
44	i	1209	0	1182	7	0
45	4	40	0	54	0	0
45	6	51	0	82	3	0
45	A	51	0	82	1	0
45	H	51	0	82	3	0
45	J	40	0	54	5	0
45	L	82	0	118	0	0
45	M	44	0	65	0	0
45	N	51	0	82	2	0
45	V	64	0	75	4	0
45	i	51	0	82	1	0
45	o	31	0	36	1	0
46	6	46	0	69	0	0
46	9	54	0	88	0	0
46	L	54	0	88	1	0
46	M	108	0	176	6	0
47	k	31	0	12	1	0
48	k	1	0	0	0	0
49	s	15	0	27	0	0
50	j	34	0	40	1	0
50	t	31	0	34	1	0
51	1	8	0	0	0	0
51	3	16	0	0	0	0
51	6	8	0	0	0	0
51	9	16	0	0	0	0
52	1	31	0	19	0	0
53	1	44	0	27	2	0
54	2	4	0	0	1	0
54	3	4	0	0	0	0
55	3	1	0	0	0	0
56	4	29	0	0	0	0
57	b	1	0	0	0	0
58	d	48	0	26	0	0
All	All	67257	0	67811	626	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 626 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:a:72:SER:HG	36:a:75:HIS:HD1	1.24	0.82
5:L:67:HIS:HE2	5:L:70:THR:HG1	1.37	0.71
29:1:302:SER:HB2	29:1:350:LEU:HD11	1.73	0.70
45:H:401:3PE:H2F2	45:H:401:3PE:H371	1.75	0.69
32:4:152:MET:HE1	34:6:60:MET:HE1	1.75	0.68

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	105 (93%)	8 (7%)	0	100	100
2	H	316/318 (99%)	307 (97%)	9 (3%)	0	100	100
3	J	173/175 (99%)	165 (95%)	8 (5%)	0	100	100
4	K	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
5	L	604/606 (100%)	575 (95%)	29 (5%)	0	100	100
6	M	457/459 (100%)	451 (99%)	6 (1%)	0	100	100
7	N	345/347 (99%)	335 (97%)	10 (3%)	0	100	100
8	V	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
9	W	137/189 (72%)	136 (99%)	1 (1%)	0	100	100
10	X	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
10	j	80/87 (92%)	77 (96%)	3 (4%)	0	100	100
11	Y	169/171 (99%)	167 (99%)	2 (1%)	0	100	100
12	Z	169/175 (97%)	168 (99%)	1 (1%)	0	100	100
13	k	317/355 (89%)	303 (96%)	14 (4%)	0	100	100
14	l	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
15	m	78/84 (93%)	73 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	n	77/98 (79%)	74 (96%)	3 (4%)	0	100	100
17	o	118/122 (97%)	116 (98%)	2 (2%)	0	100	100
18	p	126/130 (97%)	125 (99%)	1 (1%)	0	100	100
19	q	137/144 (95%)	135 (98%)	2 (2%)	0	100	100
20	r	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
21	s	120/137 (88%)	118 (98%)	2 (2%)	0	100	100
22	t	175/179 (98%)	172 (98%)	3 (2%)	0	100	100
23	u	63/108 (58%)	62 (98%)	1 (2%)	0	100	100
24	v	153/186 (82%)	149 (97%)	4 (3%)	0	100	100
25	w	99/154 (64%)	96 (97%)	3 (3%)	0	100	100
26	x	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
27	y	48/58 (83%)	46 (96%)	2 (4%)	0	100	100
28	z	68/70 (97%)	68 (100%)	0	0	100	100
29	1	428/464 (92%)	412 (96%)	16 (4%)	0	100	100
30	2	211/246 (86%)	196 (93%)	15 (7%)	0	100	100
31	3	686/727 (94%)	668 (97%)	18 (3%)	0	100	100
32	4	427/463 (92%)	407 (95%)	20 (5%)	0	100	100
33	5	206/266 (77%)	199 (97%)	7 (3%)	0	100	100
34	6	154/223 (69%)	151 (98%)	3 (2%)	0	100	100
35	9	174/217 (80%)	168 (97%)	6 (3%)	0	100	100
36	a	42/109 (38%)	41 (98%)	1 (2%)	0	100	100
37	b	93/124 (75%)	92 (99%)	1 (1%)	0	100	100
38	c	124/170 (73%)	121 (98%)	3 (2%)	0	100	100
39	d	338/380 (89%)	328 (97%)	10 (3%)	0	100	100
40	e	84/99 (85%)	81 (96%)	3 (4%)	0	100	100
41	f	111/116 (96%)	108 (97%)	3 (3%)	0	100	100
42	g	112/140 (80%)	108 (96%)	4 (4%)	0	100	100
43	h	93/113 (82%)	89 (96%)	4 (4%)	0	100	100
44	i	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
All	All	8133/9105 (89%)	7883 (97%)	250 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	103/103 (100%)	103 (100%)	0	100	100
2	H	278/278 (100%)	278 (100%)	0	100	100
3	J	144/144 (100%)	144 (100%)	0	100	100
4	K	86/86 (100%)	86 (100%)	0	100	100
5	L	538/538 (100%)	538 (100%)	0	100	100
6	M	411/411 (100%)	411 (100%)	0	100	100
7	N	315/315 (100%)	315 (100%)	0	100	100
8	V	101/101 (100%)	101 (100%)	0	100	100
9	W	122/160 (76%)	122 (100%)	0	100	100
10	X	80/80 (100%)	80 (100%)	0	100	100
10	j	76/80 (95%)	76 (100%)	0	100	100
11	Y	154/154 (100%)	154 (100%)	0	100	100
12	Z	155/157 (99%)	155 (100%)	0	100	100
13	k	283/309 (92%)	283 (100%)	0	100	100
14	l	94/95 (99%)	94 (100%)	0	100	100
15	m	69/72 (96%)	69 (100%)	0	100	100
16	n	61/76 (80%)	61 (100%)	0	100	100
17	o	107/109 (98%)	107 (100%)	0	100	100
18	p	114/116 (98%)	114 (100%)	0	100	100
19	q	119/122 (98%)	119 (100%)	0	100	100
20	r	95/122 (78%)	95 (100%)	0	100	100
21	s	110/120 (92%)	110 (100%)	0	100	100
22	t	159/161 (99%)	159 (100%)	0	100	100
23	u	59/84 (70%)	59 (100%)	0	100	100
24	v	140/160 (88%)	140 (100%)	0	100	100
25	w	92/130 (71%)	91 (99%)	1 (1%)	65	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	x	44/67 (66%)	44 (100%)	0	100	100
27	y	46/54 (85%)	46 (100%)	0	100	100
28	z	59/59 (100%)	59 (100%)	0	100	100
29	1	344/368 (94%)	344 (100%)	0	100	100
30	2	183/210 (87%)	183 (100%)	0	100	100
31	3	578/608 (95%)	578 (100%)	0	100	100
32	4	370/391 (95%)	370 (100%)	0	100	100
33	5	189/230 (82%)	189 (100%)	0	100	100
34	6	132/181 (73%)	132 (100%)	0	100	100
35	9	151/179 (84%)	151 (100%)	0	100	100
36	a	43/93 (46%)	43 (100%)	0	100	100
37	b	79/97 (81%)	79 (100%)	0	100	100
38	c	113/150 (75%)	113 (100%)	0	100	100
39	d	294/326 (90%)	294 (100%)	0	100	100
40	e	76/82 (93%)	76 (100%)	0	100	100
41	f	101/102 (99%)	101 (100%)	0	100	100
42	g	107/124 (86%)	107 (100%)	0	100	100
43	h	84/94 (89%)	84 (100%)	0	100	100
44	i	131/131 (100%)	131 (100%)	0	100	100
All	All	7189/7829 (92%)	7188 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	w	27	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
24	v	55	GLN
44	i	72	ASN
30	2	67	ASN
43	h	20	GLN
39	d	44	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	2MR	4	85	32	10,12,13	0.20	0	5,13,15	0.14	0
5	FME	L	1	5	8,9,10	0.92	0	7,9,11	1.01	1 (14%)
13	SEP	k	36	13	8,9,10	0.26	0	8,12,14	1.03	1 (12%)
6	FME	M	1	6	8,9,10	0.92	0	7,9,11	0.81	0
4	FME	K	1	4	8,9,10	0.94	0	7,9,11	0.88	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	2MR	4	85	32	-	0/10/13/15	-
5	FME	L	1	5	-	2/7/9/11	-
13	SEP	k	36	13	-	1/5/8/10	-
6	FME	M	1	6	-	6/7/9/11	-
4	FME	K	1	4	-	2/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	k	36	SEP	P-OG-CB	2.67	125.66	118.30
5	L	1	FME	C-CA-N	2.04	113.41	109.73

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	1	FME	CA-CB-CG-SD
6	M	1	FME	C-CA-CB-CG
6	M	1	FME	O-C-CA-CB
13	k	36	SEP	N-CA-CB-OG
5	L	1	FME	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	1	FME	1	0
6	M	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 3 are monoatomic - leaving 34 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	$\# Z > 2$
58	NDP	d	401	-	49,52,52	0.35	0	66,80,80	0.34	0
46	PC1	6	202	-	45,45,53	0.31	0	51,53,61	0.30	0
45	3PE	N	401	-	50,50,50	0.33	0	53,55,55	0.47	0
46	PC1	M	502	-	53,53,53	0.29	0	59,61,61	0.31	0
51	SF4	1	501	29	0,12,12	-	-	-	-	-
53	NAI	1	503	-	45,48,48	0.32	0	60,73,73	0.38	0
54	FES	3	803	31	0,4,4	-	-	-	-	-
51	SF4	3	801	31	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	FMN	1	502	-	33,33,33	0.33	0	48,50,50	0.42	0
51	SF4	3	802	31	0,12,12	-	-	-		
51	SF4	9	403	35	0,12,12	-	-	-		
45	3PE	M	501	-	43,43,50	0.33	0	46,48,55	0.34	0
45	3PE	V	201	-	26,26,50	0.48	0	30,31,55	0.52	1 (3%)
45	3PE	A	201	-	50,50,50	0.31	0	53,55,55	0.32	0
46	PC1	L	1003	-	53,53,53	0.31	0	59,61,61	0.55	1 (1%)
56	A1JBT	4	502	-	31,33,33	0.29	0	31,49,49	0.60	0
45	3PE	4	501	-	39,39,50	0.33	0	42,44,55	0.30	0
45	3PE	L	1001	-	50,50,50	0.30	0	53,55,55	0.31	0
45	3PE	L	1002	-	30,30,50	0.40	0	33,35,55	0.72	1 (3%)
45	3PE	J	201	-	39,39,50	0.34	0	42,44,55	0.31	0
50	ZMP	j	101	-	27,33,36	0.65	0	32,40,45	1.12	2 (6%)
51	SF4	6	201	34	0,12,12	-	-	-		
45	3PE	H	401	-	50,50,50	0.31	0	53,55,55	0.34	0
45	3PE	6	203	-	50,50,50	0.30	0	53,55,55	0.30	0
49	MYR	s	201	21	14,14,15	0.21	0	13,13,15	0.17	0
45	3PE	o	501	-	30,30,50	0.38	0	33,35,55	0.34	0
54	FES	2	300	30	0,4,4	-	-	-		
45	3PE	V	202	-	36,36,50	0.35	0	39,41,55	0.33	0
46	PC1	9	401	-	53,53,53	0.30	0	59,61,61	0.46	0
46	PC1	M	503	-	53,53,53	0.30	0	59,61,61	0.30	0
47	DGT	k	401	48	29,33,33	0.31	0	44,52,52	0.32	0
45	3PE	i	201	-	50,50,50	0.30	0	53,55,55	0.31	0
51	SF4	9	402	35	0,12,12	-	-	-		
50	ZMP	t	201	-	24,30,36	0.81	1 (4%)	29,37,45	0.99	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	NDP	d	401	-	-	4/34/77/77	0/5/5/5
46	PC1	6	202	-	-	13/49/49/57	-
45	3PE	N	401	-	-	13/54/54/54	-
46	PC1	M	502	-	-	12/57/57/57	-
53	NAI	1	503	-	-	5/29/72/72	0/5/5/5
51	SF4	1	501	29	-	-	0/6/5/5
54	FES	3	803	31	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	SF4	3	801	31	-	-	0/6/5/5
52	FMN	1	502	-	-	8/18/18/18	0/3/3/3
51	SF4	3	802	31	-	-	0/6/5/5
51	SF4	9	403	35	-	-	0/6/5/5
45	3PE	M	501	-	-	10/47/47/54	-
45	3PE	V	201	-	-	5/27/27/54	-
45	3PE	A	201	-	-	14/54/54/54	-
46	PC1	L	1003	-	-	15/57/57/57	-
56	A1JBT	4	502	-	-	4/8/29/29	0/5/5/5
45	3PE	4	501	-	-	9/43/43/54	-
45	3PE	L	1001	-	-	13/54/54/54	-
45	3PE	L	1002	-	-	6/34/34/54	-
45	3PE	J	201	-	-	11/43/43/54	-
50	ZMP	j	101	-	-	4/38/40/43	-
51	SF4	6	201	34	-	-	0/6/5/5
45	3PE	H	401	-	-	15/54/54/54	-
45	3PE	6	203	-	-	8/54/54/54	-
49	MYR	s	201	21	-	1/11/12/13	-
45	3PE	o	501	-	-	6/34/34/54	-
54	FES	2	300	30	-	-	0/1/1/1
45	3PE	V	202	-	-	9/40/40/54	-
46	PC1	9	401	-	-	14/57/57/57	-
46	PC1	M	503	-	-	16/57/57/57	-
47	DGT	k	401	48	-	4/22/34/34	0/3/3/3
45	3PE	i	201	-	-	9/54/54/54	-
51	SF4	9	402	35	-	-	0/6/5/5
50	ZMP	t	201	-	-	6/35/37/43	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	t	201	ZMP	C9-C10	2.59	1.53	1.50

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	j	101	ZMP	O1-C10-C9	-2.90	120.57	123.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	t	201	ZMP	O1-C10-C9	-2.59	120.93	123.99
50	j	101	ZMP	C14-C15-N2	-2.25	107.35	111.90
46	L	1003	PC1	C2-O21-C21	2.21	123.23	117.79
45	V	201	3PE	O12-P-O14	2.13	119.03	110.68

There are no chirality outliers.

