



wwPDB EM Validation Summary Report ⓘ

Dec 7, 2022 – 10:13 AM JST

PDB ID : 5XTD
EMDB ID : EMD-6773
Title : Cryo-EM structure of human respiratory complex I
Authors : Gu, J.; Wu, M.; Yang, M.
Deposited on : 2017-06-19
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

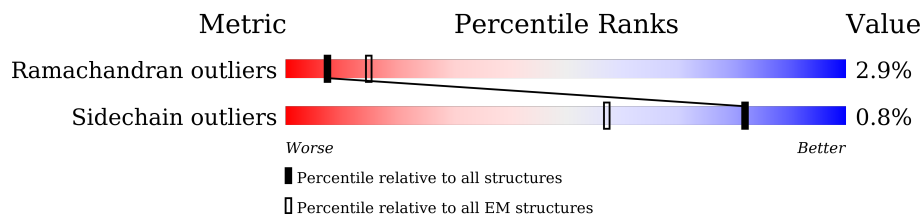
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 3.70 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	431	
2	B	176	
3	C	156	
4	E	113	
5	F	83	
6	G	85	
6	X	85	
7	H	112	
8	I	110	

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Mol	Chain	Length	Quality of chain
9	J	337	32% 97%
10	K	33	64% 91% 9%
11	L	118	56% 97%
12	M	687	52% 96%
13	N	143	34% 95% 5%
14	O	212	61% 97%
15	P	208	31% 95% 5%
16	Q	430	18% 98%
17	S	70	97%
18	T	95	47% 96%
19	U	83	99%
20	V	140	14% 98%
21	W	138	97%
22	Y	59	75% 24%
23	Z	80	100%
24	a	138	96%
25	b	128	15% 87% 9%
26	c	153	95% 5%
27	d	171	95% 5%
28	e	97	10% 97%
29	f	47	19% 98%
30	g	119	95% 5%
31	h	104	94% 6%
32	i	347	98%
33	j	115	24% 97%

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Mol	Chain	Length	Quality of chain
34	k	97	<p>10% 93% 6%</p>
35	l	603	<p>94% 5%</p>
36	m	174	<p>10% 94% 6%</p>
37	n	56	<p>11% 96%</p>
38	o	128	<p>97%</p>
39	p	172	<p>98%</p>
40	r	459	<p>98%</p>
41	s	318	<p>97%</p>
42	u	169	<p>97%</p>
43	v	137	<p>10% 77% 19%</p>
44	w	320	<p>18% 97%</p>

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 66789 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 dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	431	3322	2096	594	612	20	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	176	1420	893	243	271	13	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	156	1249	794	227	214	14	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	113	968	623	178	162	5	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	83	670	422	124	122	2	0	0

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	85	672	434	99	134	5	0	0
6	X	85	686	442	101	138	5	0	0

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	112	922	593	157	169	3	0	0

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	95	769	483	146	138	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	337	2712	1759	482	463	8	0	0

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	33	274	173	47	53	1	0	0

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	118	964	608	173	179	4	0	0

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	687	5274	3310	917	1009	38	0	0

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	143	1195	770	210	212	3	0	0

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	212	1643	1047	276	310	10	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P	208	1730	1117	297	313	3	0	0

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	430	3460	2214	599	624	23	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	S	70	568	367	101	96	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	T	95	742	459	138	142	3	0	0

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	U	83	647	427	105	113	2	0	0

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	V	140	1038	668	178	187	5	0	0

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W	138	1135	727	202	200	6	0	0

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Y	59	533	354	87	91	1	0	0

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Z	80	648	426	110	110	2	0	0

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	a	138	1174	771	199	202	2	0	0

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	b	124	1059	697	181	176	5	0	0

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	c	153	1236	795	208	222	11	0	0

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	d	171	1418	885	262	259	12	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	e	97	810	522	132	152	4	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	f	47	405	269	69	67	0	0

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	g	119	1004	658	173	169	4	0	0

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	h	104	863	546	161	150	6	0	0

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	i	347	2735	1819	421	470	25	0	0

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	j	115	919	626	132	152	9	0	0

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	k	97	740	487	113	127	13	0	0

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	l	603	4717	3119	742	823	33	0	0

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	m	174	1313	879	194	229	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	n	56	473	305	85	80	3	0	0

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

4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	o	128	1066	685	192	187	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	p	172	1495	961	265	261	8	0	0

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	r	459	3629	2411	569	619	30	0	0

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	s	318	2509	1678	380	435	16	0	0

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	u	169	1394	886	247	252	9	0	0

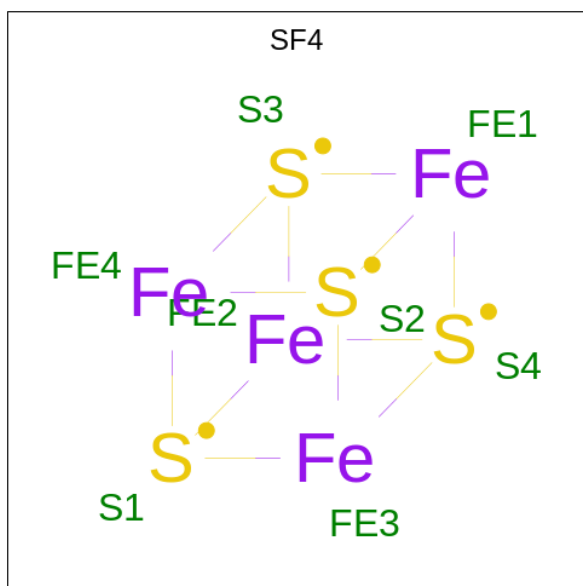
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	v	111	921	569	187	156	9	0	0

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

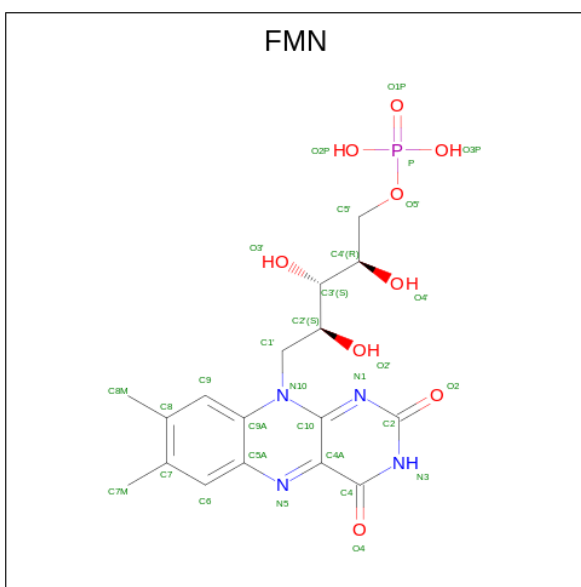
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	w	320	2474	1573	429	464	8	0	0

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



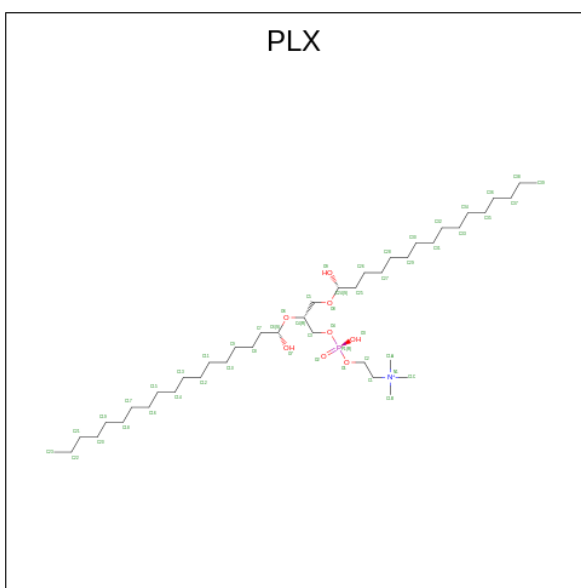
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	A	1	8	4	4	0
45	B	1	16	8	8	0
45	B	1	16	8	8	0
45	C	1	8	4	4	0
45	M	1	16	8	8	0
45	M	1	16	8	8	0

- Molecule 46 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



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

- Molecule 47 is (9R,11S)-9-((1S)-1-HYDROXYHEXADECYL)OXYMETHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOXANE (three-letter code: PLX) (formula: $C_{42}H_{89}NO_8P$).



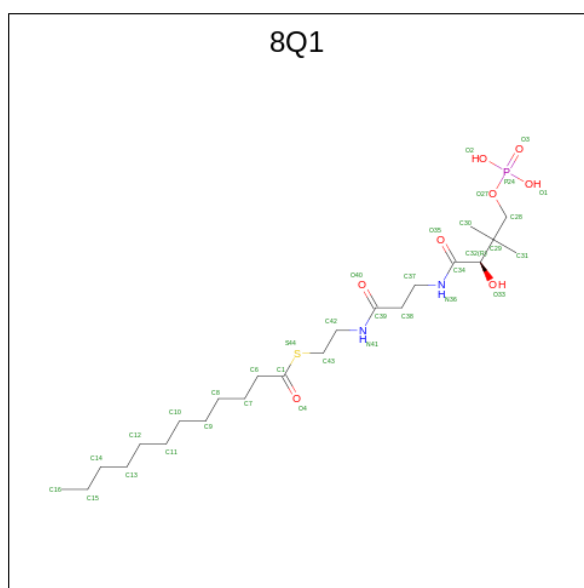
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	B	1	52	42	1	8	1	0
47	U	1	52	42	1	8	1	0

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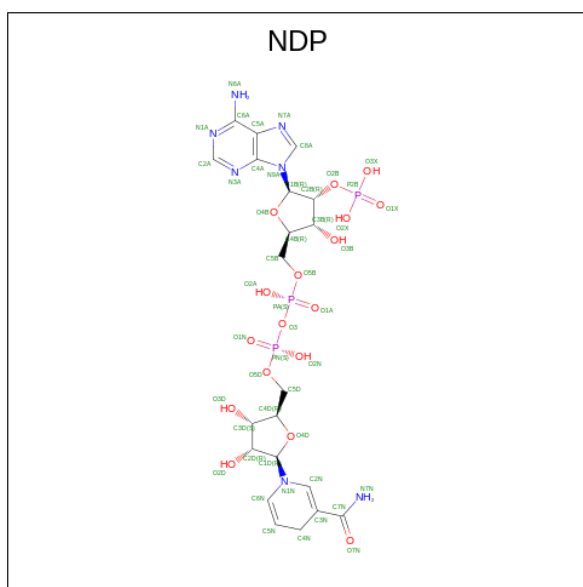
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	V	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	b	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	g	1	Total	C	N	O	P	0
			156	126	3	24	3	
47	g	1	Total	C	N	O	P	0
			156	126	3	24	3	
47	g	1	Total	C	N	O	P	0
			156	126	3	24	3	
47	r	1	Total	C	N	O	P	0
			104	84	2	16	2	
47	r	1	Total	C	N	O	P	0
			104	84	2	16	2	

- Molecule 48 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: C₂₃H₄₅N₂O₈PS).



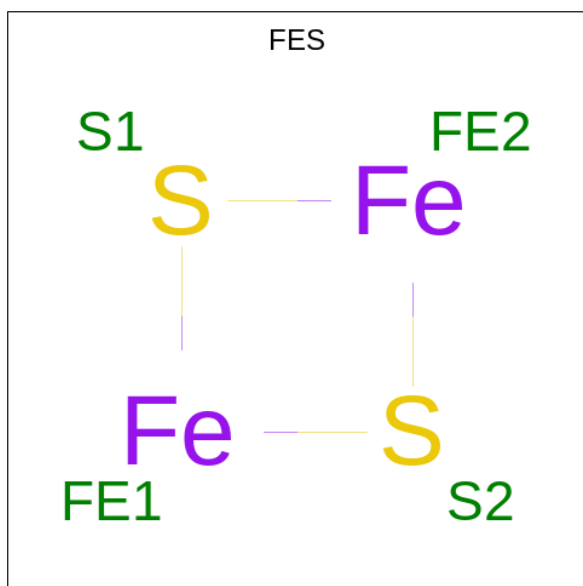
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
48	E	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
48	p	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 49 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



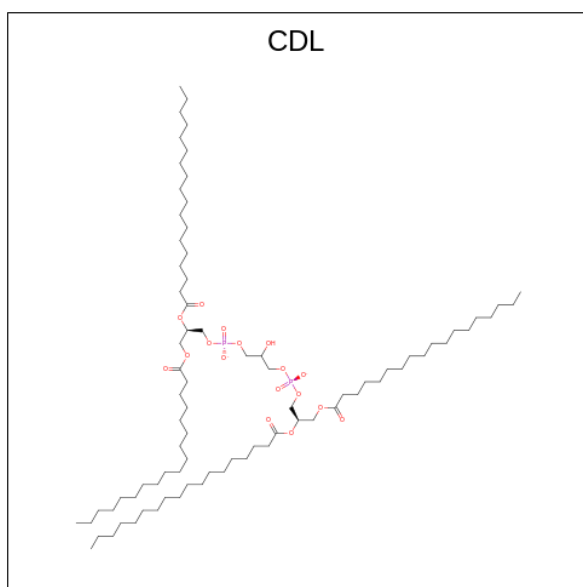
Mol	Chain	Residues	Atoms					AltConf
49	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 50 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



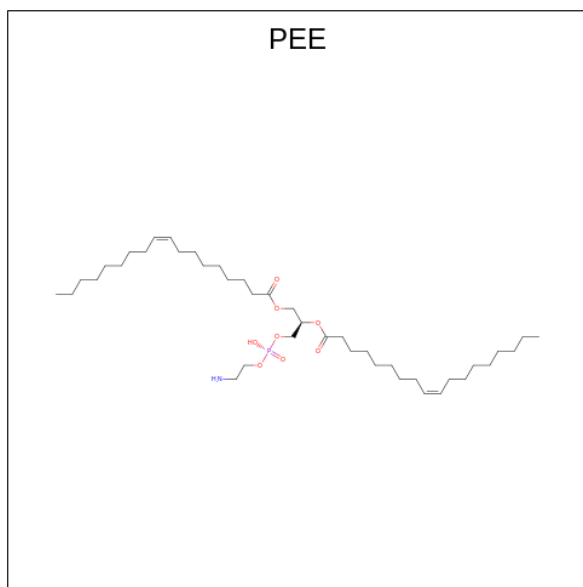
Mol	Chain	Residues	Atoms			AltConf
50	M	1	Total	Fe	S	0
			4	2	2	
50	O	1	Total	Fe	S	0
			4	2	2	

- Molecule 51 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
51	V	1	63	44	17	2	0
51	i	1	64	45	17	2	0
51	l	1	128	90	34	4	0
51	l	1	128	90	34	4	0
51	n	1	64	45	17	2	0

- Molecule 52 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).