5 of 234 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C1-O11-P-O12
45	A	201	3PE	C11-O13-P-O12
45	A	201	3PE	C11-O13-P-O14
45	H	401	3PE	C1-O11-P-O12
45	H	401	3PE	C1-O11-P-O14

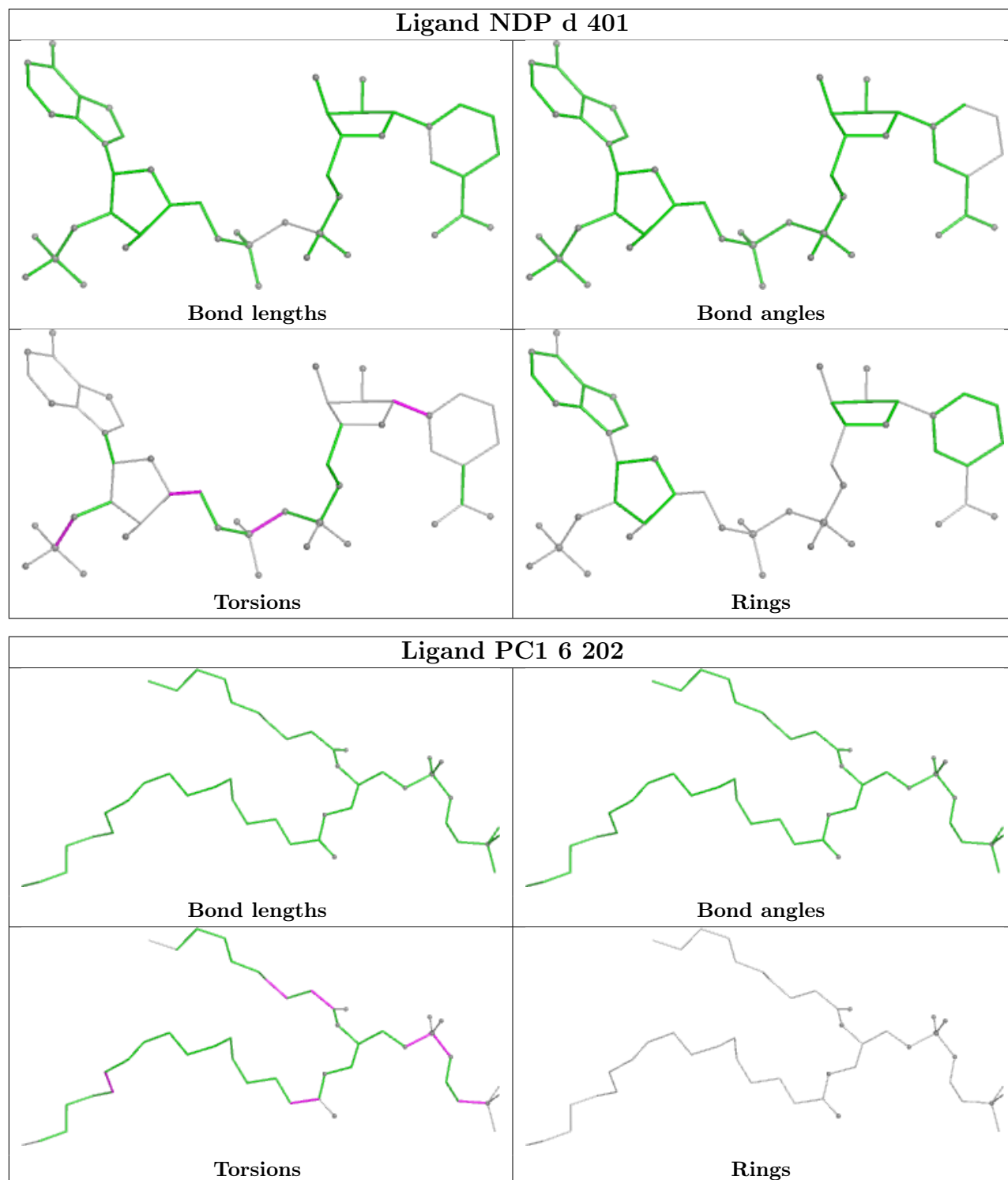
There are no ring outliers.

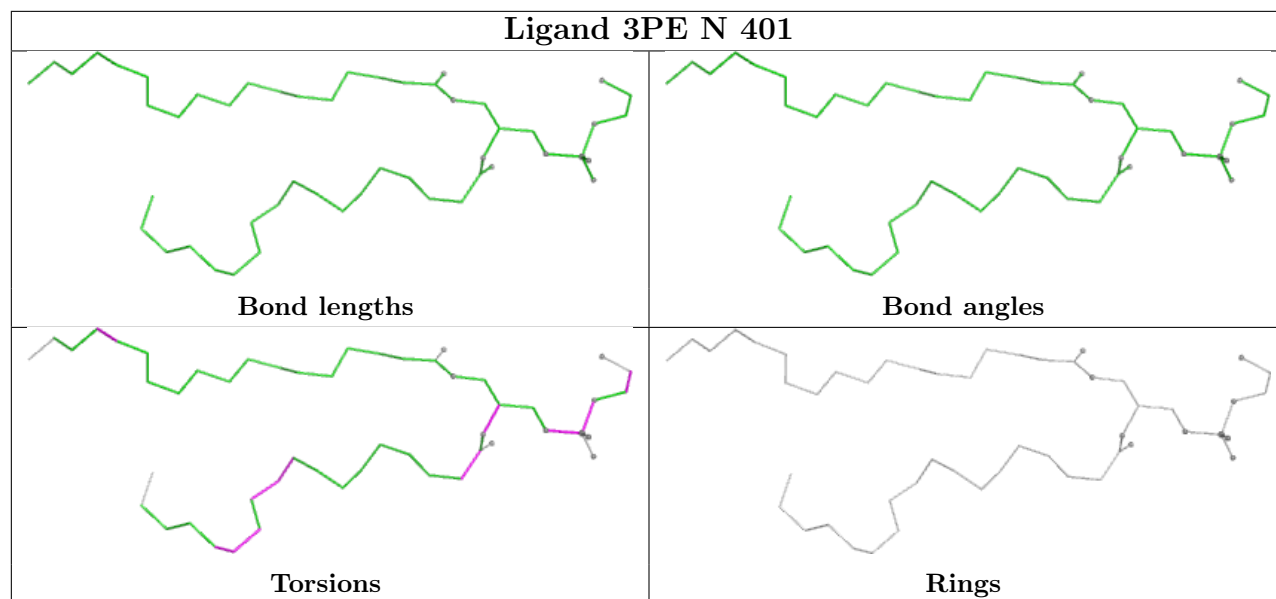
17 monomers are involved in 32 short contacts:

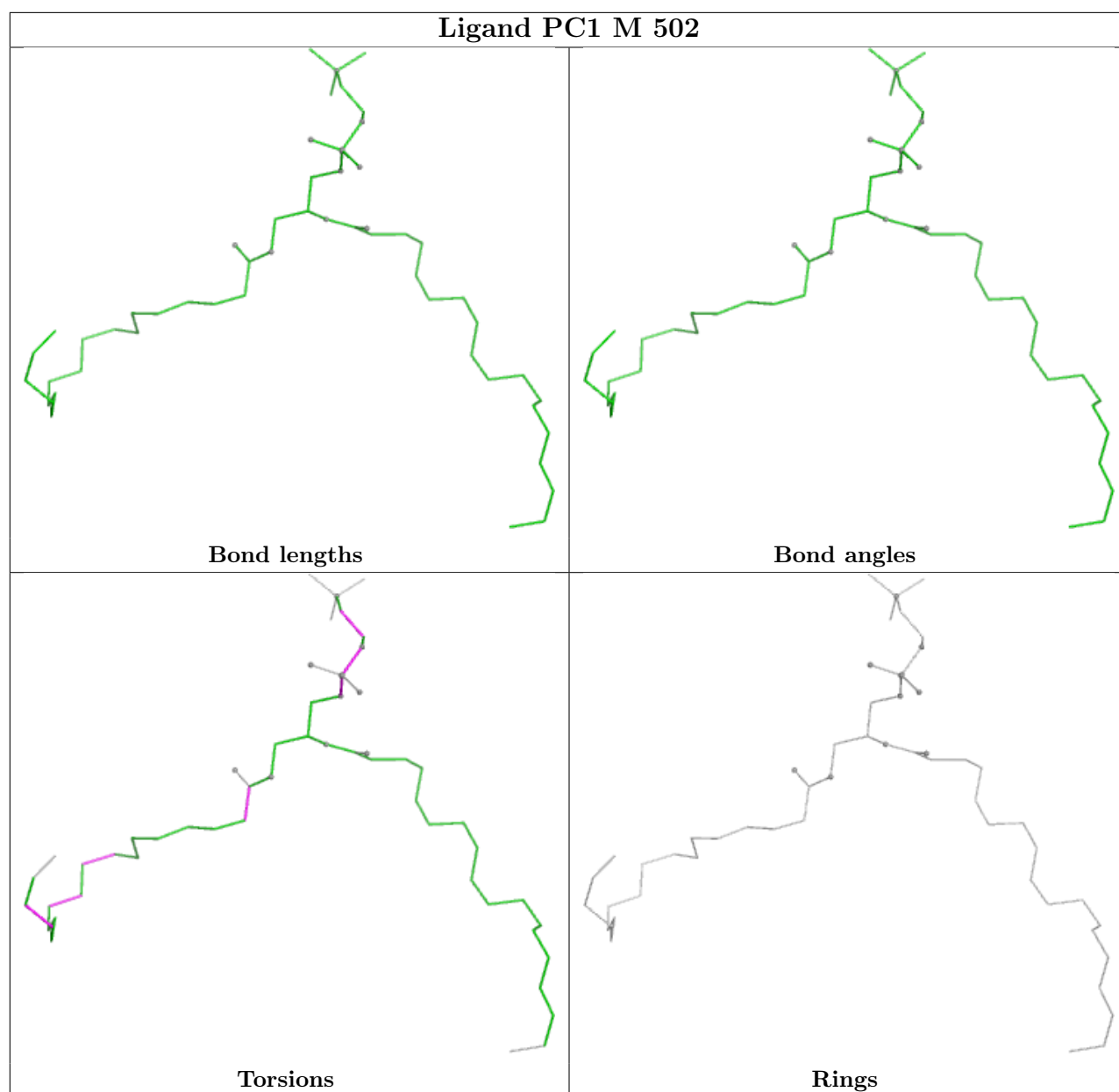
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	N	401	3PE	2	0
46	M	502	PC1	2	0
53	1	503	NAI	2	0
45	V	201	3PE	1	0
45	A	201	3PE	1	0
46	L	1003	PC1	1	0
45	J	201	3PE	5	0
50	j	101	ZMP	1	0
45	H	401	3PE	3	0
45	6	203	3PE	3	0
45	o	501	3PE	1	0
54	2	300	FES	1	0
45	V	202	3PE	3	0
46	M	503	PC1	4	0
47	k	401	DGT	1	0
45	i	201	3PE	1	0
50	t	201	ZMP	1	0

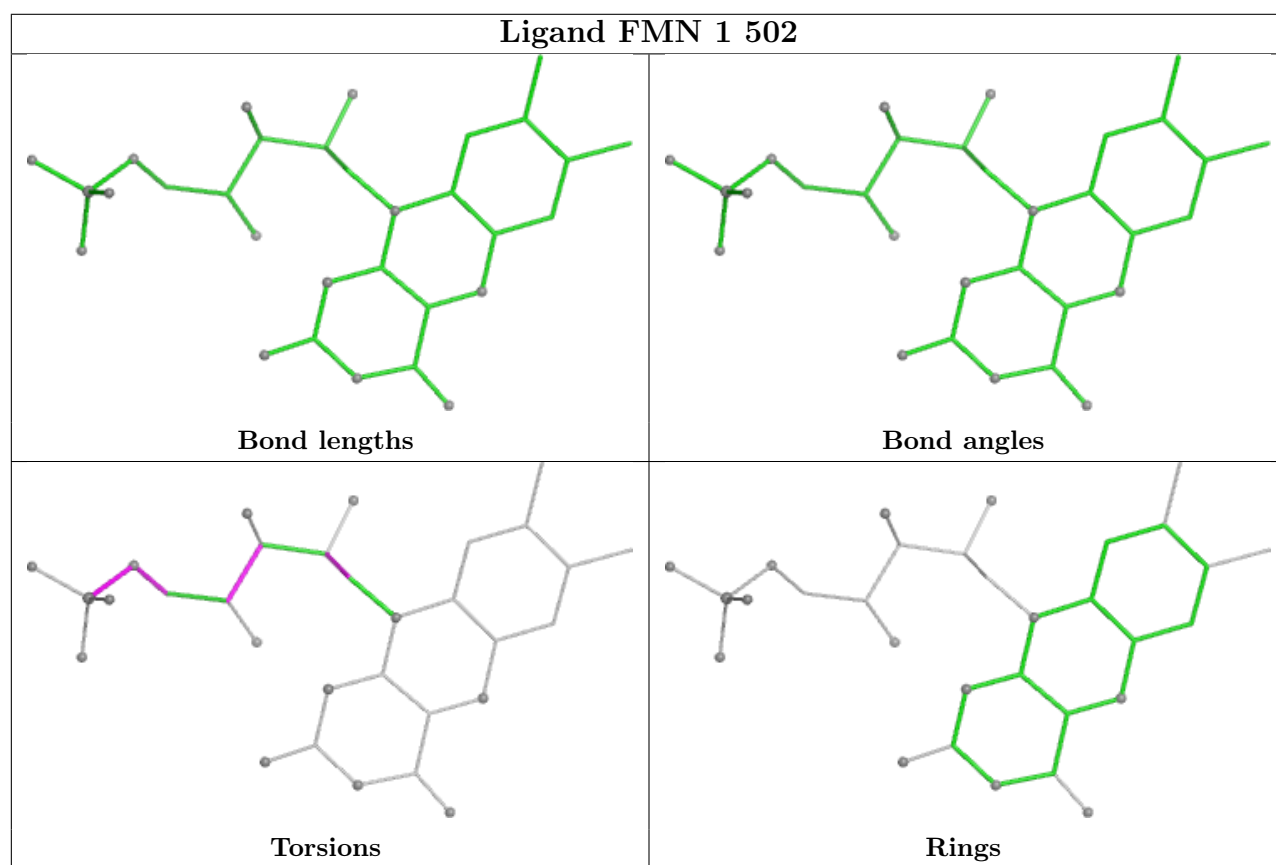
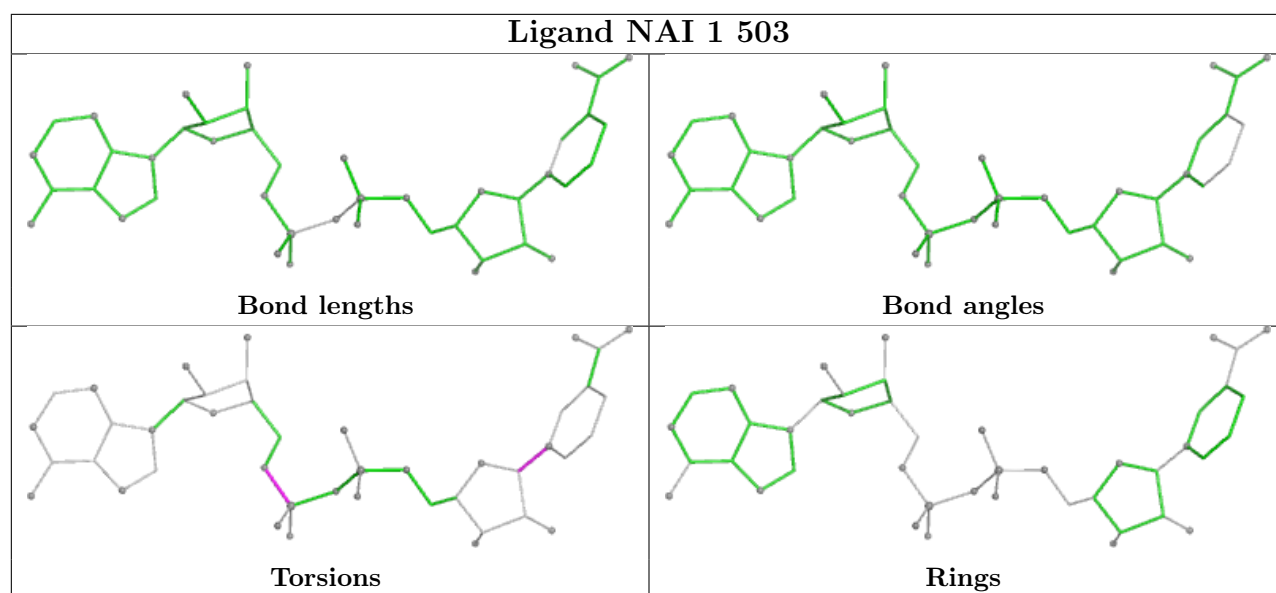
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

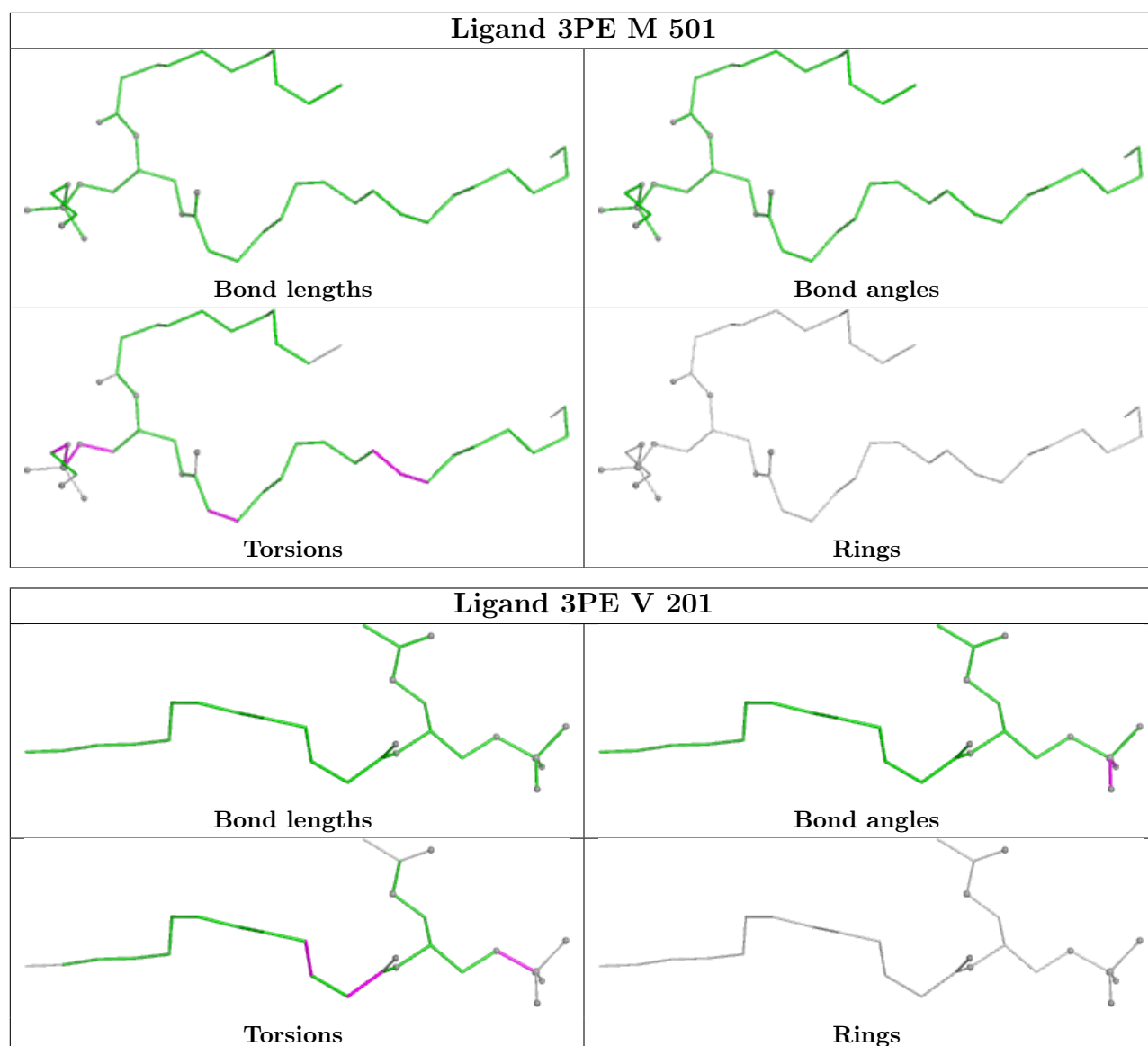
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

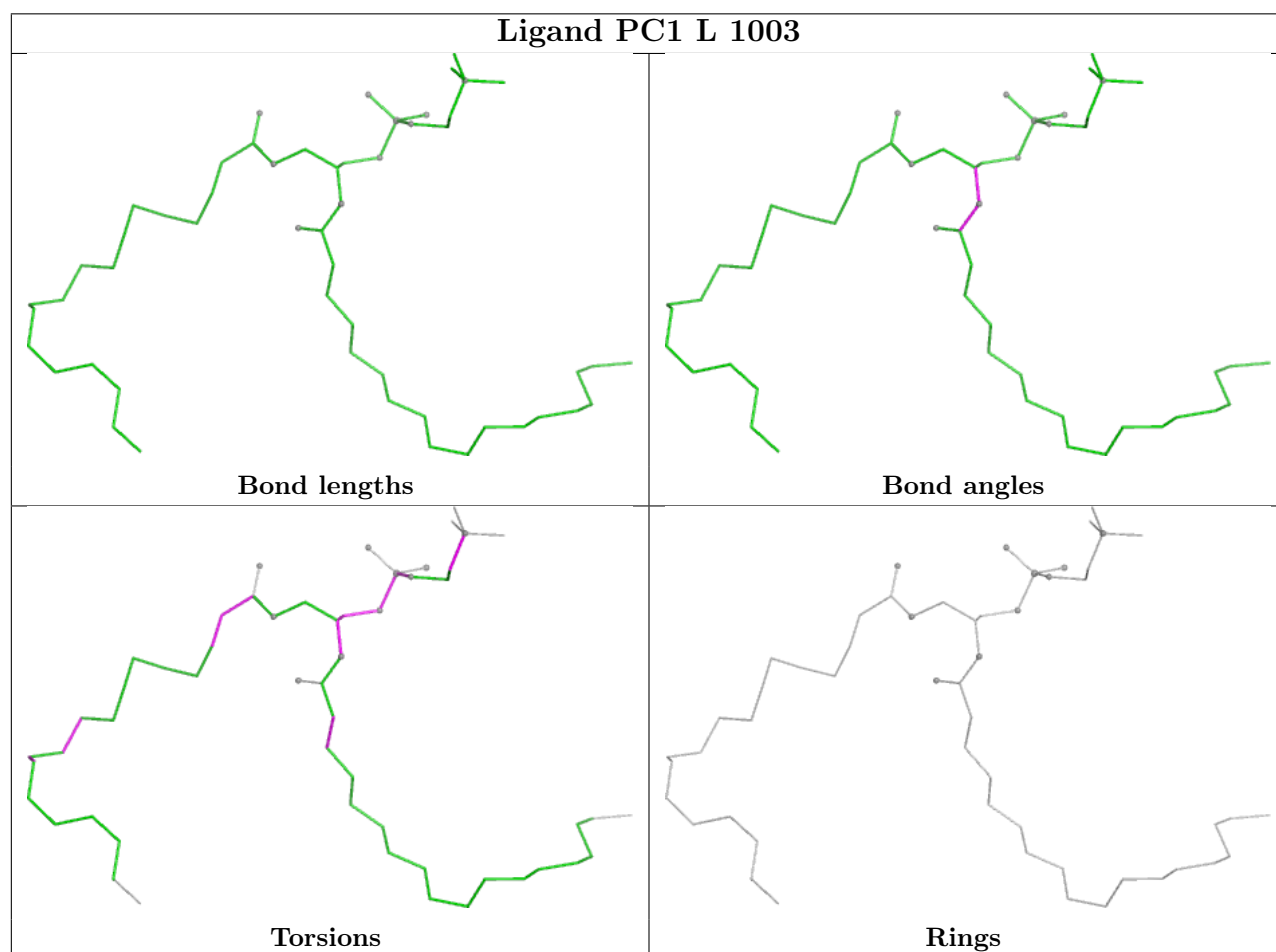
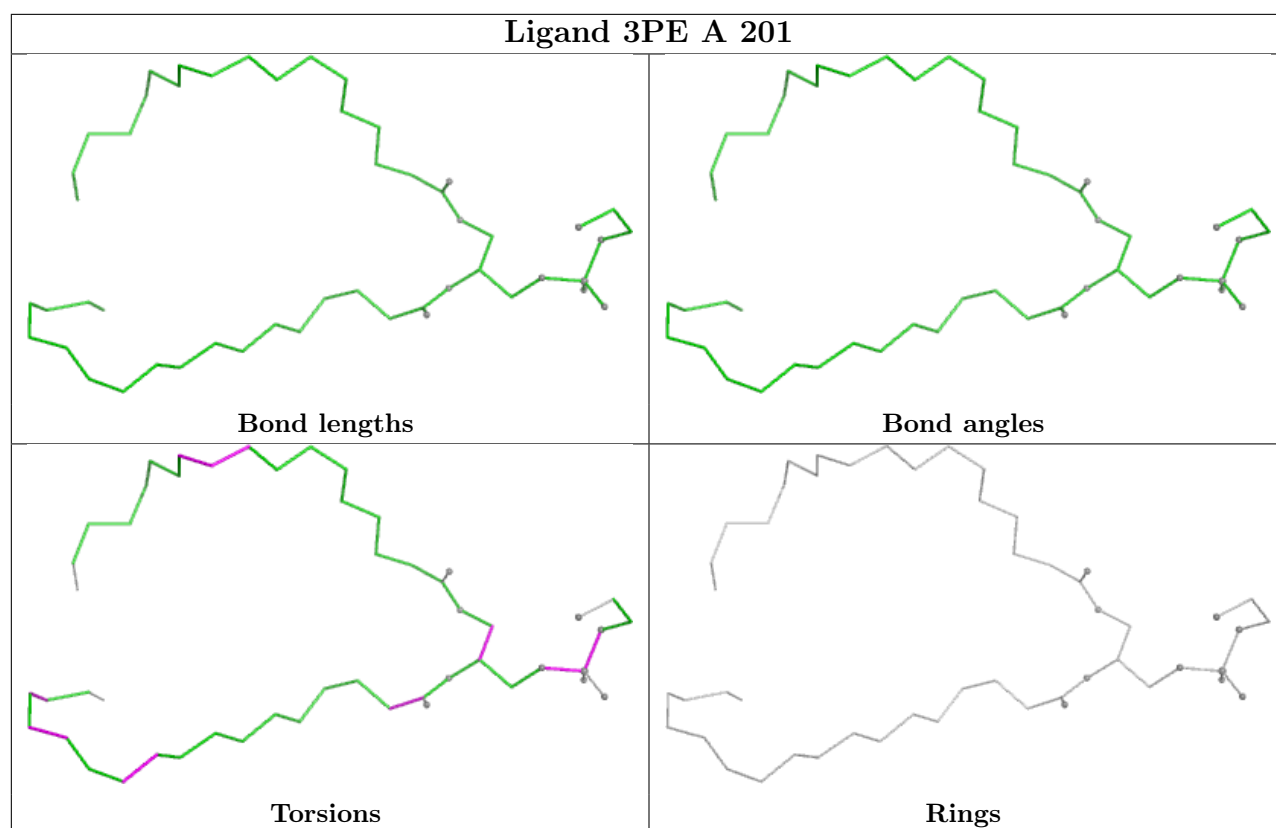