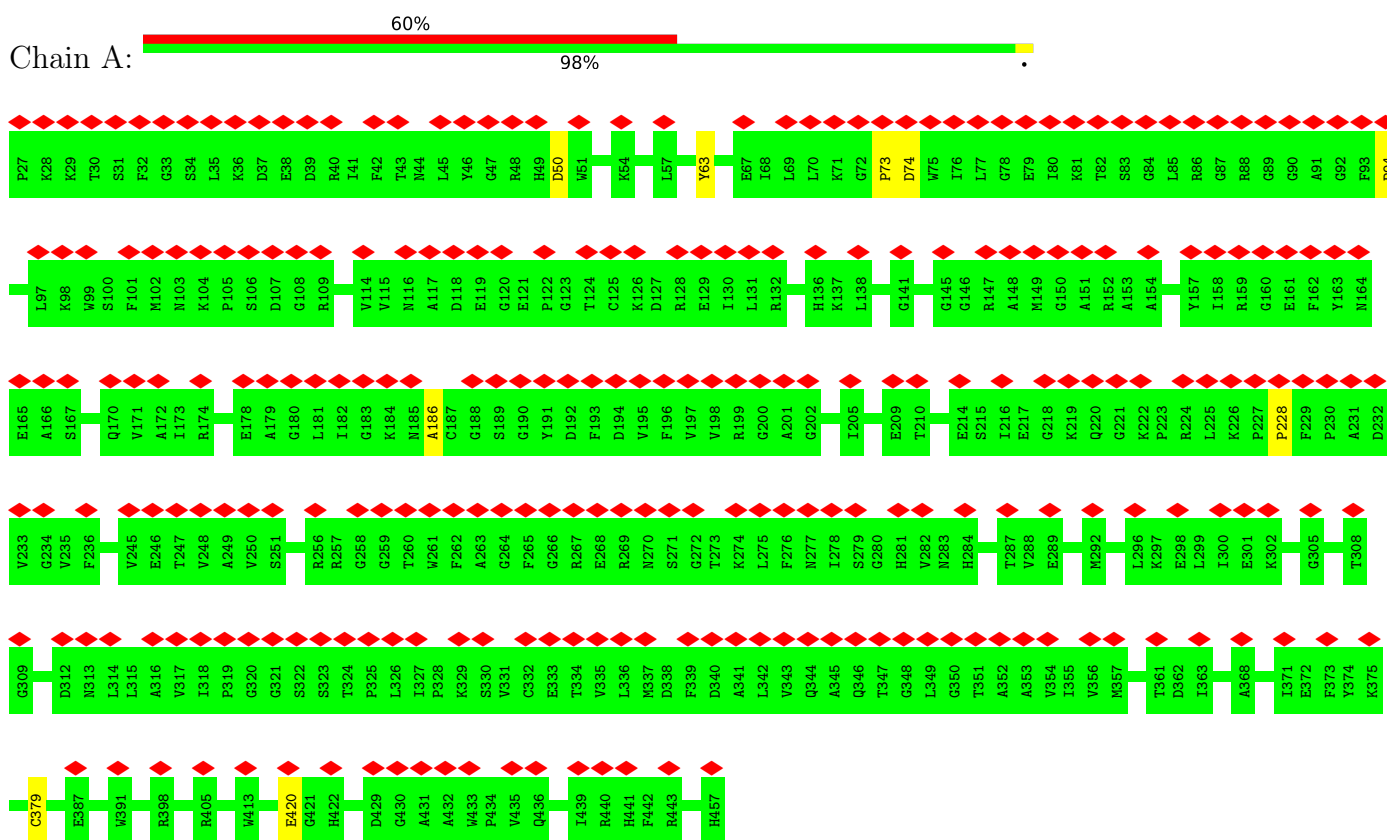


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
52	V	1	Total 51	41	1	8	1	0
52	W	1	Total 51	41	1	8	1	0
52	1	1	Total 100	80	2	16	2	0
52	1	1	Total 100	80	2	16	2	0

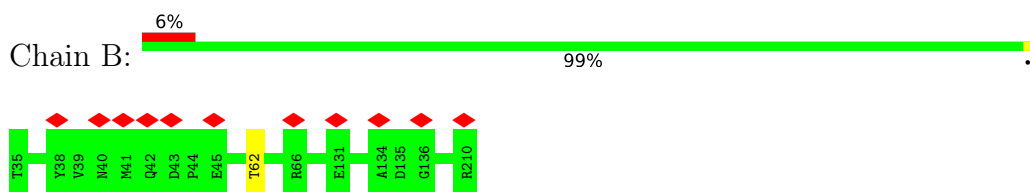
3 Residue-property plots

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 dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

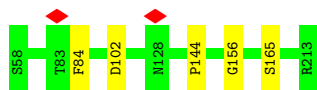


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

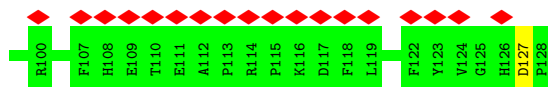
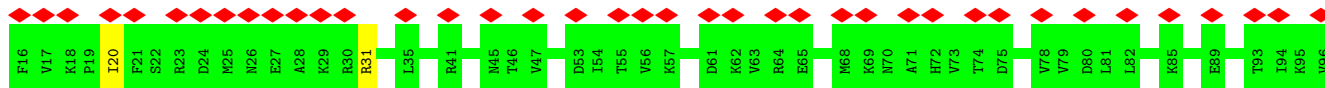


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

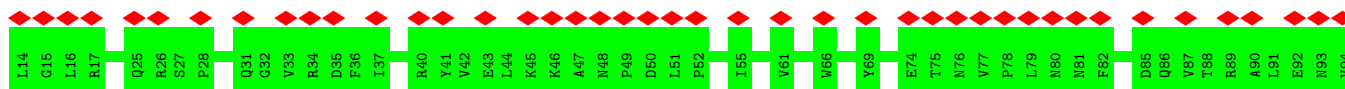




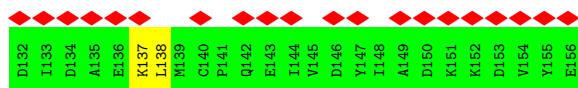
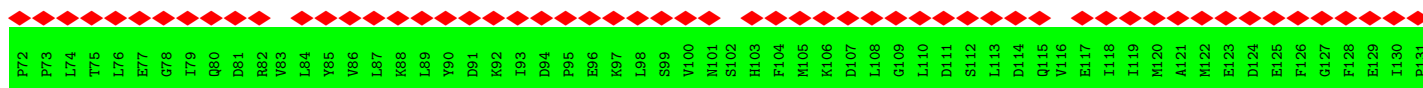
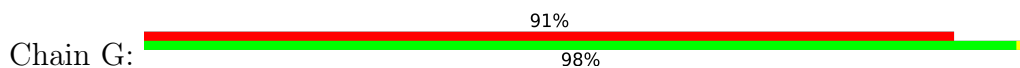
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 6: Acyl carrier protein, mitochondrial

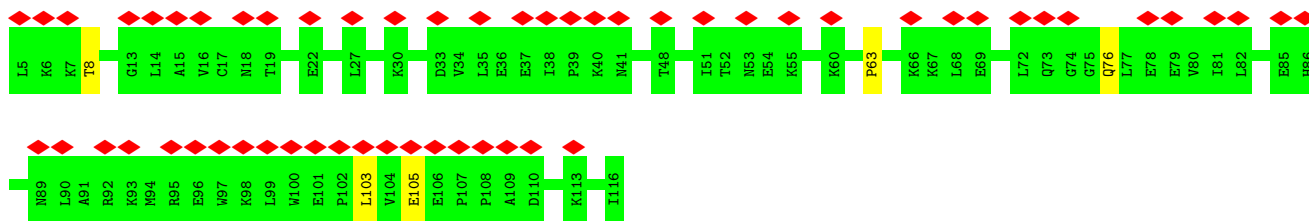


- Molecule 6: Acyl carrier protein, mitochondrial

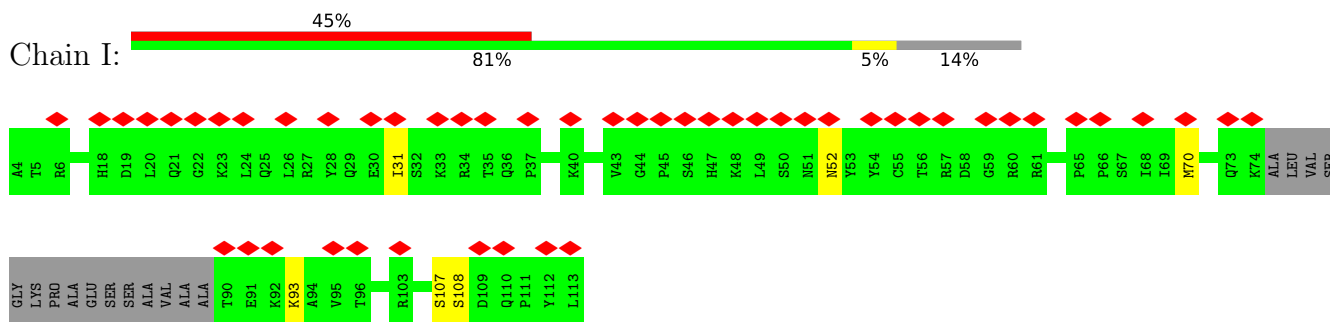


- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

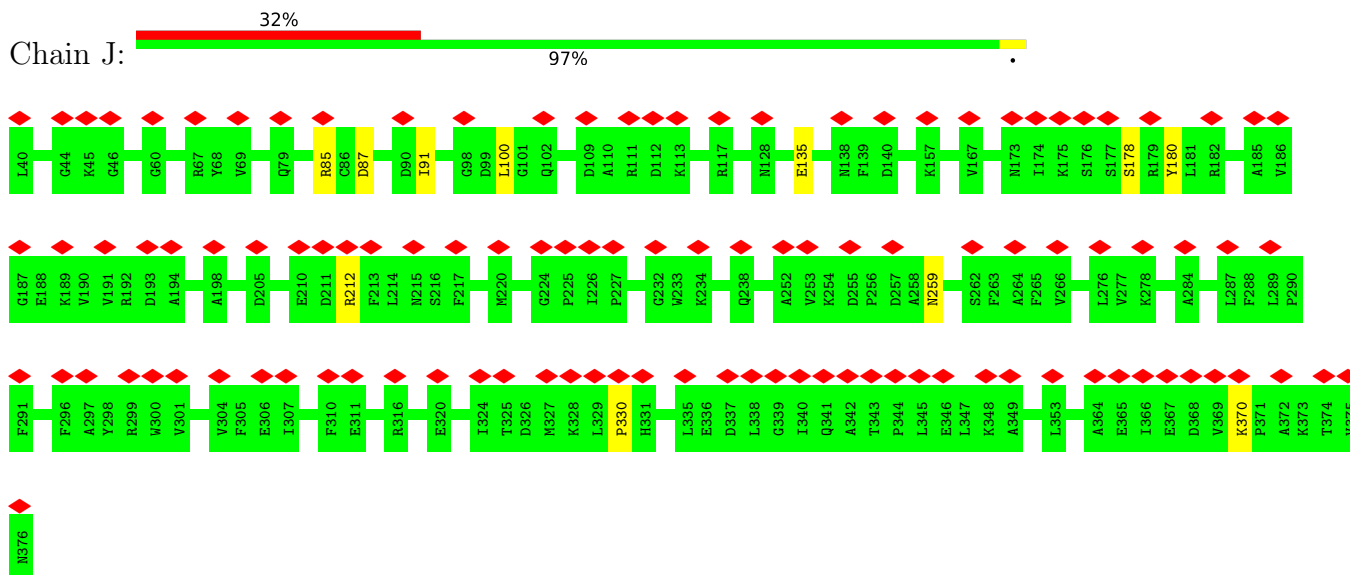




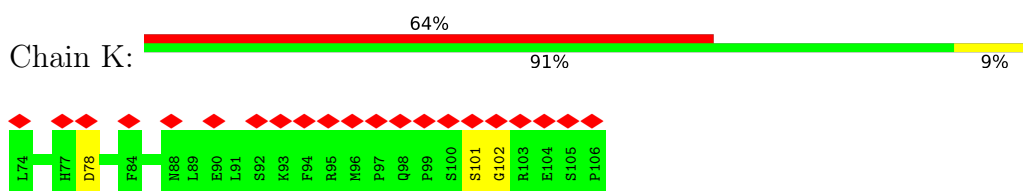
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