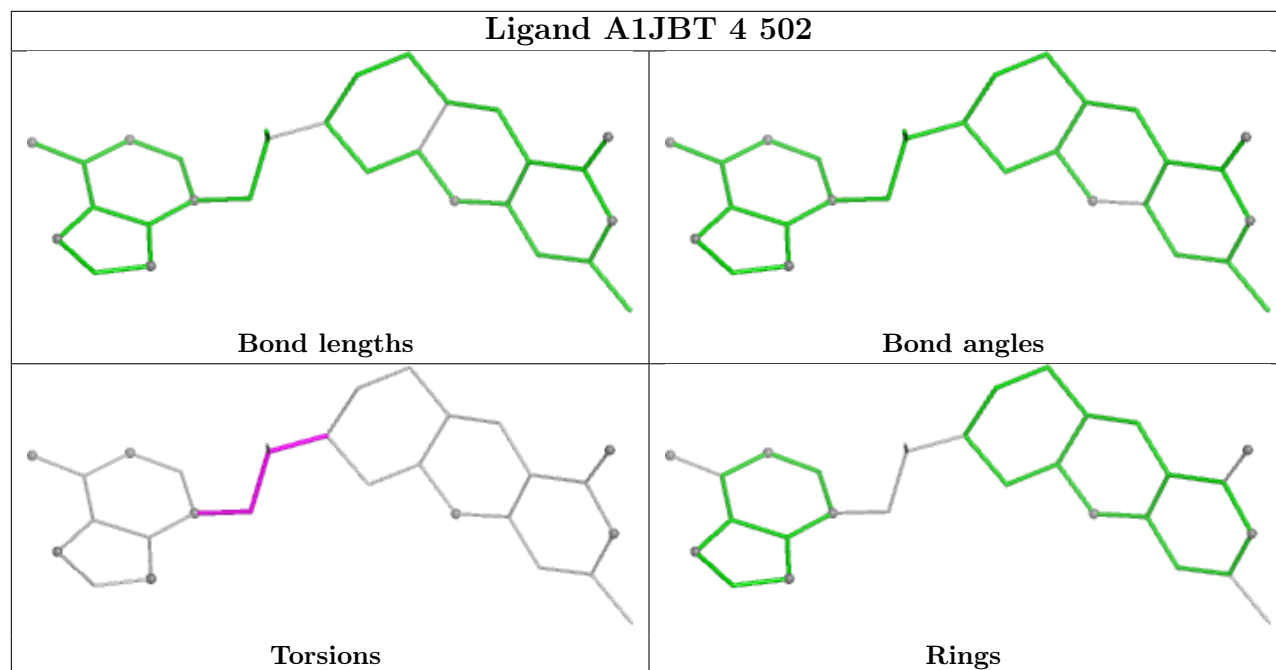
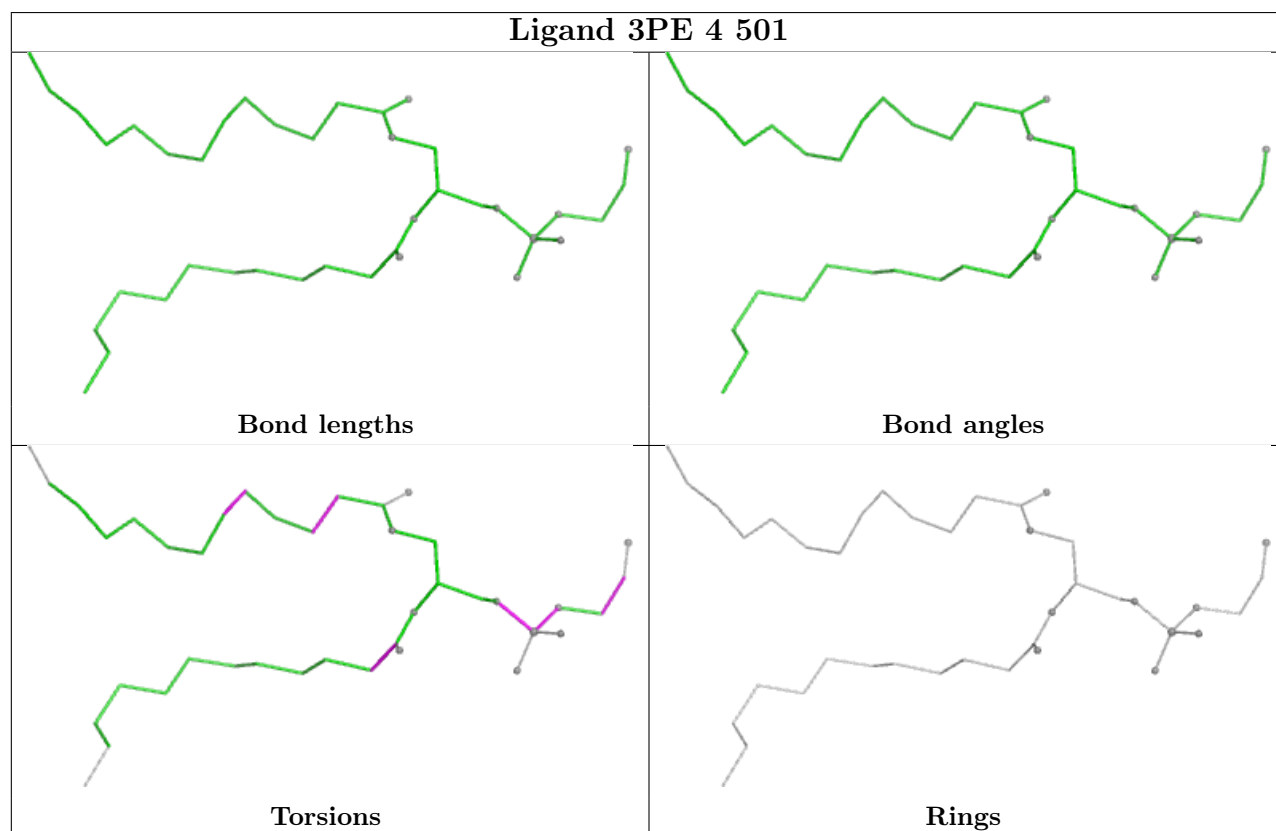


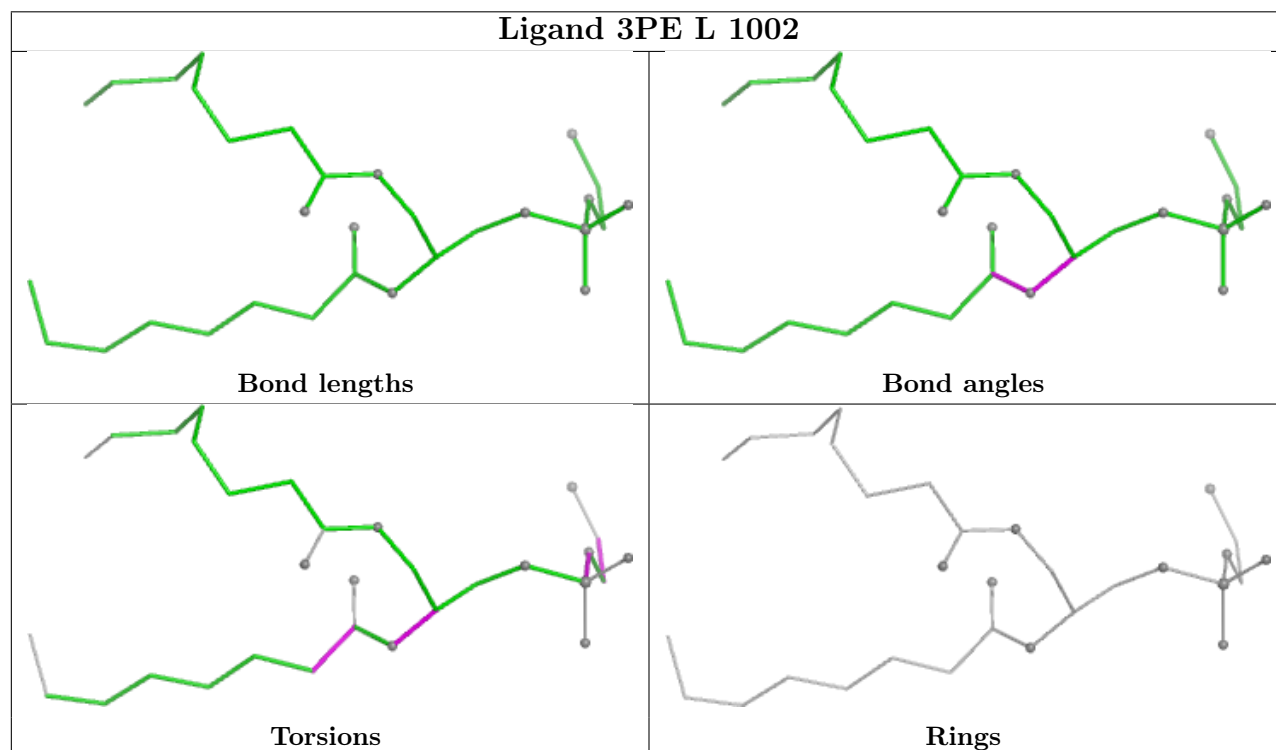
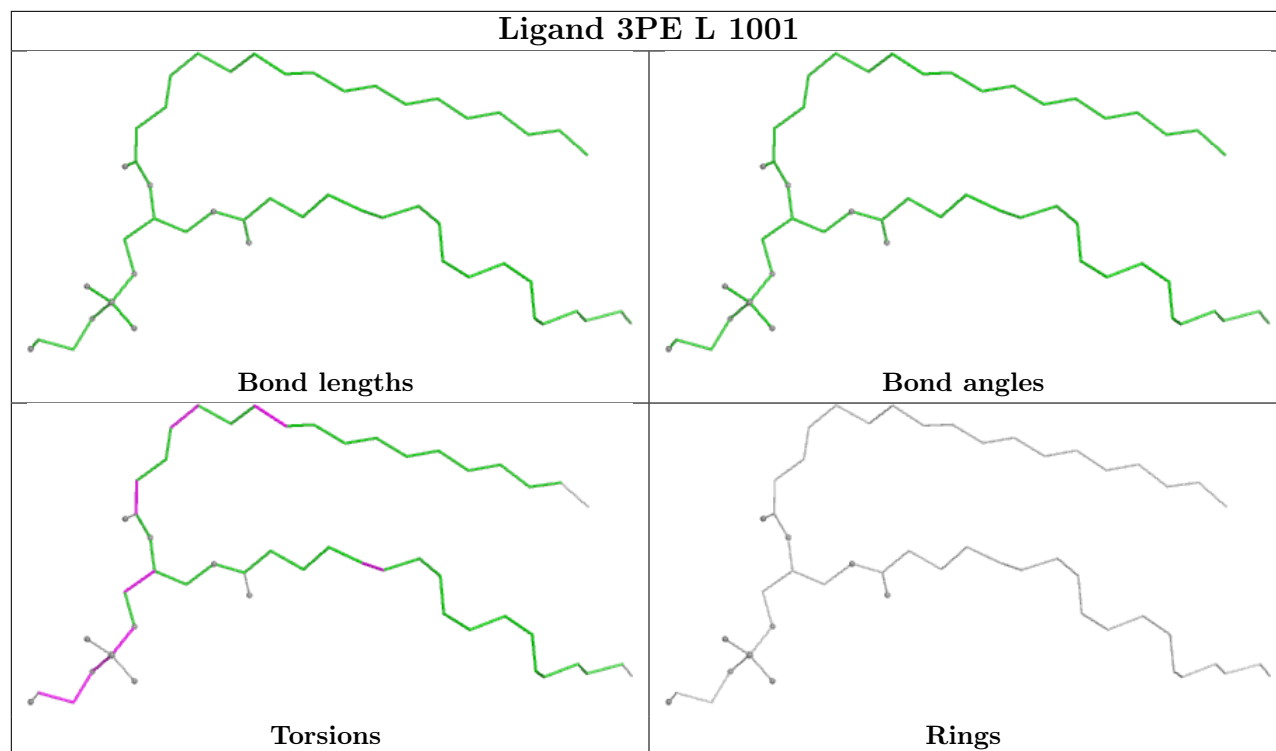


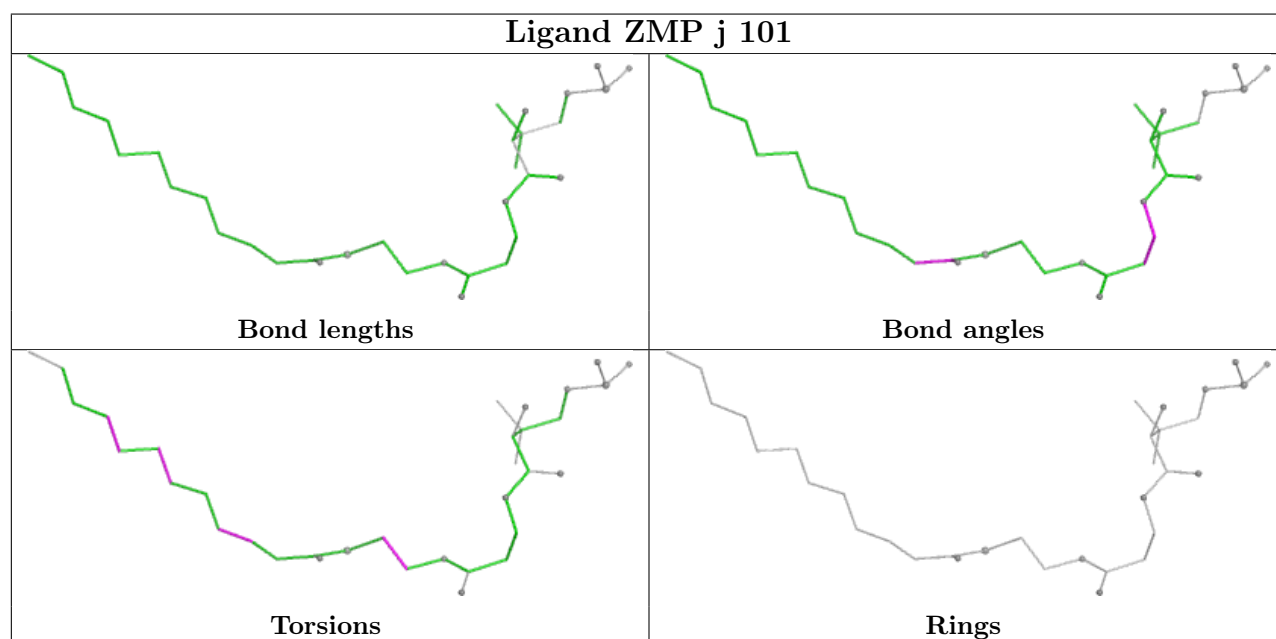
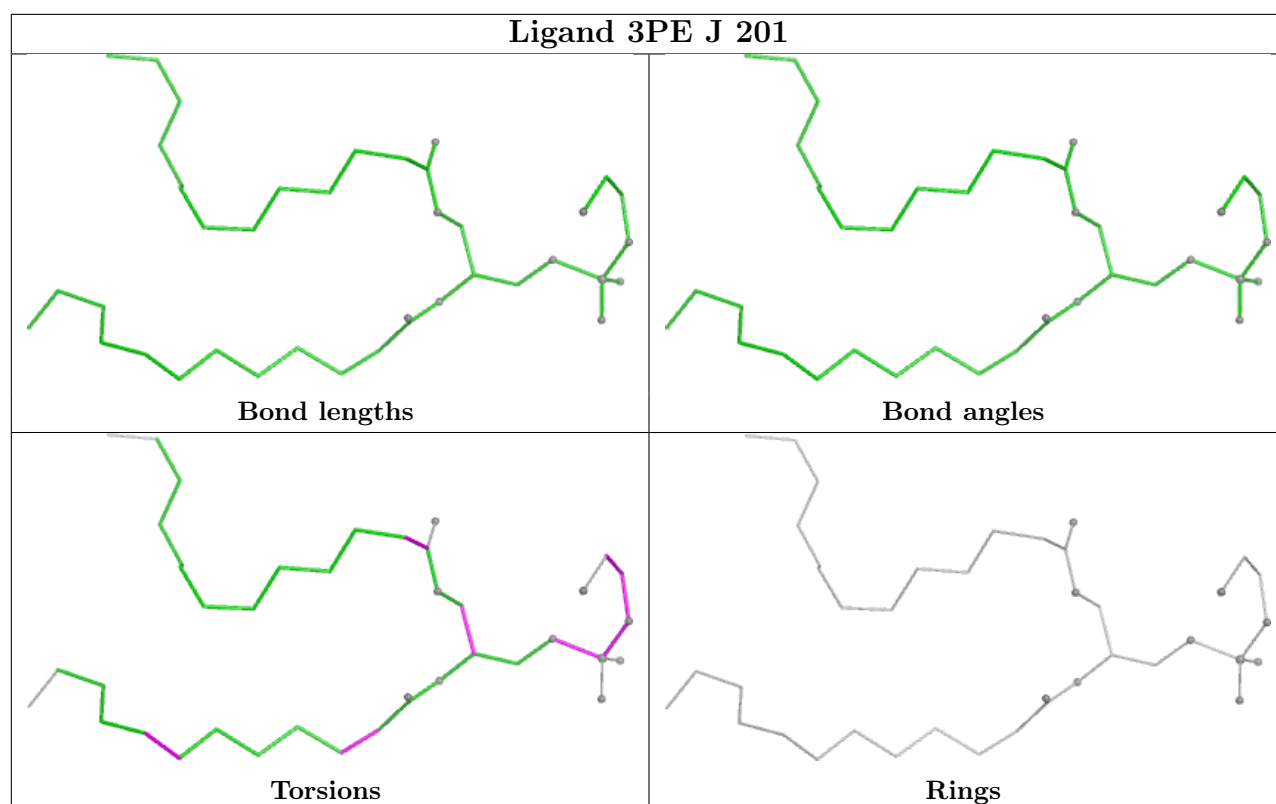


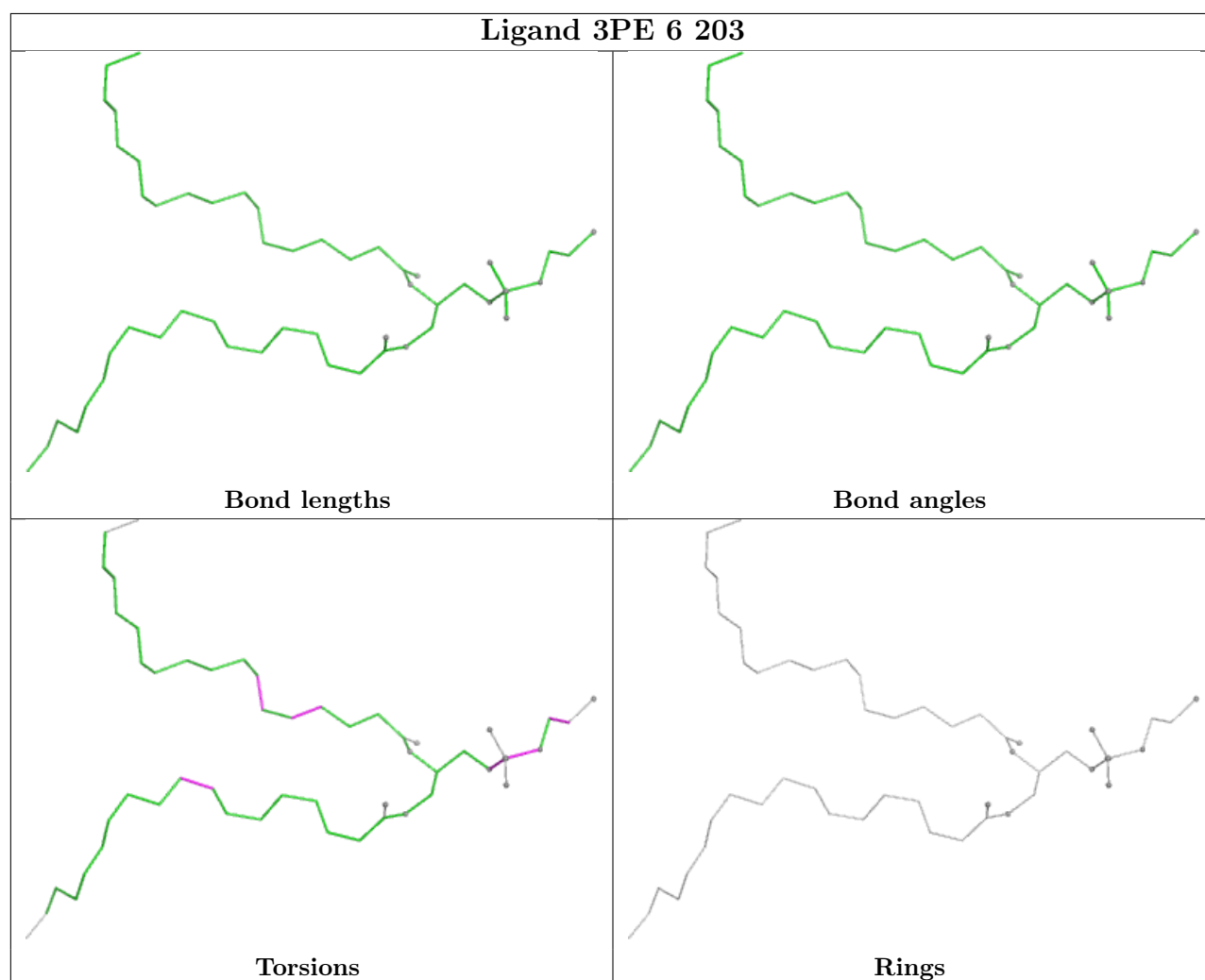
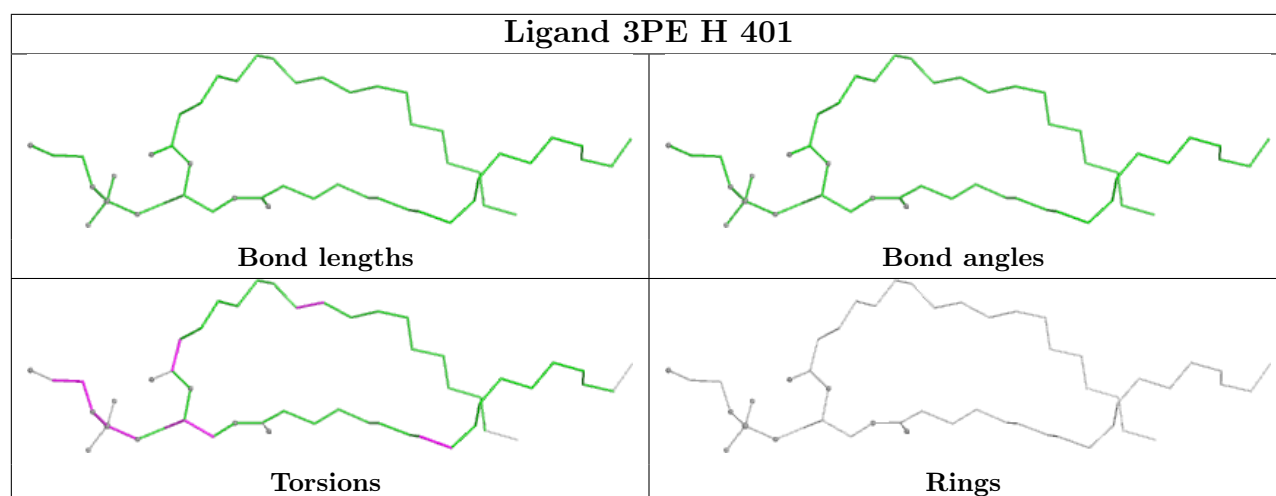