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

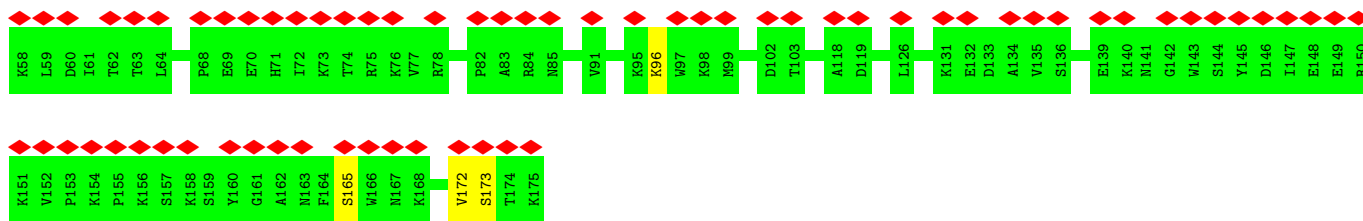


- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



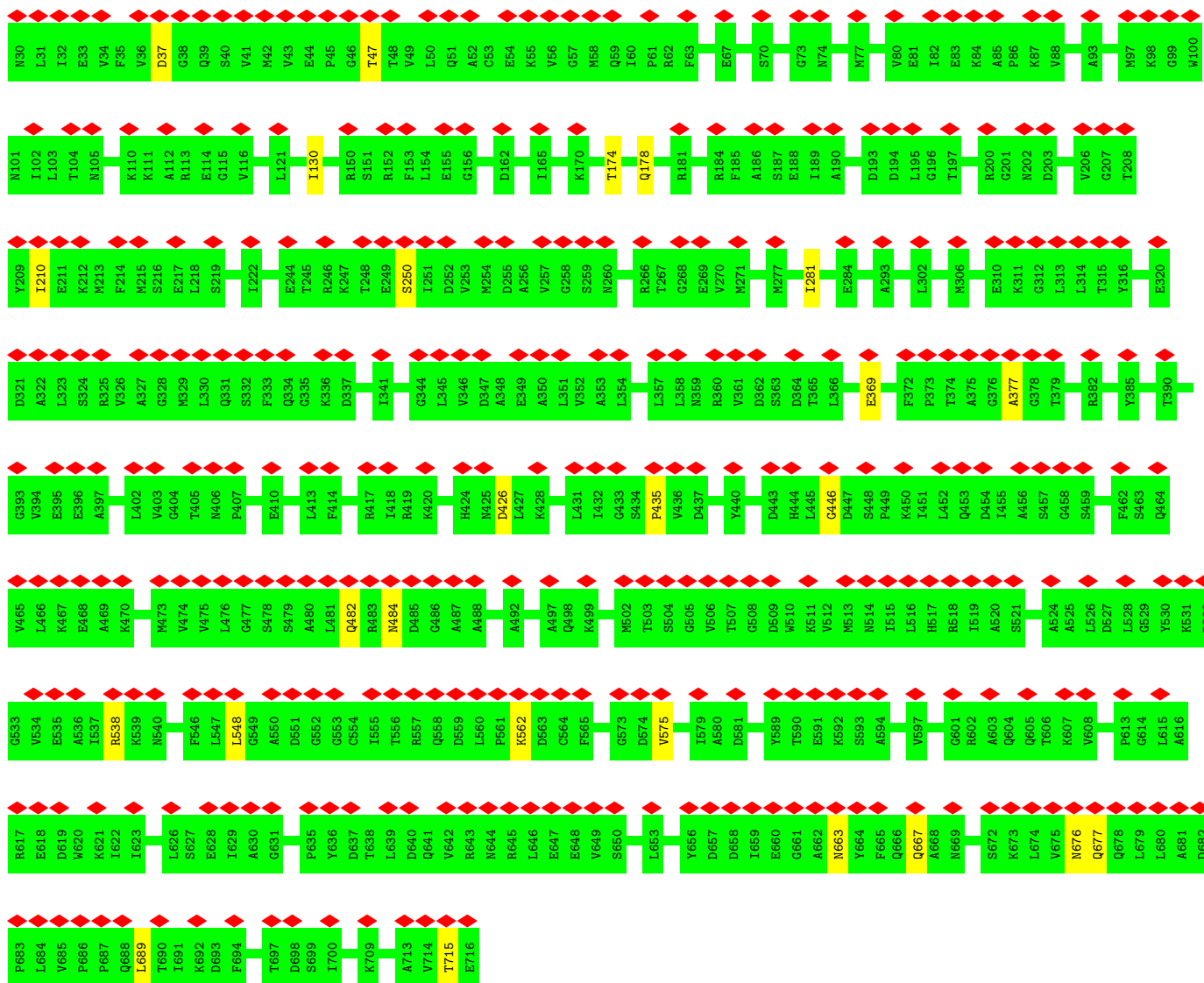
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial





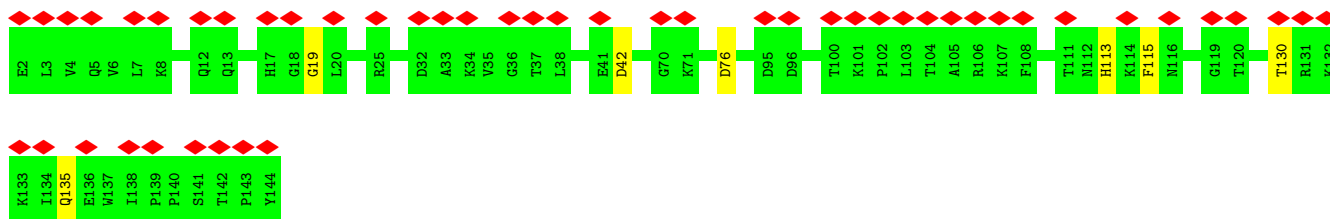
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain M: 52% 96%

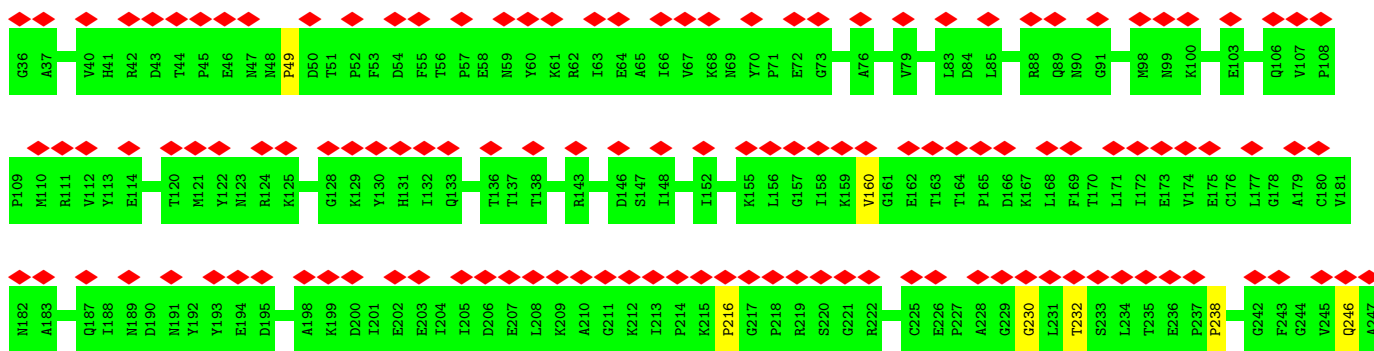


- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

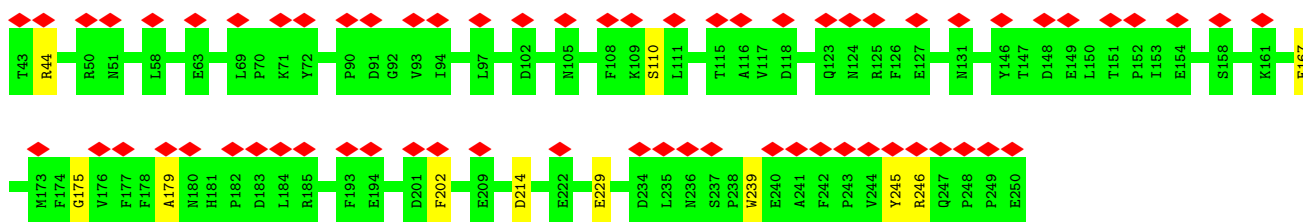
Chain N: 34% 95% 5%



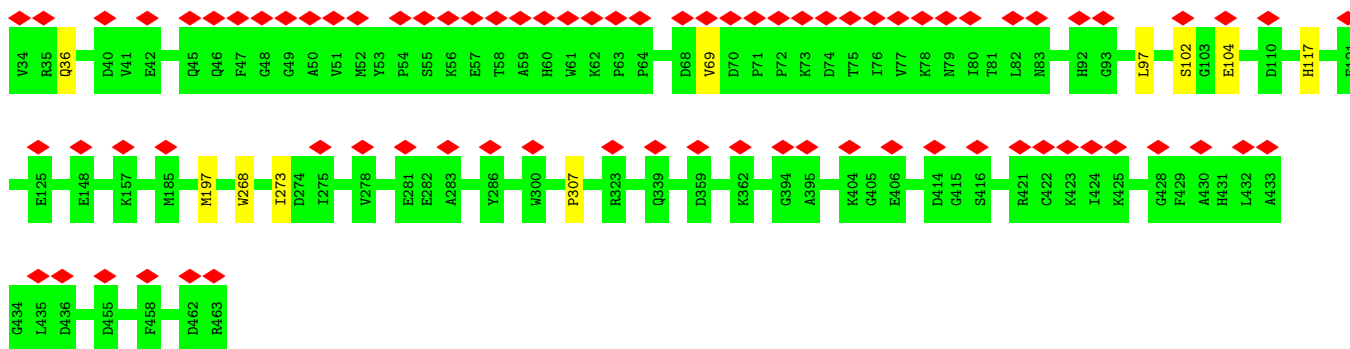
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



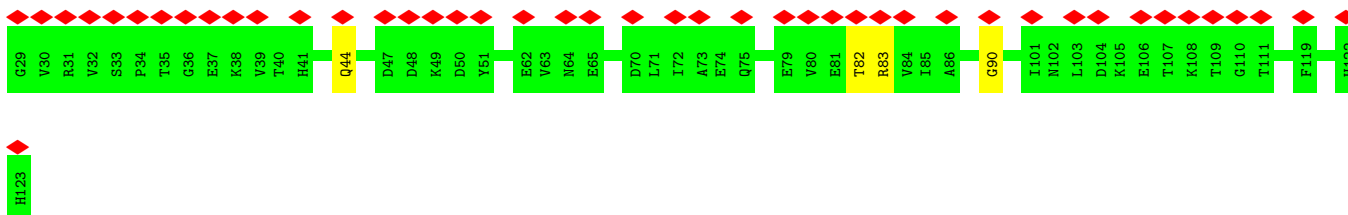
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S:  97%



- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T:  47% 96%



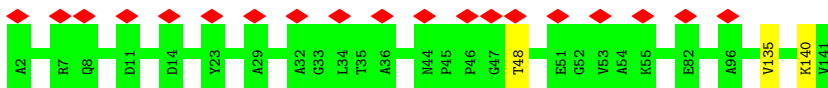
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:  99%



- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:  14% 98%




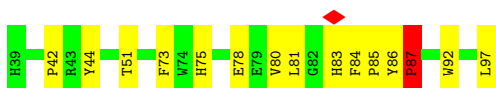
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:  97%



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y:  75% 24%



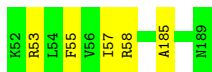
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z:  100%


There are no outlier residues recorded for this chain.