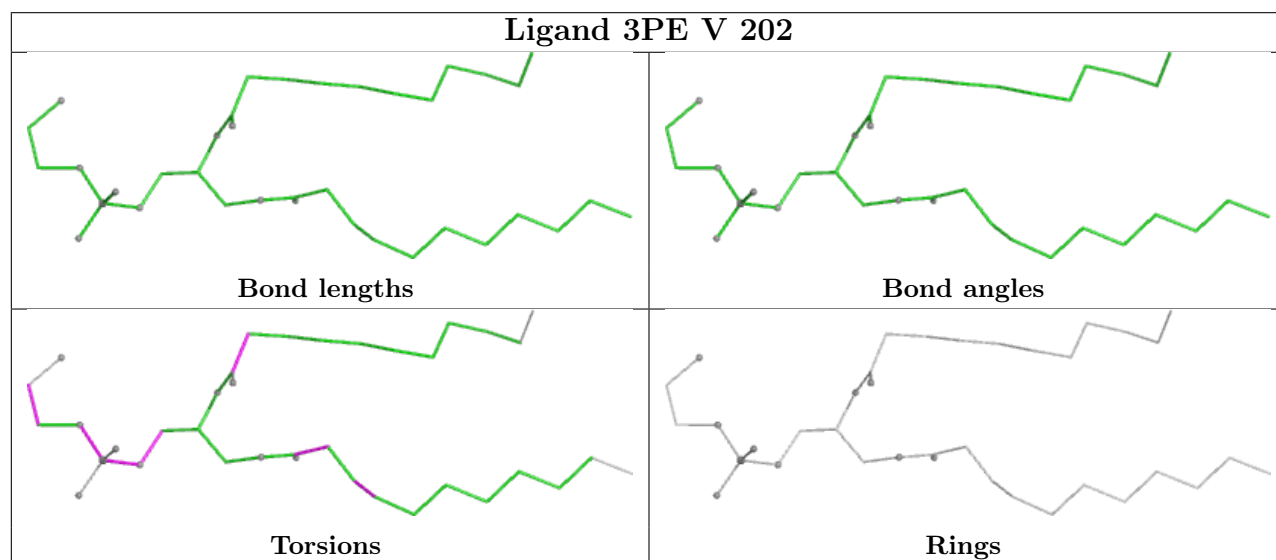
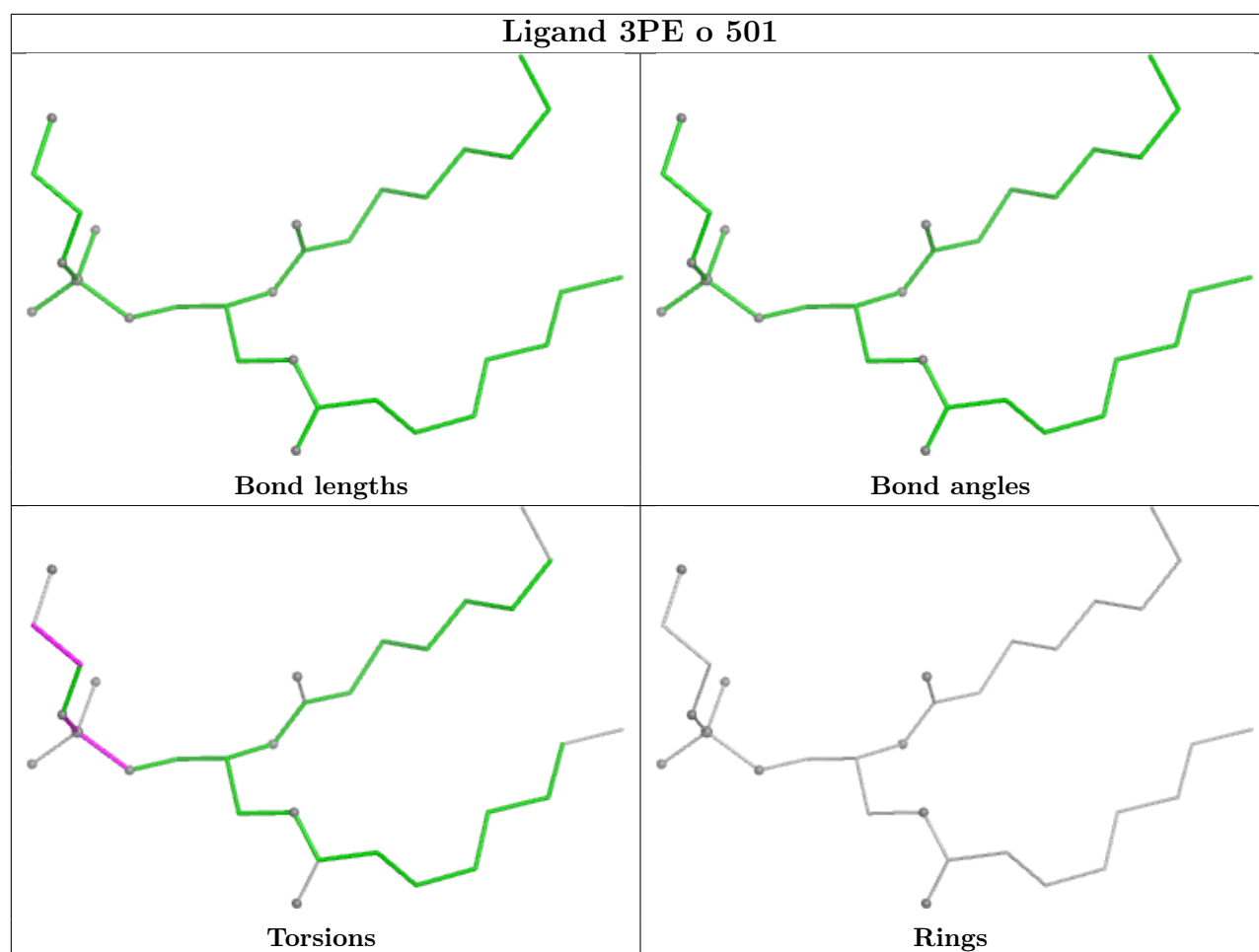


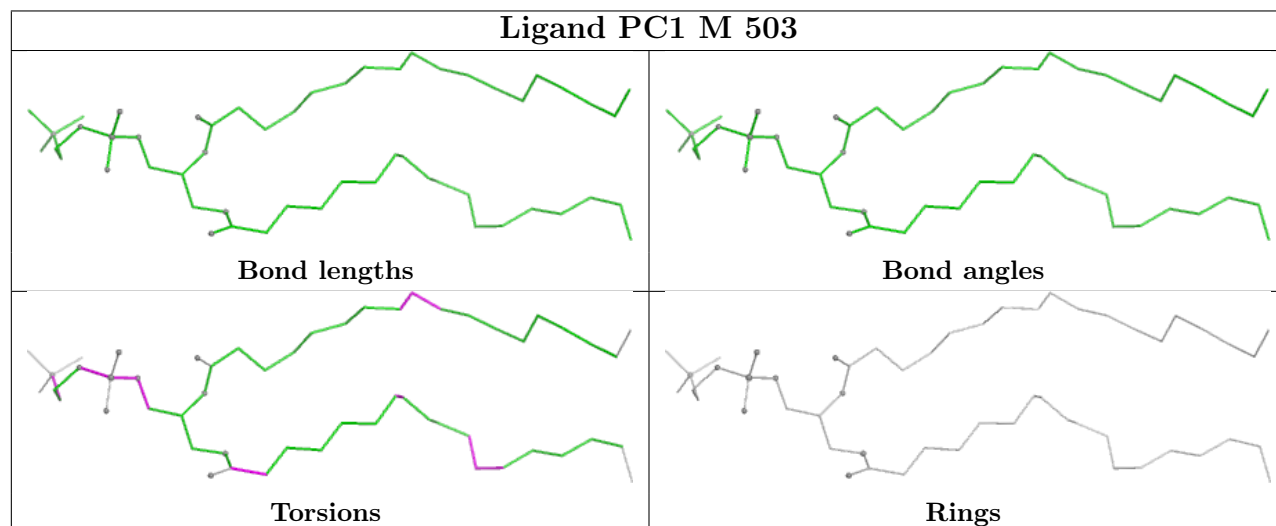
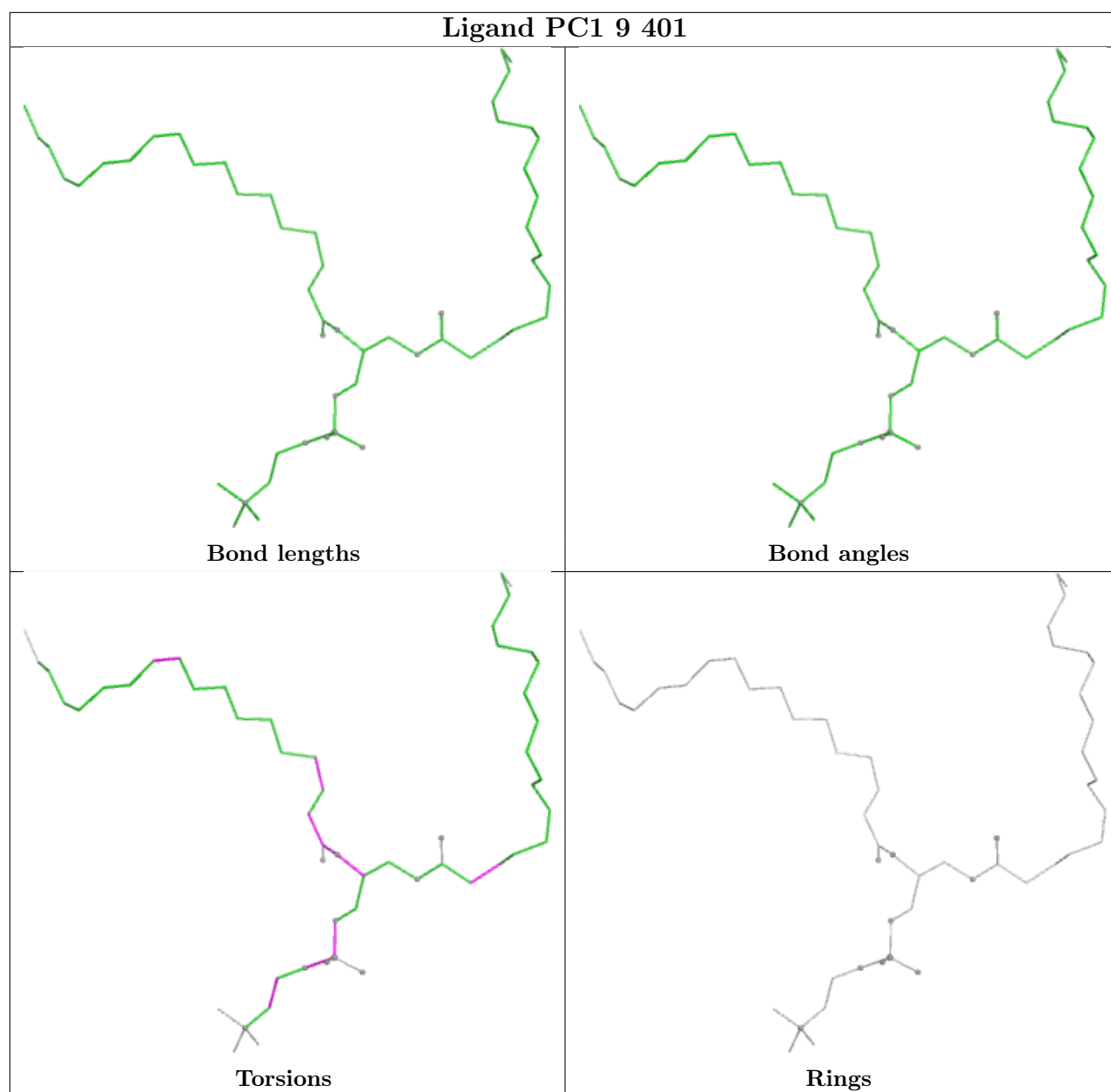
Ligand A1JBT 4 502**Ligand 3PE 4 501**

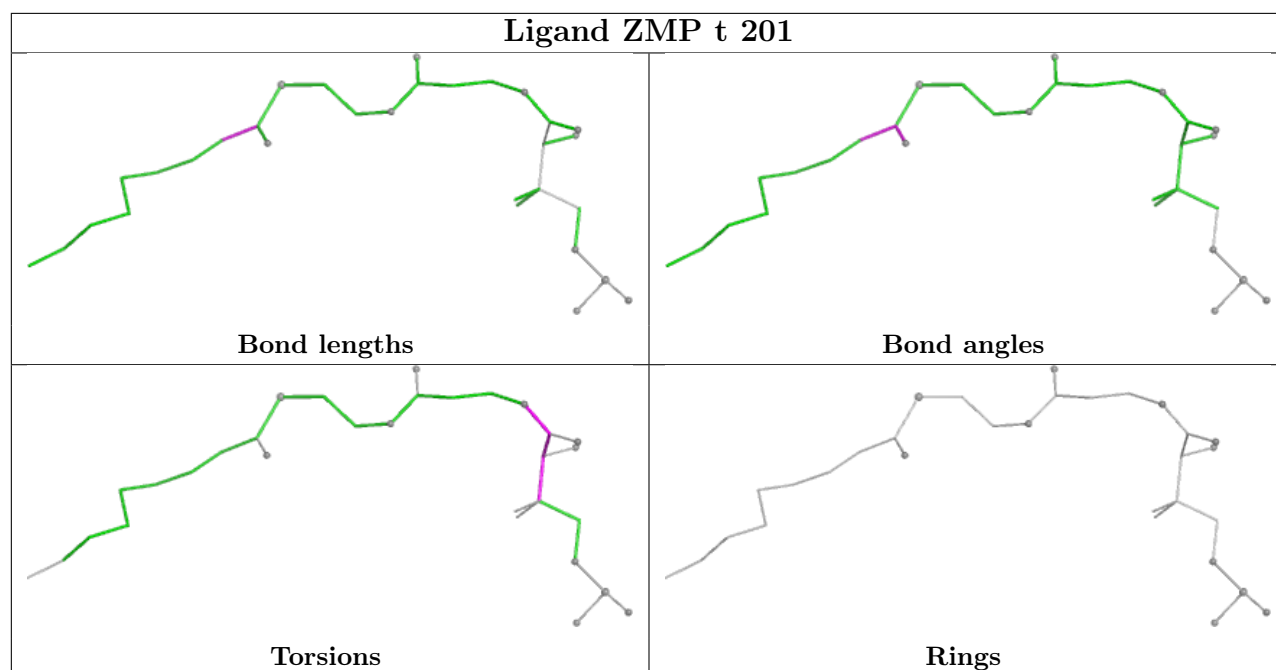
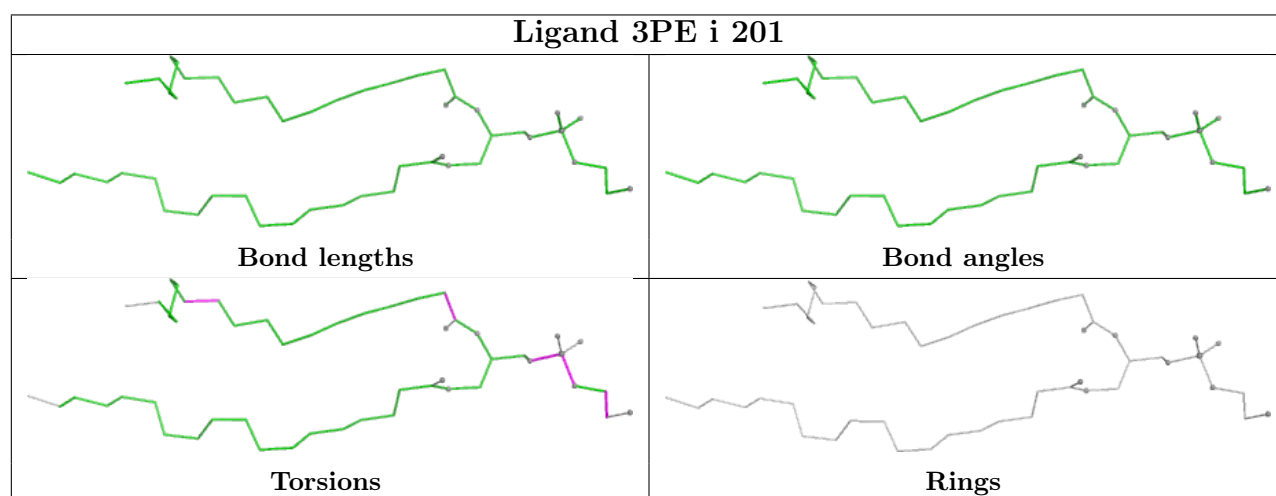
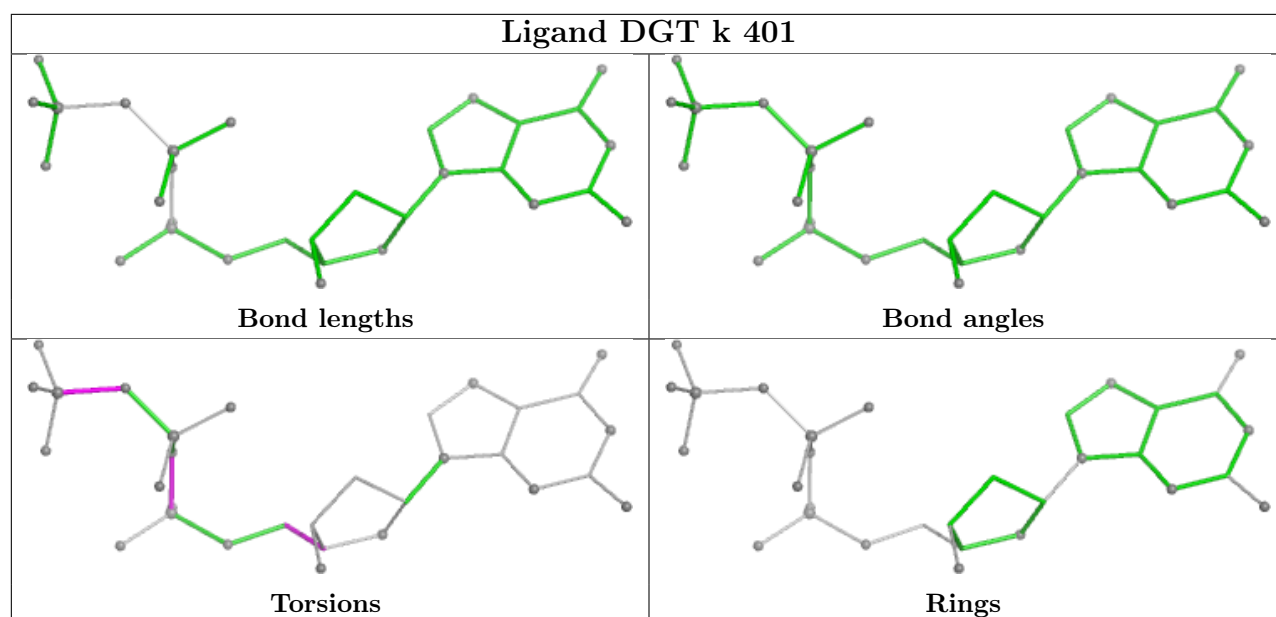