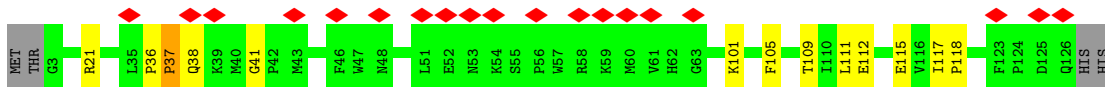
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:  96%



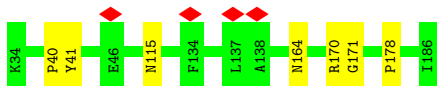
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain b:  15% 87% 9%



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c:  95% 5%



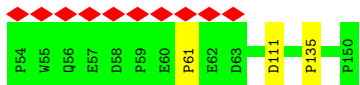
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d:  95% 5%



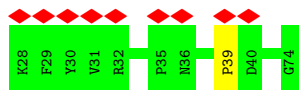
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e:  10% 97%



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f:  19% 98%



- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



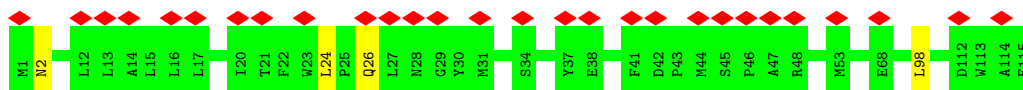
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



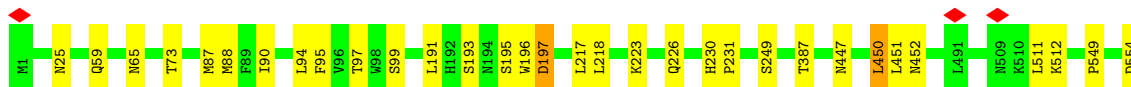
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

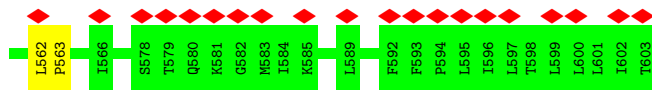


- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

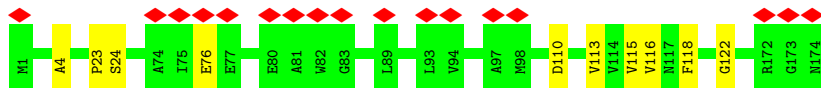
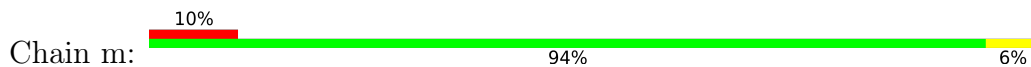


- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

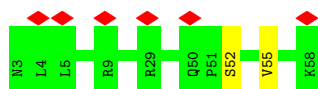




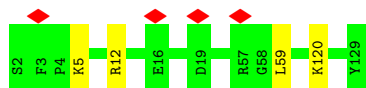
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6



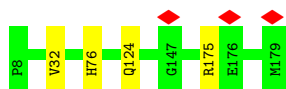
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

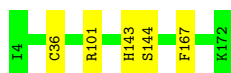


- Molecule 41: NADH-ubiquinone oxidoreductase chain 1




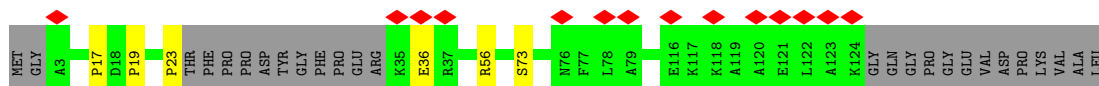
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:  97%



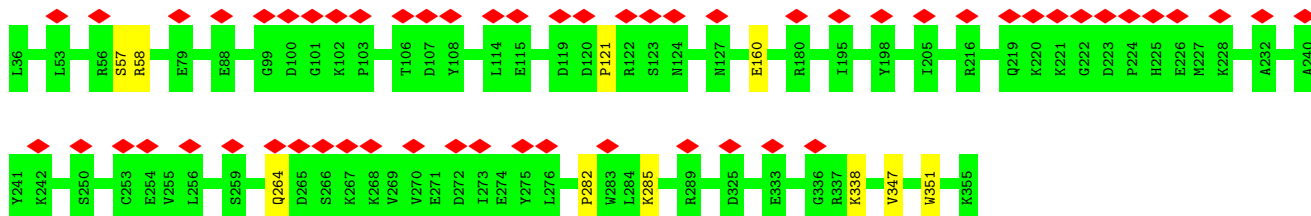
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v:  10% 77% 19%



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain w:  18% 97%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	167761	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 ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.325	Depositor
Minimum map value	-0.134	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0525	Depositor
Map size (\AA)	519.83997, 519.83997, 519.83997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.083, 1.083, 1.083	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: PLX, PEE, SF4, NDP, CDL, FES, 8Q1, FMN

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	0.30	0/3398	0.49	0/4590
2	B	0.50	0/1452	0.57	0/1964
3	C	0.58	0/1280	0.57	0/1732
4	E	0.34	0/993	0.54	0/1335
5	F	0.28	0/682	0.52	0/922
6	G	0.33	0/684	0.53	0/926
6	X	0.57	0/698	0.61	0/942
7	H	0.33	0/941	0.59	0/1275
8	I	0.29	0/788	0.54	0/1066
9	J	0.34	0/2785	0.52	0/3771
10	K	0.27	0/282	0.47	0/381
11	L	0.33	0/987	0.53	0/1331
12	M	0.32	0/5362	0.53	0/7266
13	N	0.37	0/1236	0.55	0/1681
14	O	0.29	0/1682	0.51	0/2289
15	P	0.38	0/1780	0.59	0/2424
16	Q	0.43	0/3552	0.59	1/4815 (0.0%)
17	S	0.60	0/583	0.64	0/785
18	T	0.31	0/755	0.47	0/1017
19	U	0.52	0/670	0.63	0/920
20	V	0.51	0/1065	0.61	0/1450
21	W	0.57	0/1166	0.66	0/1579
22	Y	0.52	0/559	0.73	3/763 (0.4%)
23	Z	0.45	0/669	0.53	0/899
24	a	0.68	0/1209	0.65	0/1639
25	b	0.59	1/1095 (0.1%)	0.69	4/1480 (0.3%)
26	c	0.58	0/1287	0.58	0/1761
27	d	0.63	0/1445	0.65	1/1945 (0.1%)
28	e	0.61	0/835	0.62	0/1134
29	f	0.48	0/418	0.58	0/566
30	g	0.64	0/1035	0.63	0/1398
31	h	0.62	0/884	0.65	0/1182

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.67	0/2808	0.77	2/3843 (0.1%)
33	j	0.55	0/945	0.69	1/1292 (0.1%)
34	k	0.68	1/751 (0.1%)	0.79	1/1019 (0.1%)
35	l	0.61	1/4840 (0.0%)	0.69	3/6611 (0.0%)
36	m	0.68	0/1346	0.67	0/1832
37	n	0.49	0/484	0.62	0/652
38	o	0.54	0/1093	0.61	0/1479
39	p	0.59	0/1549	0.59	0/2098
40	r	0.70	0/3723	0.76	2/5089 (0.0%)
41	s	0.62	0/2580	0.73	0/3539
42	u	0.57	0/1433	0.61	0/1937
43	v	0.48	0/934	0.67	3/1241 (0.2%)
44	w	0.44	0/2533	0.56	0/3440
All	All	0.51	3/67276 (0.0%)	0.62	21/91300 (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
44	w	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	118	PRO	N-CD	5.18	1.55	1.47
34	k	2	PRO	N-CD	5.14	1.55	1.47
35	l	231	PRO	N-CD	5.05	1.54	1.47

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	i	323	THR	C-N-CD	-7.37	104.38	120.60
22	Y	92	TRP	N-CA-C	-7.00	92.10	111.00
27	d	2	PRO	N-CA-CB	6.79	111.44	103.30
22	Y	87	PRO	CA-N-CD	-6.57	102.30	111.50
25	b	36	PRO	C-N-CD	6.22	141.46	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	w	338	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	A	429/431 (100%)	396 (92%)	24 (6%)	9 (2%)	7	38
2	B	174/176 (99%)	163 (94%)	10 (6%)	1 (1%)	25	62
3	C	154/156 (99%)	136 (88%)	13 (8%)	5 (3%)	4	31
4	E	111/113 (98%)	101 (91%)	8 (7%)	2 (2%)	8	41
5	F	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
6	G	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	6	35
6	X	83/85 (98%)	73 (88%)	6 (7%)	4 (5%)	2	22
7	H	110/112 (98%)	100 (91%)	5 (4%)	5 (4%)	2	23
8	I	91/110 (83%)	79 (87%)	6 (7%)	6 (7%)	1	16
9	J	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	7	38
10	K	31/33 (94%)	27 (87%)	1 (3%)	3 (10%)	0	8
11	L	116/118 (98%)	104 (90%)	8 (7%)	4 (3%)	3	30
12	M	685/687 (100%)	608 (89%)	54 (8%)	23 (3%)	3	30
13	N	141/143 (99%)	119 (84%)	15 (11%)	7 (5%)	2	22
14	O	210/212 (99%)	188 (90%)	15 (7%)	7 (3%)	4	31
15	P	206/208 (99%)	173 (84%)	22 (11%)	11 (5%)	2	21
16	Q	428/430 (100%)	397 (93%)	24 (6%)	7 (2%)	9	43
17	S	68/70 (97%)	61 (90%)	5 (7%)	2 (3%)	4	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	T	93/95 (98%)	87 (94%)	2 (2%)	4 (4%)	2	24
19	U	81/83 (98%)	76 (94%)	4 (5%)	1 (1%)	13	48
20	V	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	6	37
21	W	136/138 (99%)	127 (93%)	5 (4%)	4 (3%)	4	32
22	Y	57/59 (97%)	50 (88%)	1 (2%)	6 (10%)	0	6
23	Z	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
24	a	136/138 (99%)	121 (89%)	12 (9%)	3 (2%)	6	37
25	b	122/128 (95%)	107 (88%)	10 (8%)	5 (4%)	3	26
26	c	151/153 (99%)	129 (85%)	15 (10%)	7 (5%)	2	23
27	d	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	25	62
28	e	95/97 (98%)	83 (87%)	9 (10%)	3 (3%)	4	31
29	f	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	6	37
30	g	117/119 (98%)	105 (90%)	6 (5%)	6 (5%)	2	21
31	h	102/104 (98%)	86 (84%)	10 (10%)	6 (6%)	1	18
32	i	345/347 (99%)	324 (94%)	15 (4%)	6 (2%)	9	42
33	j	113/115 (98%)	103 (91%)	7 (6%)	3 (3%)	5	33
34	k	95/97 (98%)	88 (93%)	4 (4%)	3 (3%)	4	31
35	l	601/603 (100%)	551 (92%)	38 (6%)	12 (2%)	7	39
36	m	172/174 (99%)	150 (87%)	12 (7%)	10 (6%)	1	19
37	n	54/56 (96%)	50 (93%)	2 (4%)	2 (4%)	3	28
38	o	126/128 (98%)	113 (90%)	9 (7%)	4 (3%)	4	31
39	p	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	8	41
40	r	457/459 (100%)	420 (92%)	28 (6%)	9 (2%)	7	39
41	s	316/318 (99%)	286 (90%)	21 (7%)	9 (3%)	5	33
42	u	167/169 (99%)	152 (91%)	10 (6%)	5 (3%)	4	32
43	v	107/137 (78%)	90 (84%)	14 (13%)	3 (3%)	5	33
44	w	318/320 (99%)	281 (88%)	28 (9%)	9 (3%)	5	33
All	All	8097/8236 (98%)	7338 (91%)	526 (6%)	233 (3%)	7	32

5 of 233 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	TYR

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Mol	Chain	Res	Type
1	A	73	PRO
1	A	379	CYS
2	B	62	THR
12	M	37	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/346 (100%)	346 (100%)	0	100	100
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	106/106 (100%)	105 (99%)	1 (1%)	78	88
5	F	74/74 (100%)	74 (100%)	0	100	100
6	G	74/79 (94%)	74 (100%)	0	100	100
6	X	78/79 (99%)	78 (100%)	0	100	100
7	H	100/100 (100%)	100 (100%)	0	100	100
8	I	87/96 (91%)	87 (100%)	0	100	100
9	J	292/292 (100%)	288 (99%)	4 (1%)	67	82
10	K	32/32 (100%)	32 (100%)	0	100	100
11	L	107/107 (100%)	107 (100%)	0	100	100
12	M	576/577 (100%)	574 (100%)	2 (0%)	92	96
13	N	129/129 (100%)	129 (100%)	0	100	100
14	O	181/181 (100%)	181 (100%)	0	100	100
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	371/371 (100%)	369 (100%)	2 (0%)	88	94
17	S	59/59 (100%)	59 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	72/72 (100%)	72 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	V	102/102 (100%)	102 (100%)	0	100	100
21	W	119/119 (100%)	119 (100%)	0	100	100
22	Y	57/57 (100%)	49 (86%)	8 (14%)	3	20
23	Z	62/63 (98%)	62 (100%)	0	100	100
24	a	124/124 (100%)	122 (98%)	2 (2%)	62	80
25	b	118/122 (97%)	114 (97%)	4 (3%)	37	64
26	c	124/137 (90%)	124 (100%)	0	100	100
27	d	145/154 (94%)	137 (94%)	8 (6%)	21	53
28	e	90/90 (100%)	90 (100%)	0	100	100
29	f	43/43 (100%)	43 (100%)	0	100	100
30	g	105/105 (100%)	105 (100%)	0	100	100
31	h	90/90 (100%)	90 (100%)	0	100	100
32	i	314/314 (100%)	314 (100%)	0	100	100
33	j	102/103 (99%)	102 (100%)	0	100	100
34	k	85/85 (100%)	82 (96%)	3 (4%)	36	63
35	l	531/532 (100%)	511 (96%)	20 (4%)	33	61
36	m	137/137 (100%)	137 (100%)	0	100	100
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	114/114 (100%)	114 (100%)	0	100	100
39	p	157/157 (100%)	156 (99%)	1 (1%)	86	93
40	r	416/416 (100%)	416 (100%)	0	100	100
41	s	278/278 (100%)	278 (100%)	0	100	100
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	89/121 (74%)	89 (100%)	0	100	100
44	w	249/288 (86%)	249 (100%)	0	100	100
All	All	7093/7209 (98%)	7038 (99%)	55 (1%)	82	89

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	d	113	GLN
35	l	59	GLN
39	p	124	GLN

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Mol	Chain	Res	Type
35	l	223	LYS
27	d	115	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 142 such sidechains are listed below:

Mol	Chain	Res	Type
38	o	62	ASN
40	r	168	HIS
42	u	99	HIS
16	Q	38	GLN
15	P	247	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

30 ligands 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	$\# Z > 2$
52	PEE	l	702	-	50,50,50	1.16	6 (12%)	53,55,55	0.99	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	SF4	M	802	12	0,12,12	-	-	-		
47	PLX	g	203	-	51,51,51	0.78	1 (1%)	55,59,59	0.58	1 (1%)
52	PEE	V	202	-	50,50,50	1.16	6 (12%)	53,55,55	0.91	2 (3%)
45	SF4	B	302	2	0,12,12	-	-	-		
51	CDL	i	401	-	63,63,99	1.21	5 (7%)	69,75,111	1.04	5 (7%)
48	8Q1	E	201	-	31,34,34	1.64	6 (19%)	40,43,43	1.39	7 (17%)
47	PLX	r	501	-	51,51,51	0.74	1 (1%)	55,59,59	0.65	1 (1%)
51	CDL	V	201	-	61,61,99	1.21	5 (8%)	64,71,111	0.94	3 (4%)
46	FMN	A	502	-	33,33,33	1.40	6 (18%)	48,50,50	1.34	8 (16%)
45	SF4	B	301	2	0,12,12	-	-	-		
49	NDP	J	401	-	45,52,52	0.95	2 (4%)	53,80,80	1.32	4 (7%)
47	PLX	V	203	-	51,51,51	0.78	1 (1%)	55,59,59	0.59	1 (1%)
48	8Q1	p	201	-	31,34,34	1.67	5 (16%)	40,43,43	1.57	5 (12%)
47	PLX	B	303	-	51,51,51	0.77	1 (1%)	55,59,59	0.68	1 (1%)
50	FES	O	301	14	0,4,4	-	-	-		
45	SF4	A	501	1	0,12,12	-	-	-		
51	CDL	n	101	-	63,63,99	1.24	5 (7%)	69,75,111	1.07	4 (5%)
47	PLX	g	202	-	51,51,51	0.75	1 (1%)	55,59,59	0.61	1 (1%)
51	CDL	l	704	-	63,63,99	1.26	5 (7%)	69,75,111	1.01	4 (5%)
52	PEE	l	701	-	48,48,50	1.34	4 (8%)	51,53,55	0.96	2 (3%)
47	PLX	g	201	-	51,51,51	0.82	1 (1%)	55,59,59	0.69	1 (1%)
47	PLX	r	502	-	51,51,51	0.64	0	55,59,59	0.67	1 (1%)
45	SF4	M	801	12	0,12,12	-	-	-		
47	PLX	b	201	-	51,51,51	0.57	0	55,59,59	0.64	0
51	CDL	l	703	-	63,63,99	1.21	5 (7%)	69,75,111	1.07	4 (5%)
52	PEE	W	201	-	50,50,50	1.14	6 (12%)	53,55,55	0.97	2 (3%)
50	FES	M	803	-	0,4,4	-	-	-		
47	PLX	U	101	-	51,51,51	0.74	1 (1%)	55,59,59	0.72	2 (3%)
45	SF4	C	301	3	0,12,12	-	-	-		

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
52	PEE	l	702	-	-	27/54/54/54	-
45	SF4	M	802	12	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	PLX	g	203	-	-	24/55/55/55	-
52	PEE	V	202	-	-	27/54/54/54	-
45	SF4	B	302	2	-	-	0/6/5/5
51	CDL	i	401	-	-	39/74/74/110	-
48	8Q1	E	201	-	-	18/41/41/41	-
47	PLX	r	501	-	-	28/55/55/55	-
51	CDL	V	201	-	-	42/69/69/110	-
46	FMN	A	502	-	-	7/18/18/18	0/3/3/3
45	SF4	B	301	2	-	-	0/6/5/5
49	NDP	J	401	-	-	15/30/77/77	0/5/5/5
47	PLX	V	203	-	-	26/55/55/55	-
48	8Q1	p	201	-	-	19/41/41/41	-
47	PLX	B	303	-	-	21/55/55/55	-
50	FES	O	301	14	-	-	0/1/1/1
45	SF4	A	501	1	-	-	0/6/5/5
51	CDL	n	101	-	-	33/74/74/110	-
47	PLX	g	202	-	-	25/55/55/55	-
51	CDL	l	704	-	-	44/74/74/110	-
52	PEE	l	701	-	-	32/52/52/54	-
47	PLX	g	201	-	-	25/55/55/55	-
47	PLX	r	502	-	-	36/55/55/55	-
47	PLX	b	201	-	-	27/55/55/55	-
51	CDL	l	703	-	-	38/74/74/110	-
45	SF4	M	801	12	-	-	0/6/5/5
52	PEE	W	201	-	-	32/54/54/54	-
50	FES	M	803	-	-	-	0/1/1/1
47	PLX	U	101	-	-	22/55/55/55	-
45	SF4	C	301	3	-	-	0/6/5/5

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	p	201	8Q1	C34-N36	5.30	1.45	1.33
48	E	201	8Q1	C34-N36	5.24	1.45	1.33
48	p	201	8Q1	C39-N41	5.24	1.45	1.33
48	E	201	8Q1	C39-N41	4.93	1.44	1.33
46	A	502	FMN	C9A-C5A	4.42	1.48	1.41

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	p	201	8Q1	C6-C1-S44	6.03	120.47	113.46
49	J	401	NDP	PN-O3-PA	-5.21	114.94	132.83
48	E	201	8Q1	C6-C1-S44	4.56	118.77	113.46
52	l	702	PEE	O2-C10-C11	4.38	120.95	111.50
51	l	703	CDL	OA6-CA5-C11	4.16	120.48	111.50

There are no chirality outliers.

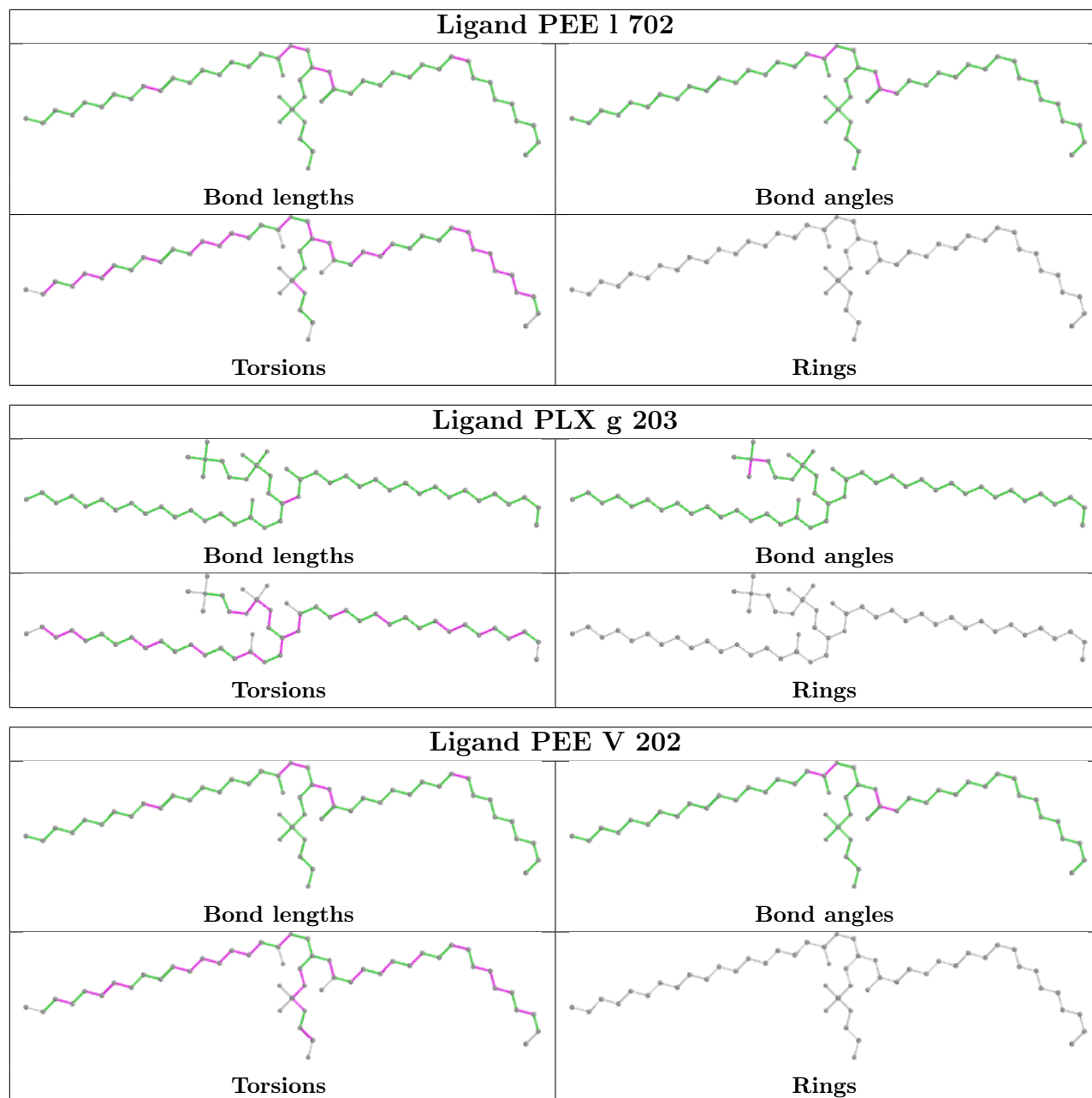
5 of 607 torsion outliers are listed below:

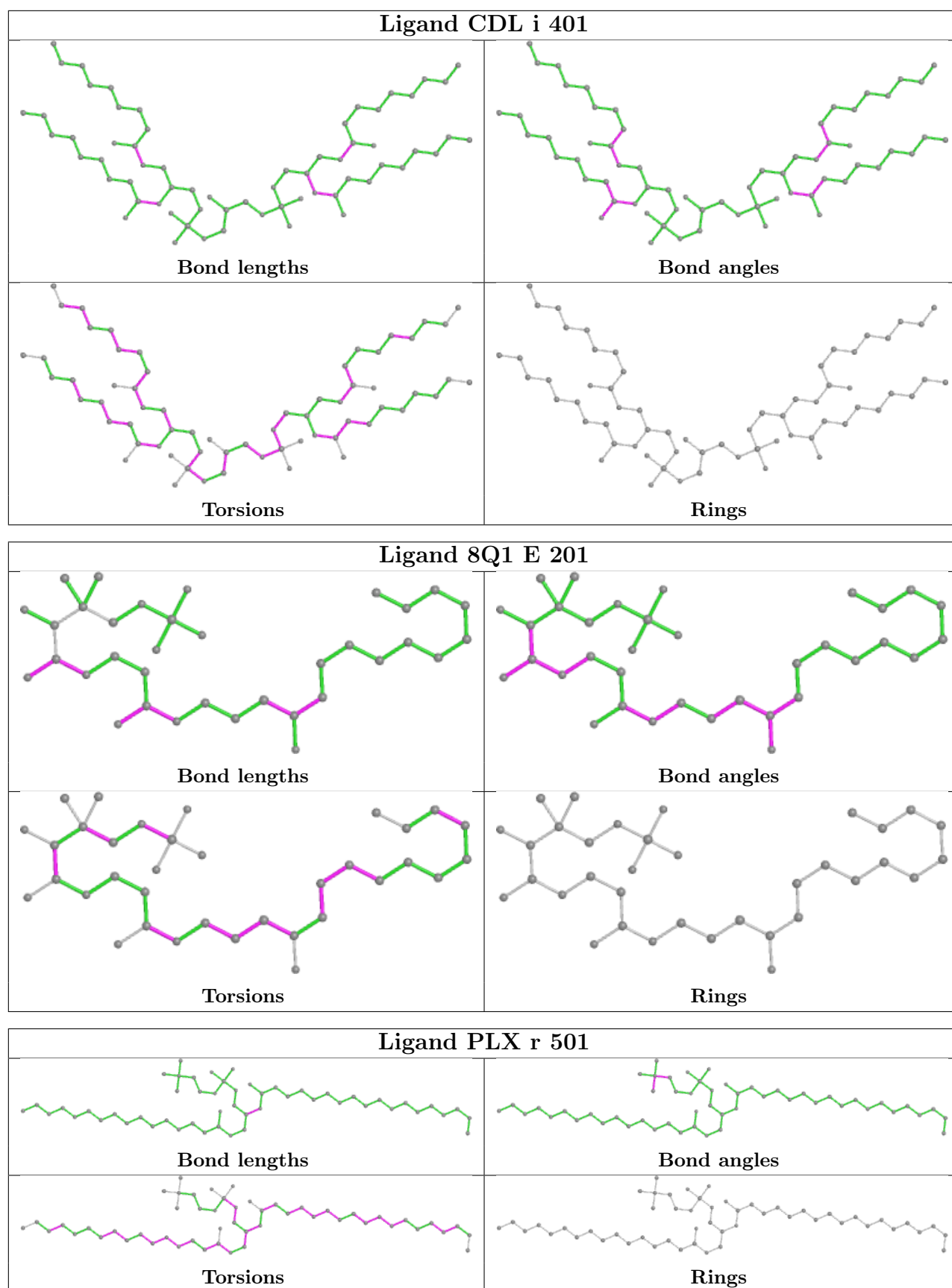
Mol	Chain	Res	Type	Atoms
46	A	502	FMN	C1'-C2'-C3'-O3'
46	A	502	FMN	C1'-C2'-C3'-C4'
46	A	502	FMN	C3'-C4'-C5'-O5'
46	A	502	FMN	O4'-C4'-C5'-O5'
47	B	303	PLX	C2-O1-P1-O2