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

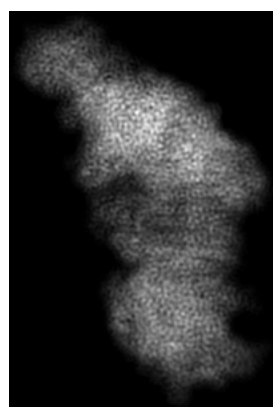
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53476. These allow visual inspection of the internal detail of the map and identification of artifacts.

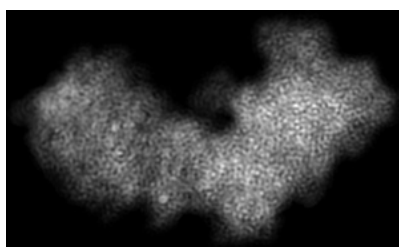
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

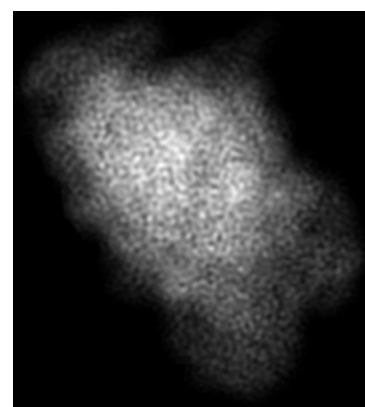
6.1.1 Primary map



X



Y



Z

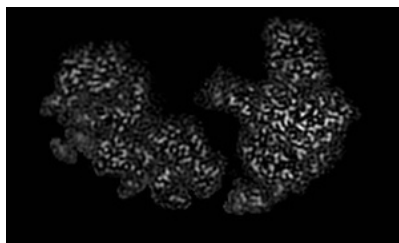
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

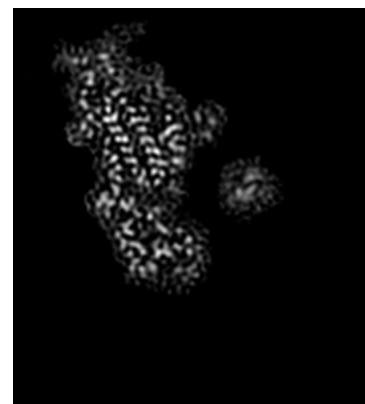
6.2.1 Primary map



X Index: 71



Y Index: 78



Z Index: 118

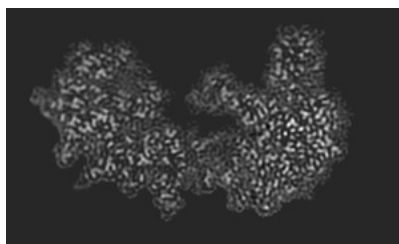
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

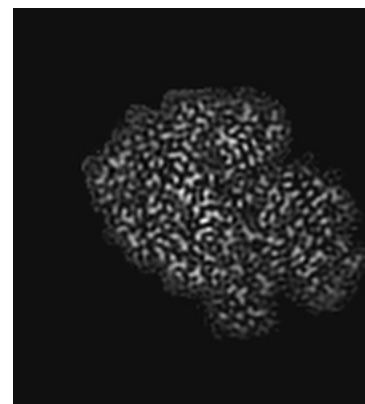
6.3.1 Primary map



X Index: 85



Y Index: 86

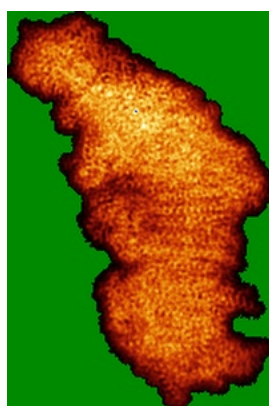


Z Index: 173

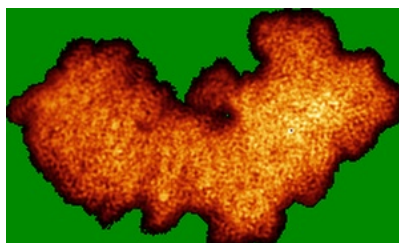
The images above show the largest variance slices of the map in three orthogonal directions.

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

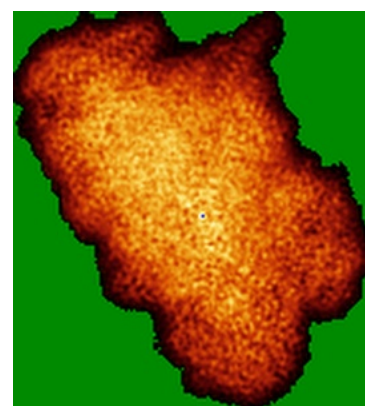
6.4.1 Primary map



X



Y

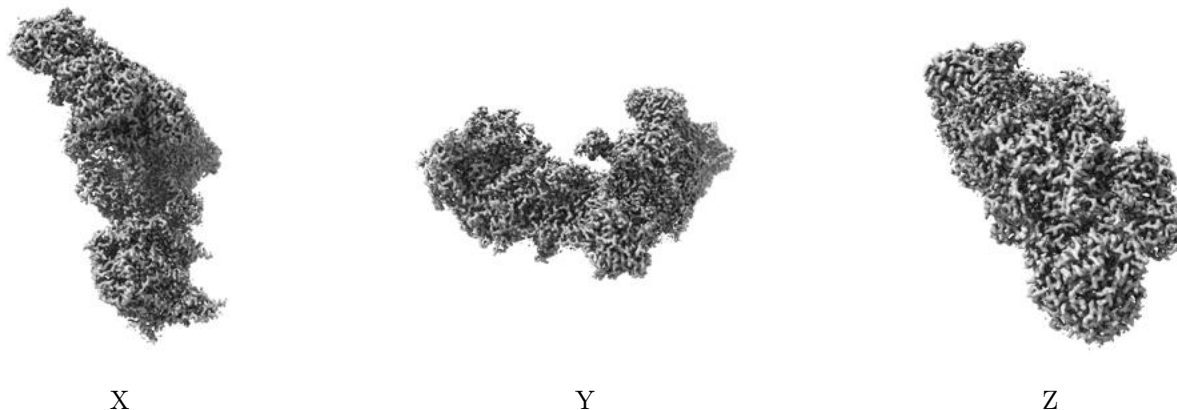


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

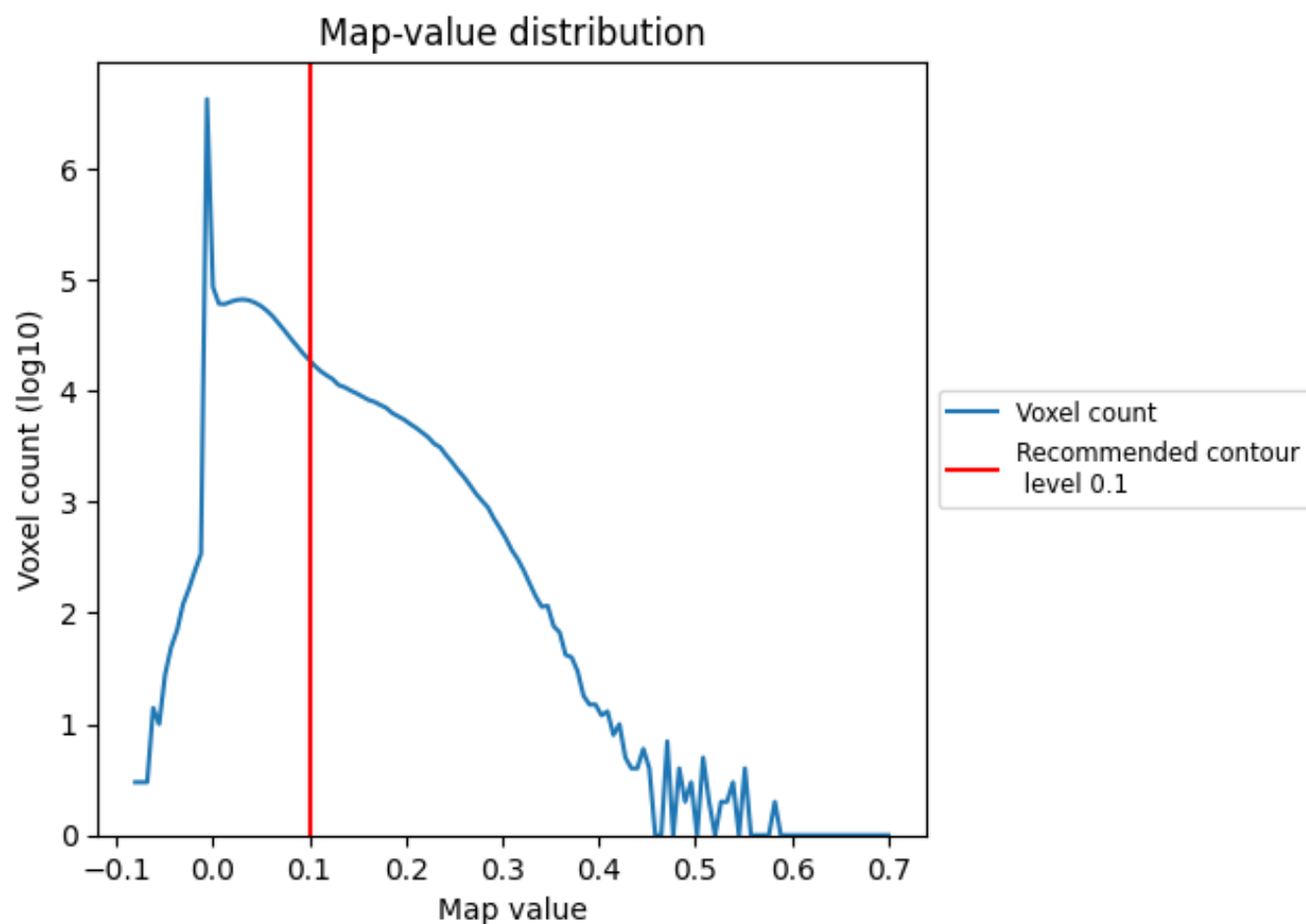
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