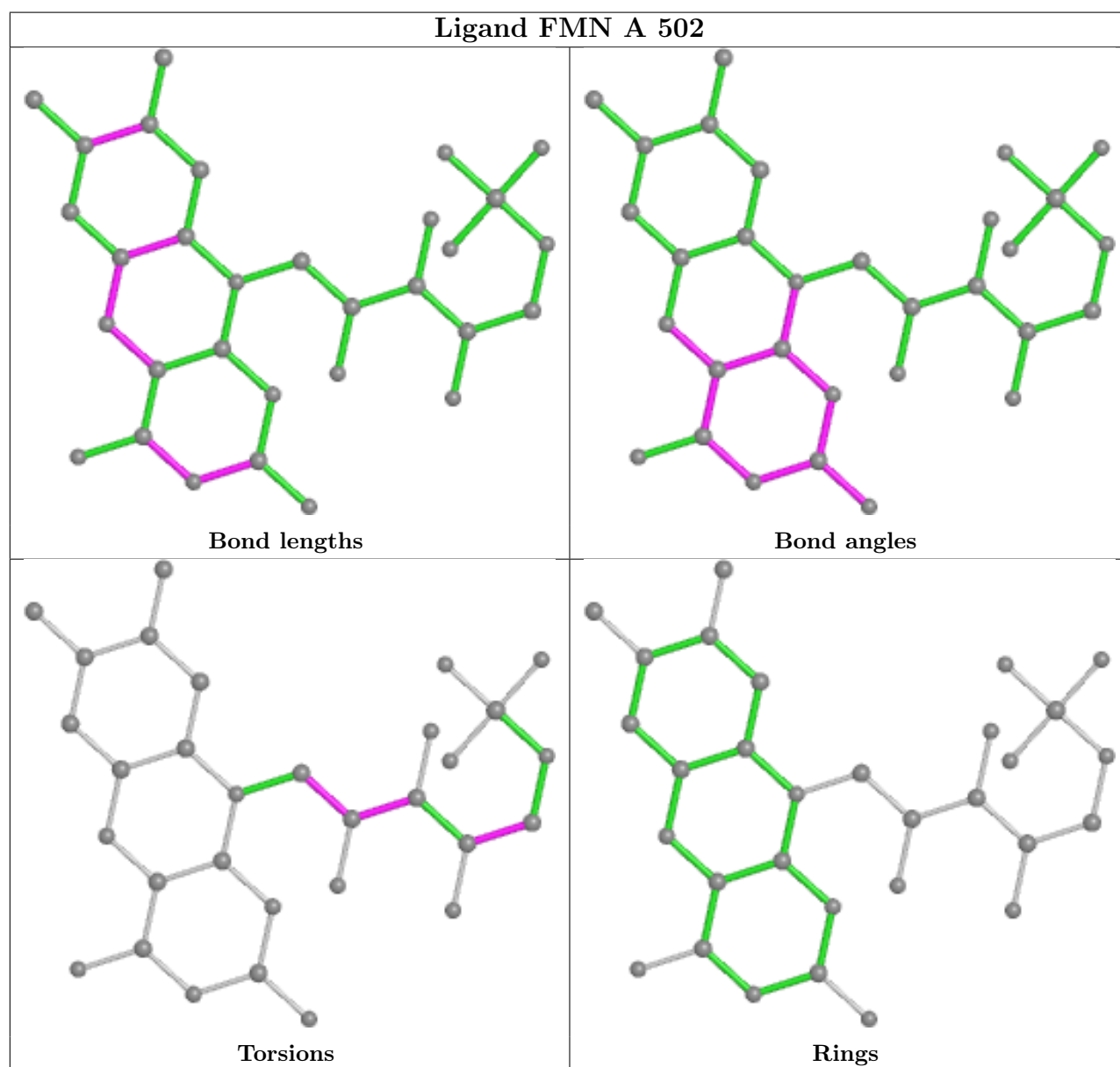
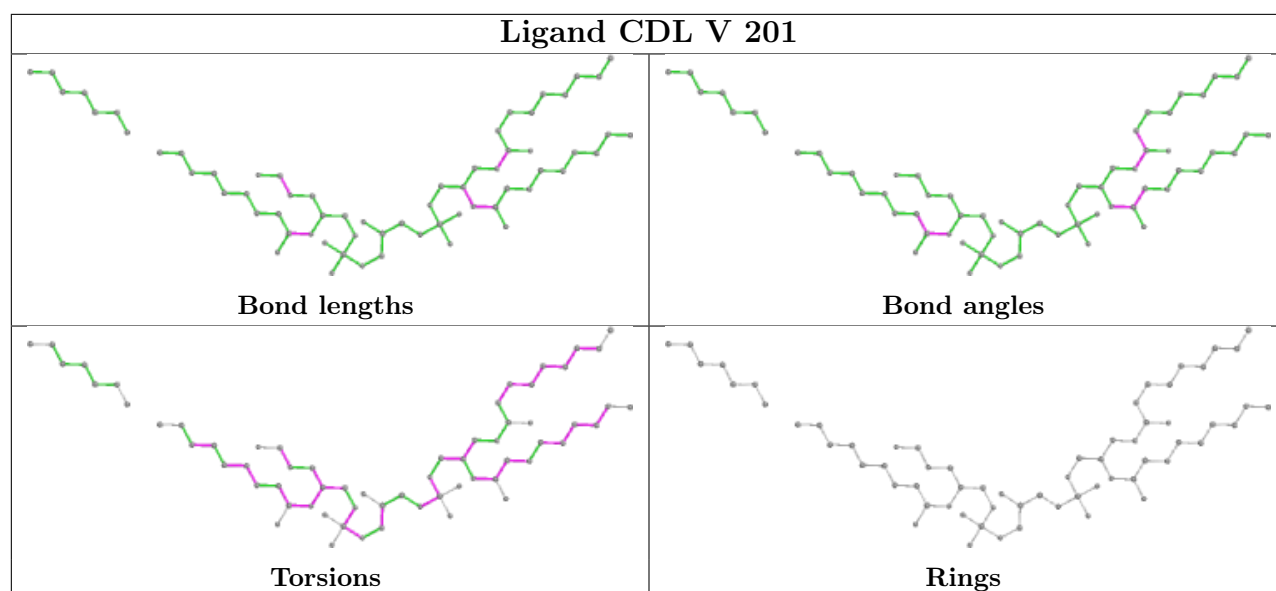
There are no ring outliers.

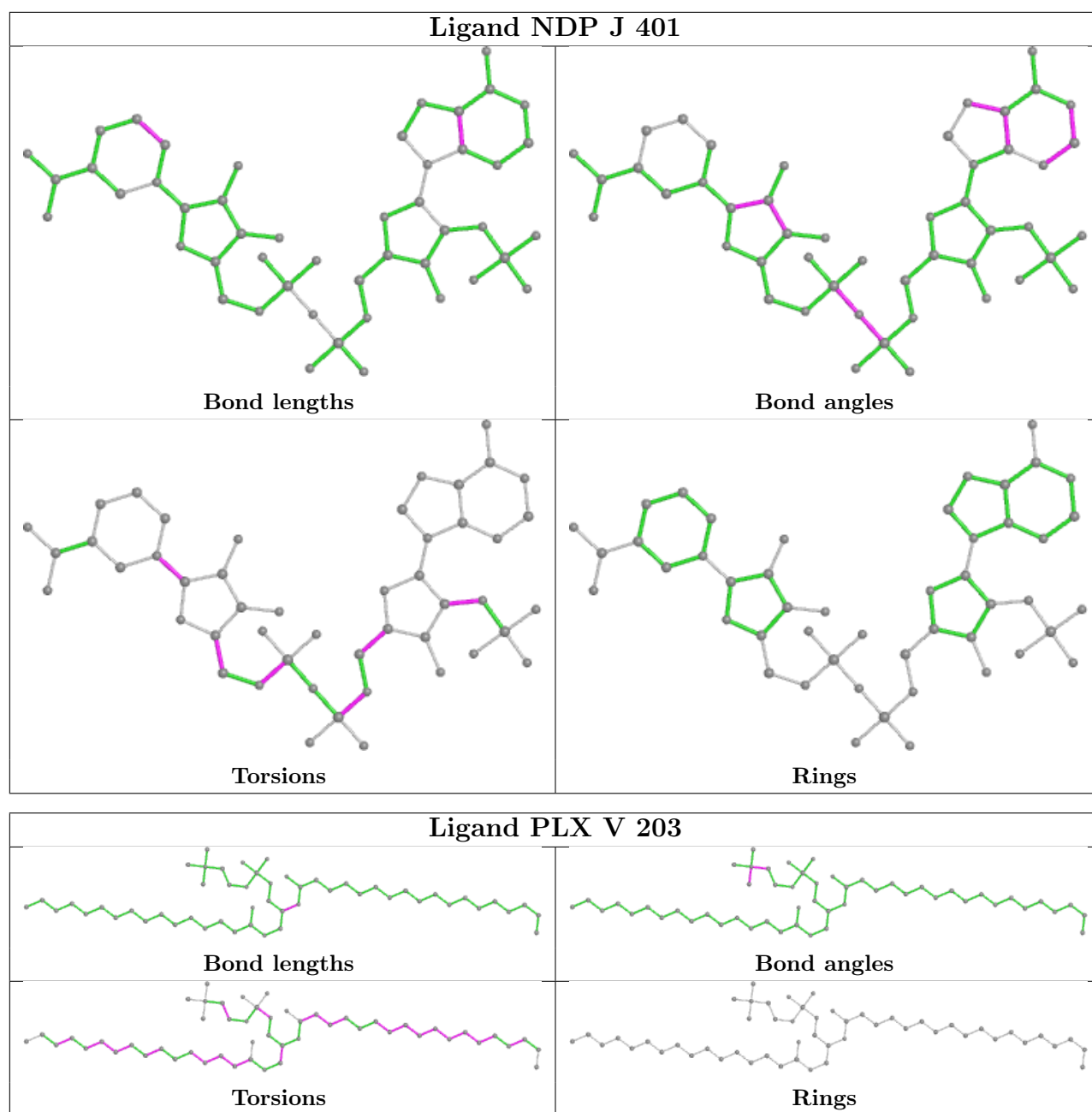
No monomer is involved in short contacts.

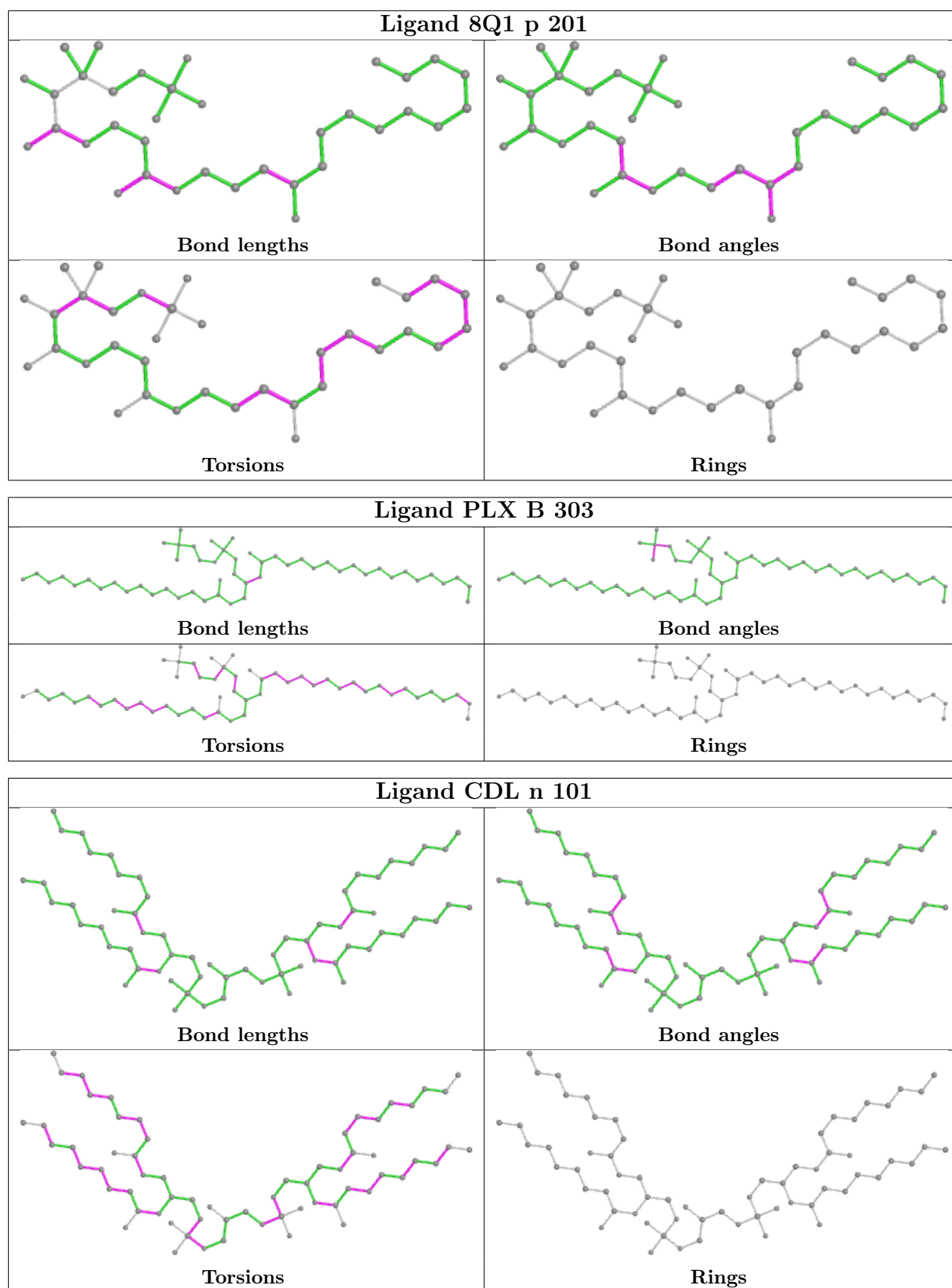
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

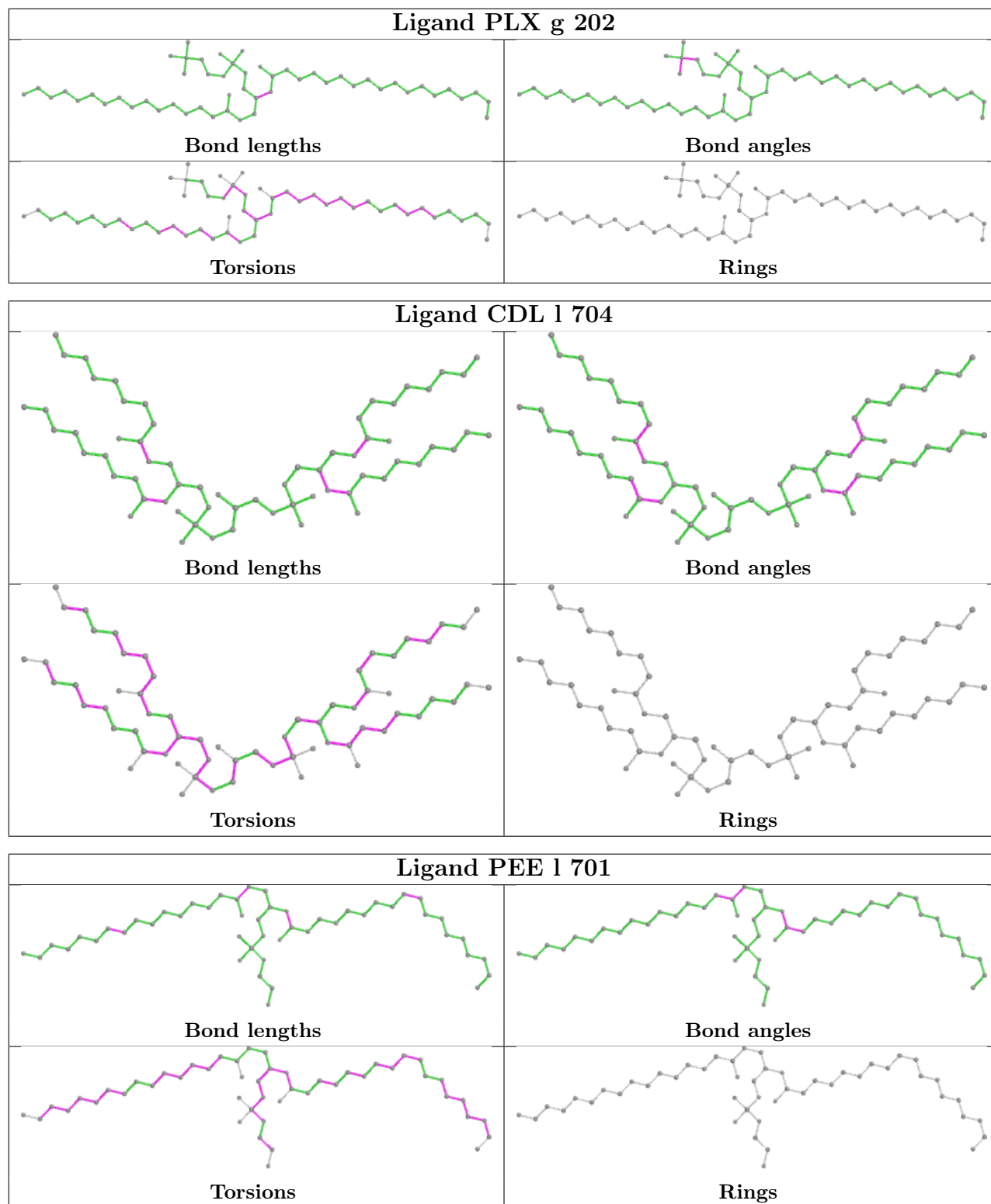


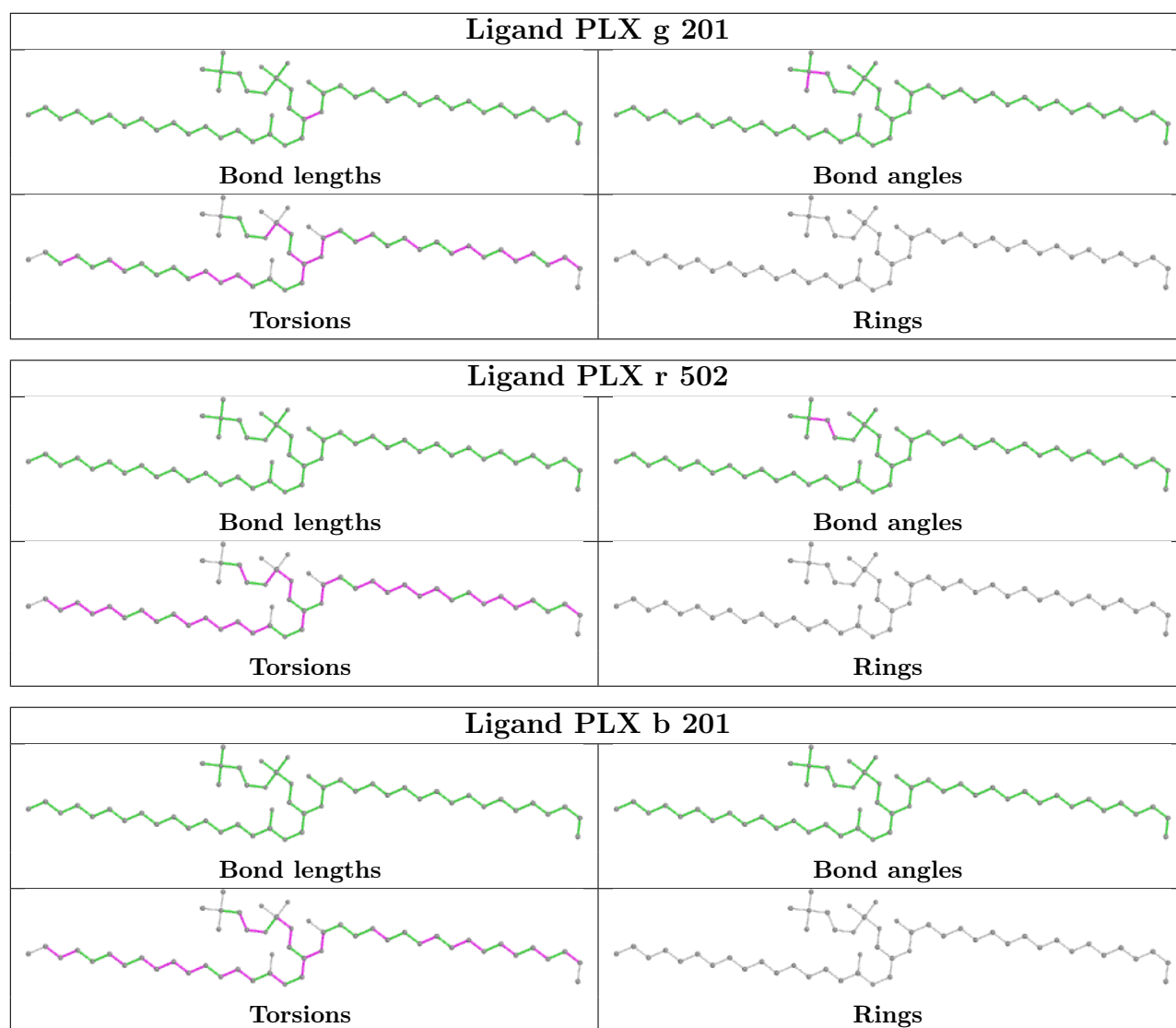


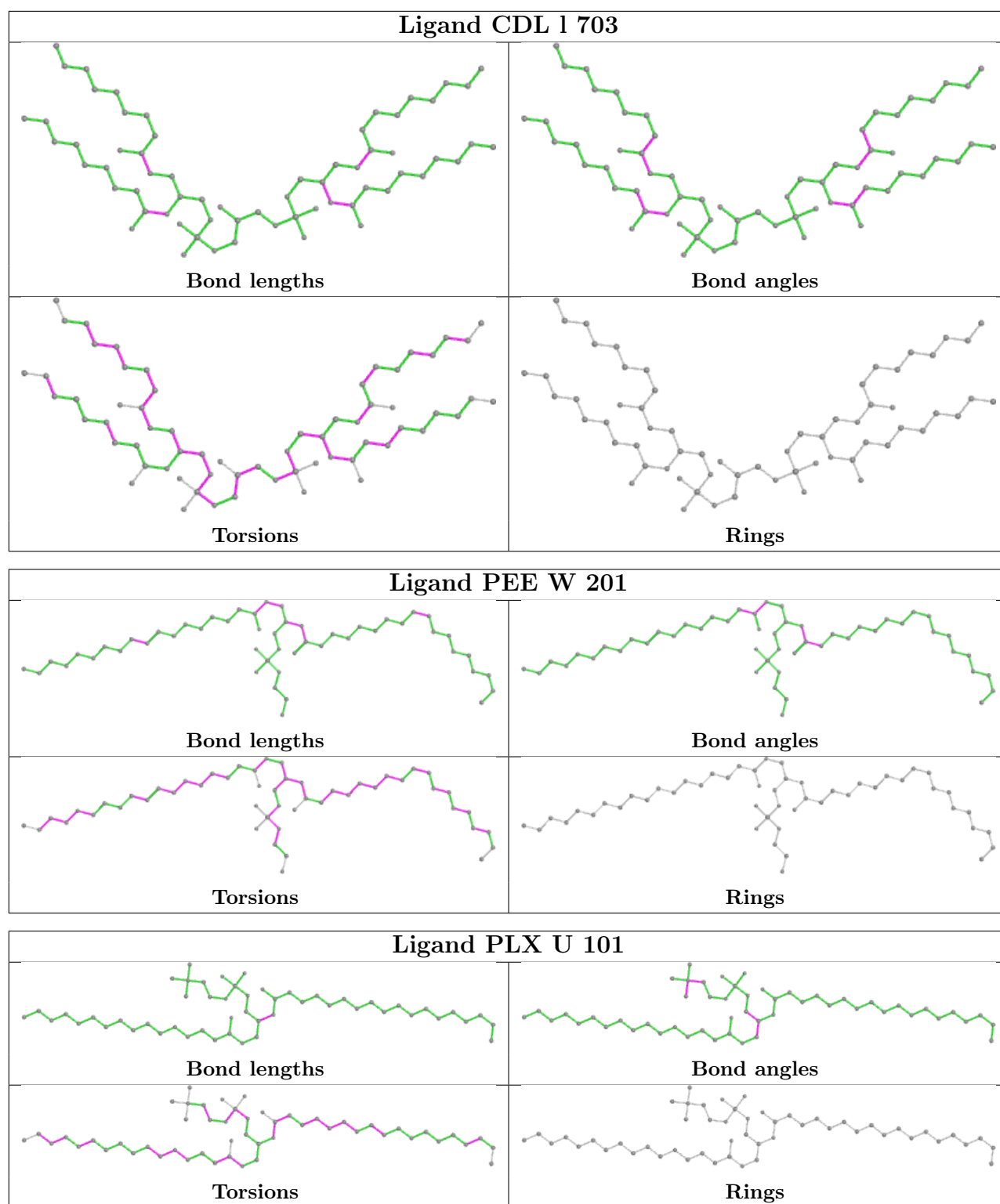












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

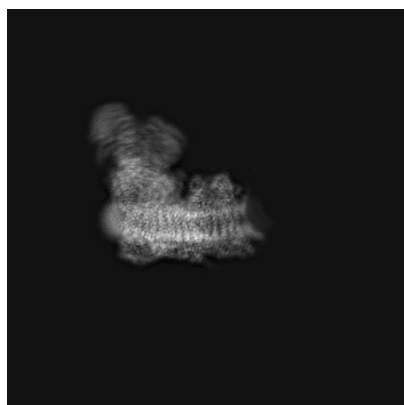
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6773. These allow visual inspection of the internal detail of the map and identification of artifacts.