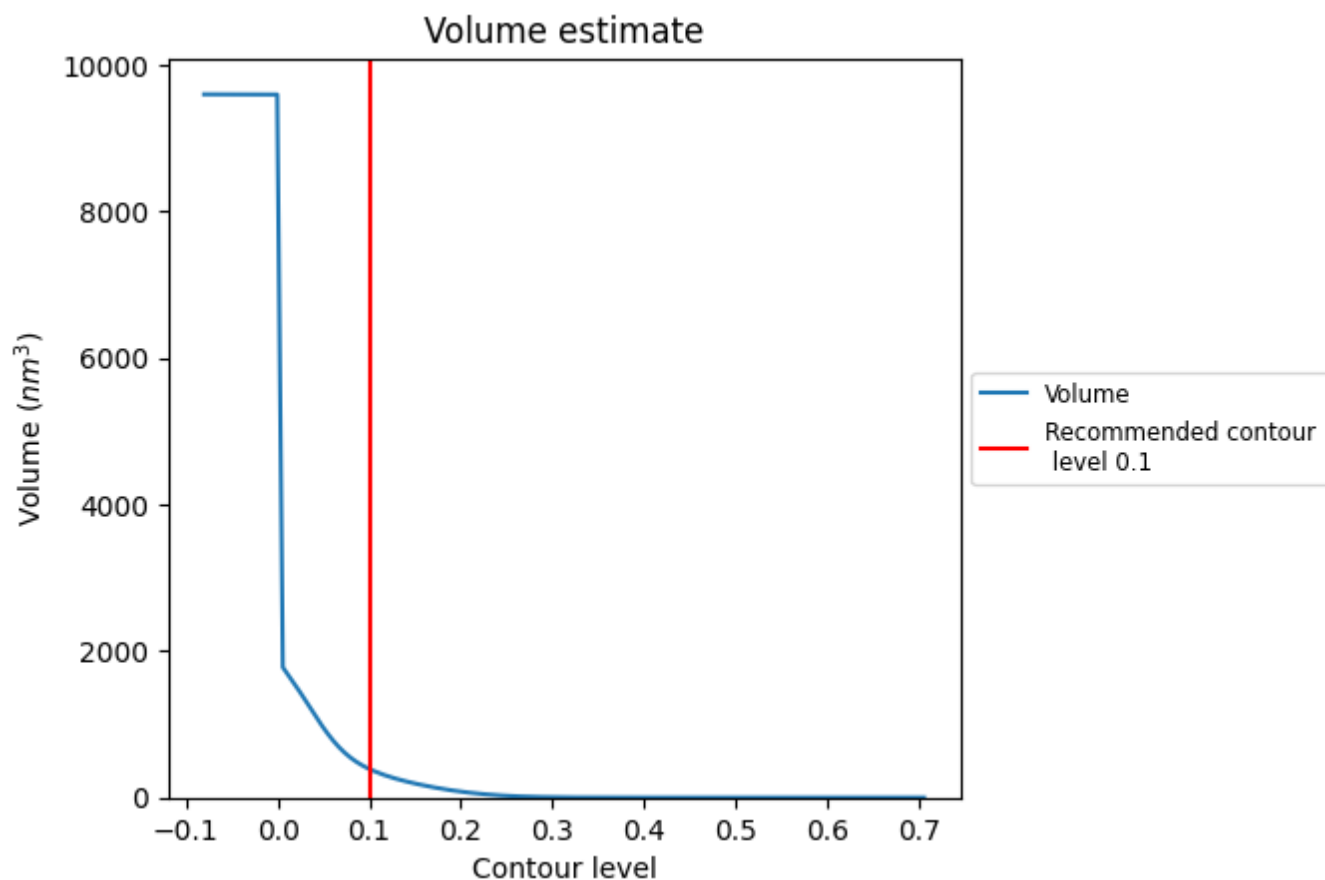
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 391 nm³; this corresponds to an approximate mass of 353 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.

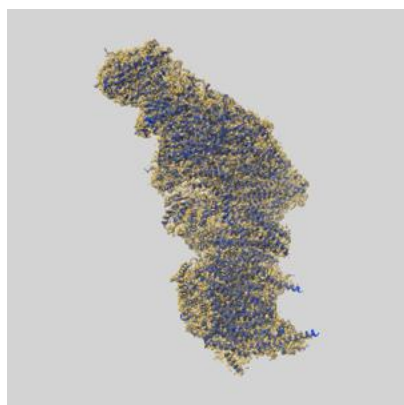
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

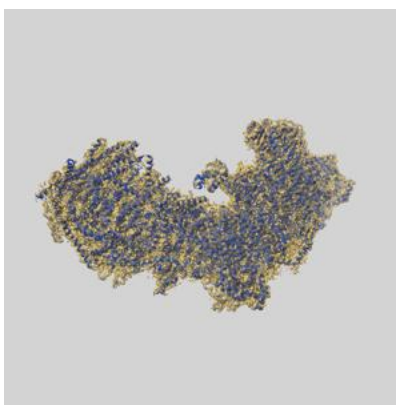
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53476 and PDB model 9R01. Per-residue inclusion information can be found in section [3](#) on page [21](#).

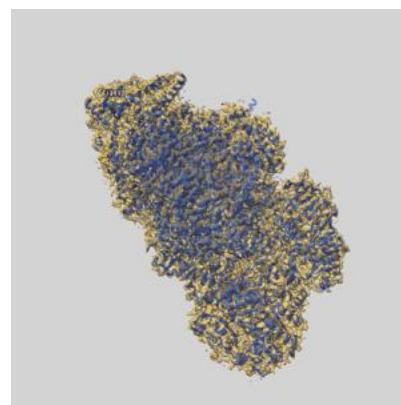
9.1 Map-model overlay [i](#)



X



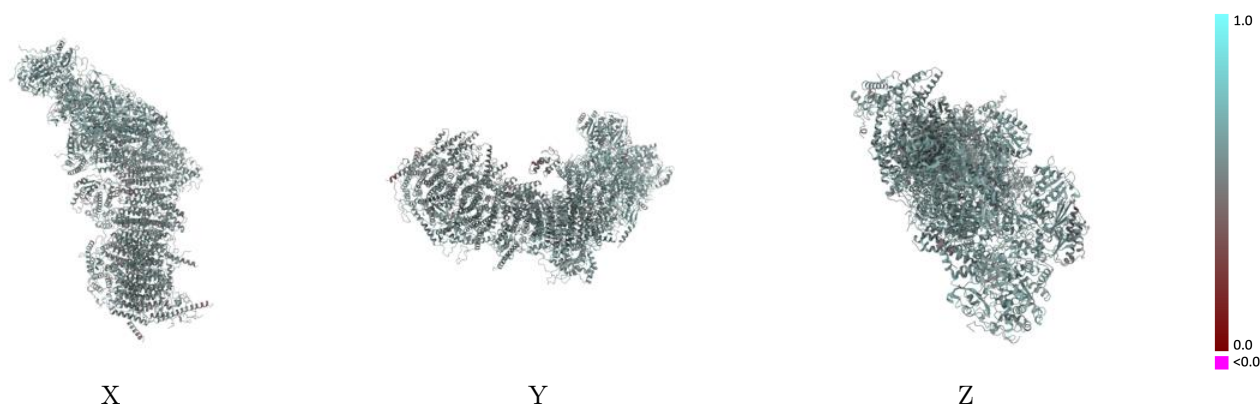
Y



Z

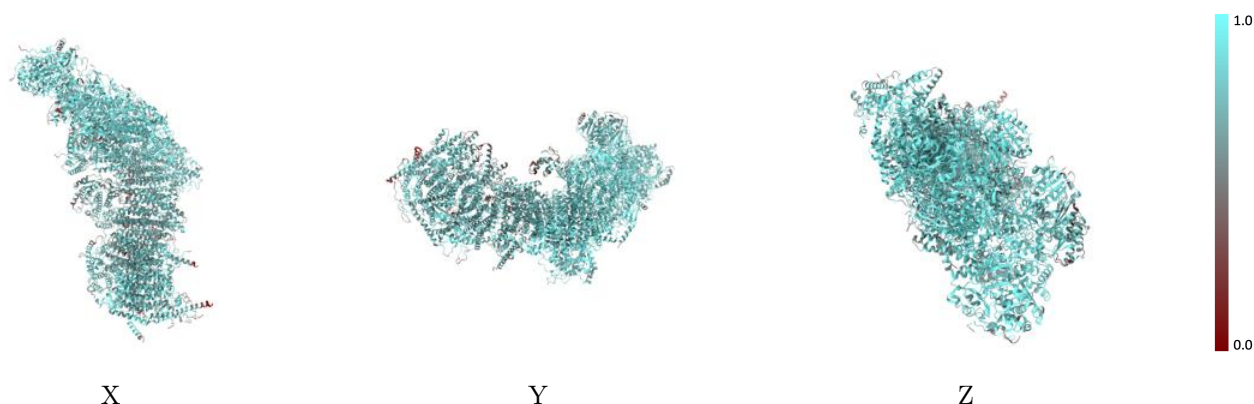
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



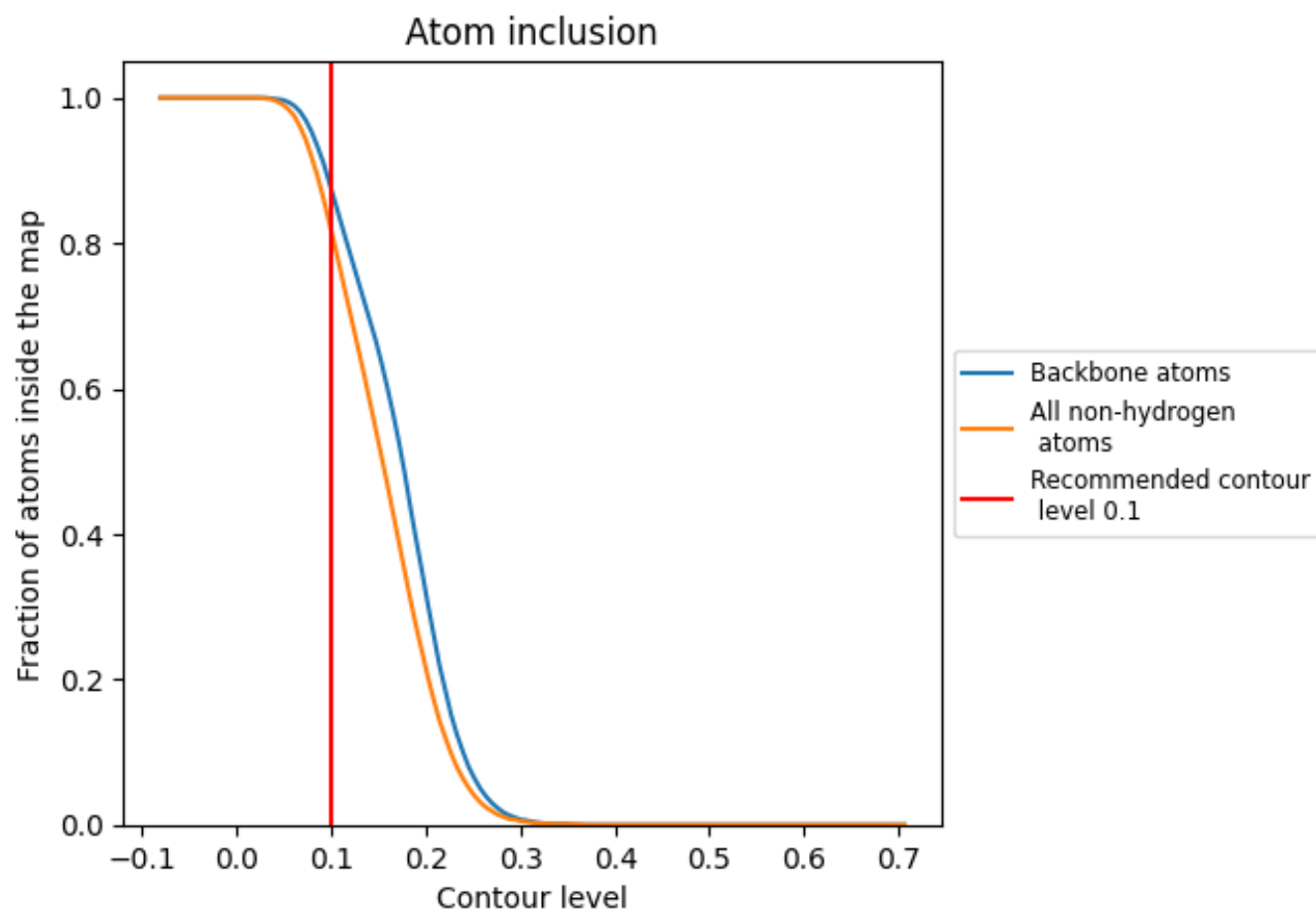
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 82% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8180	 0.5630
1	 0.8650	 0.5780
2	 0.7940	 0.5640
3	 0.8280	 0.5750
4	 0.8930	 0.5800
5	 0.9120	 0.5890
6	 0.9350	 0.5910
9	 0.9320	 0.5890
A	 0.8190	 0.5590
H	 0.9000	 0.5710
J	 0.8330	 0.5520
K	 0.8590	 0.5590
L	 0.8040	 0.5480
M	 0.8290	 0.5670
N	 0.8380	 0.5740
V	 0.6890	 0.5350
W	 0.8310	 0.5770
X	 0.7010	 0.5230
Y	 0.7820	 0.5580
Z	 0.7690	 0.5520
a	 0.7840	 0.5610
b	 0.8430	 0.5870
c	 0.8400	 0.5860
d	 0.8830	 0.5790
e	 0.7130	 0.5510
f	 0.8020	 0.5700
g	 0.8290	 0.5670
h	 0.8590	 0.5740
i	 0.8780	 0.5890
j	 0.5270	 0.4780
k	 0.7330	 0.5530
l	 0.8500	 0.5670
m	 0.8260	 0.5540
n	 0.7040	 0.5160
o	 0.7940	 0.5690



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Chain	Atom inclusion	Q-score
p	 0.7040	 0.5390
q	 0.8770	 0.5710
r	 0.7160	 0.5390
s	 0.6880	 0.5160
t	 0.7400	 0.5390
u	 0.7540	 0.5300
v	 0.7400	 0.5380
w	 0.7460	 0.5520
x	 0.7270	 0.5520
y	 0.6760	 0.5270
z	 0.9020	 0.5700