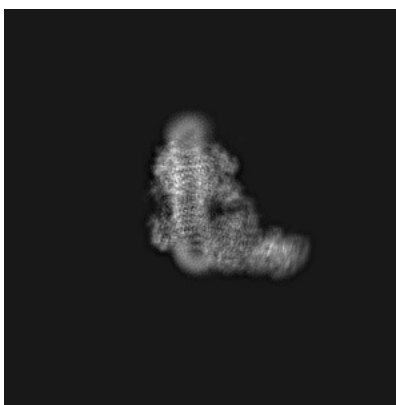
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

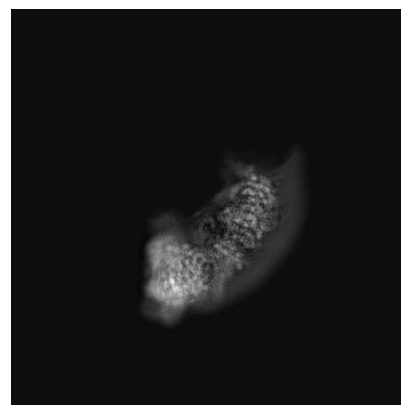
6.1.1 Primary map



X



Y



Z

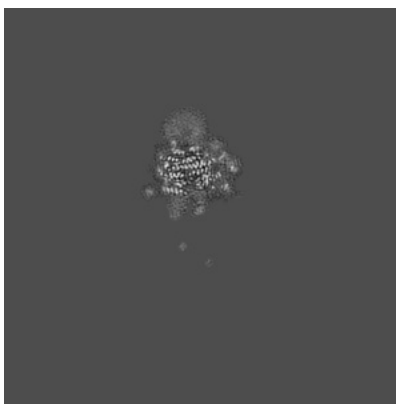
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

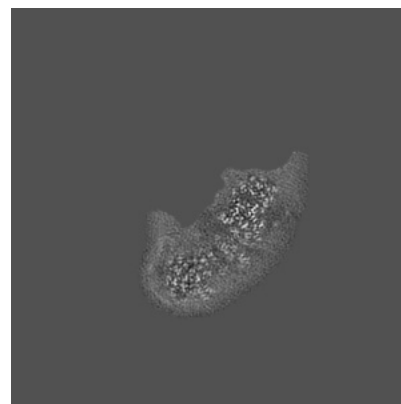
6.2.1 Primary map



X Index: 240



Y Index: 240

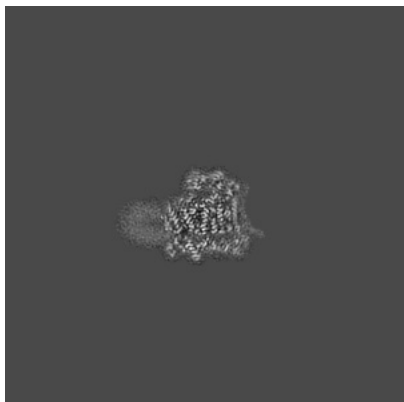


Z Index: 240

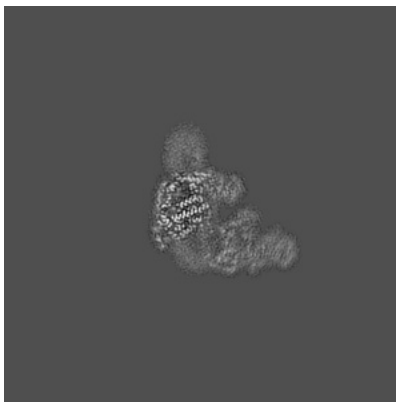
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

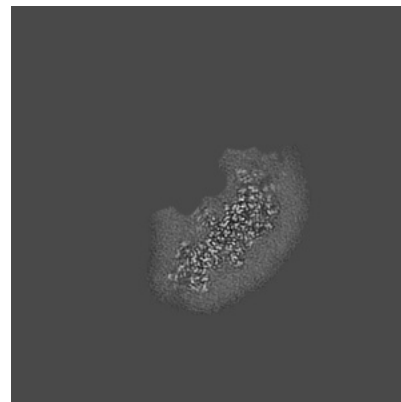
6.3.1 Primary map



X Index: 290



Y Index: 183



Z Index: 208

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 0.0525. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

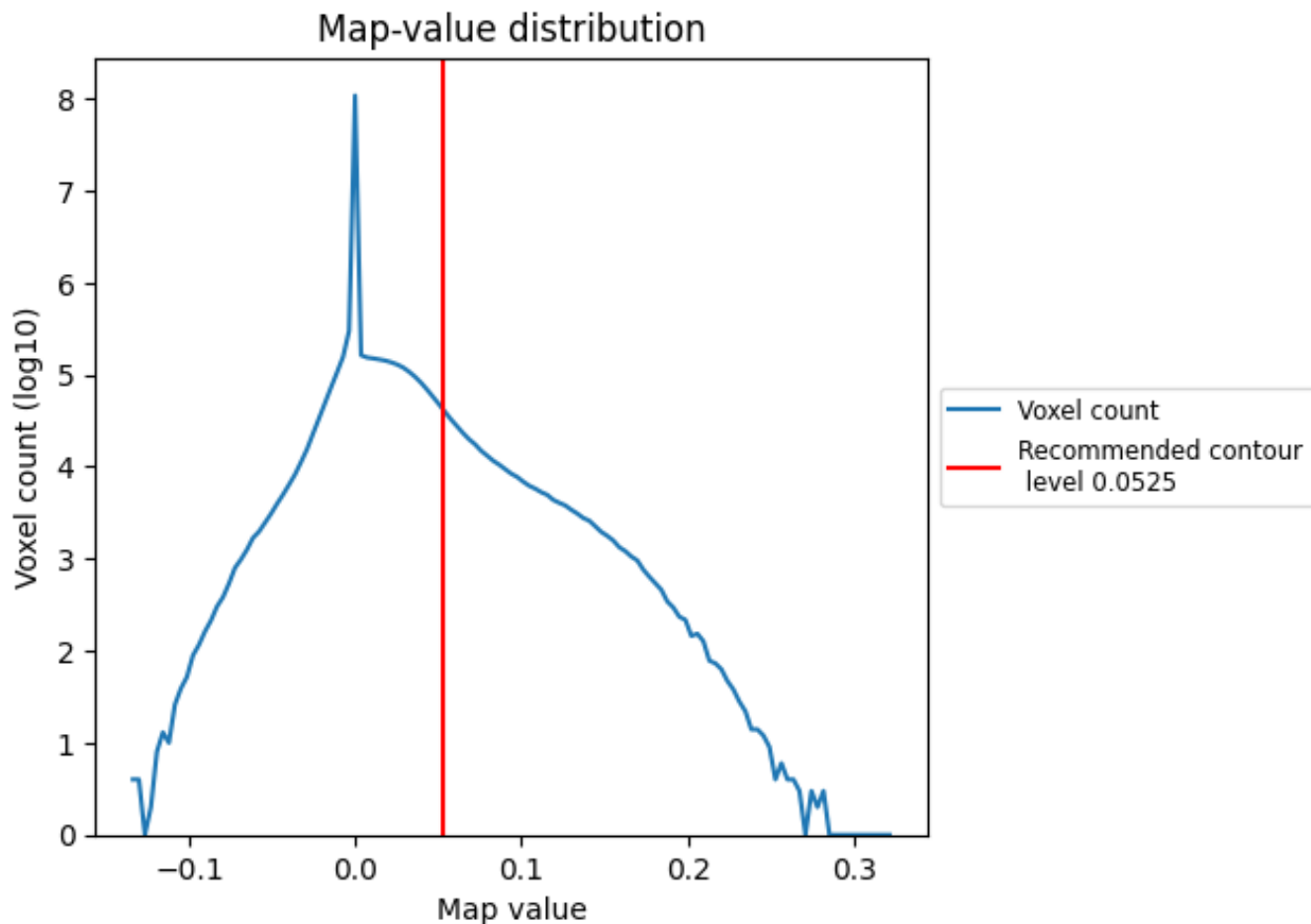
6.5 Mask visualisation

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

7 Map analysis [i](#)

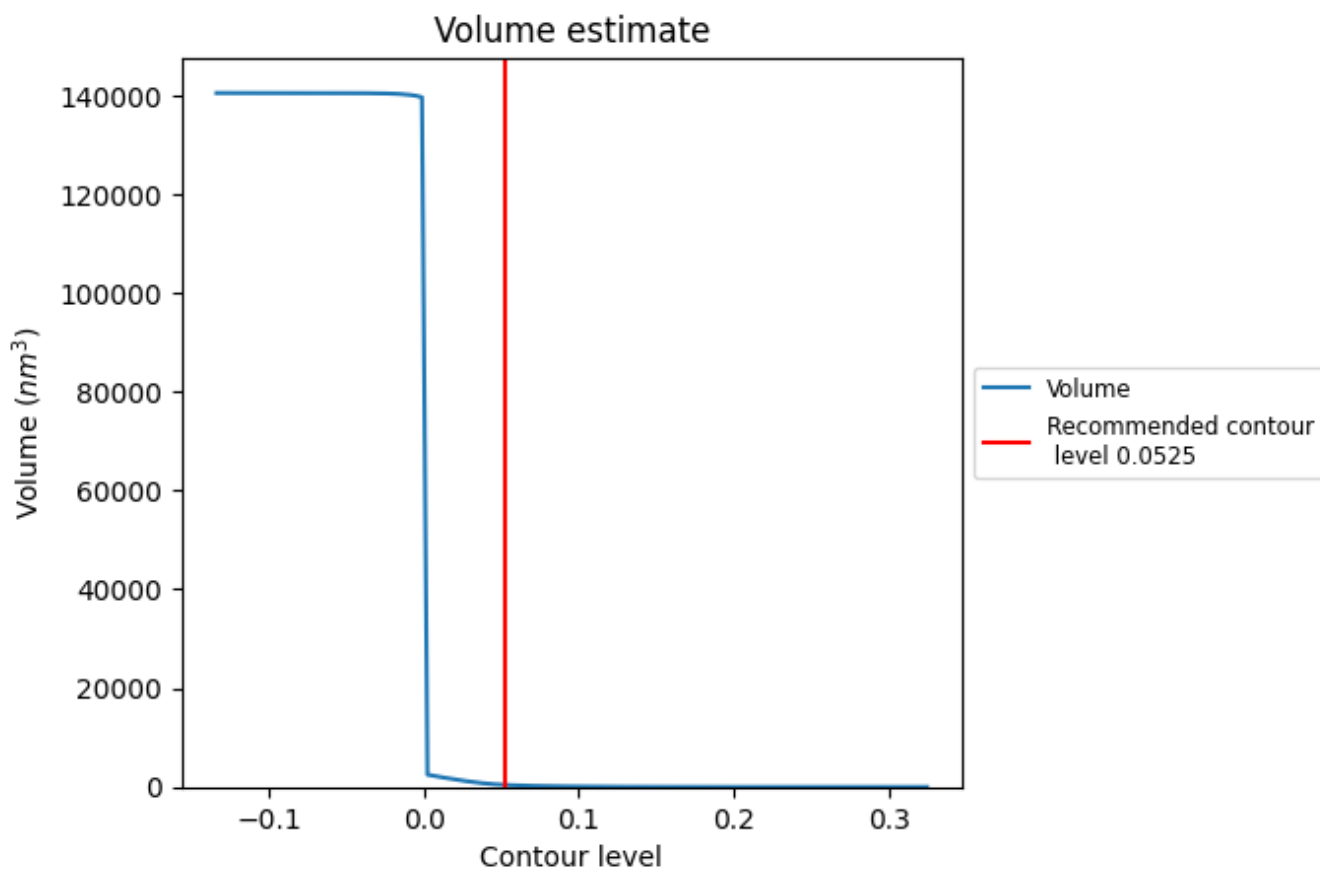
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

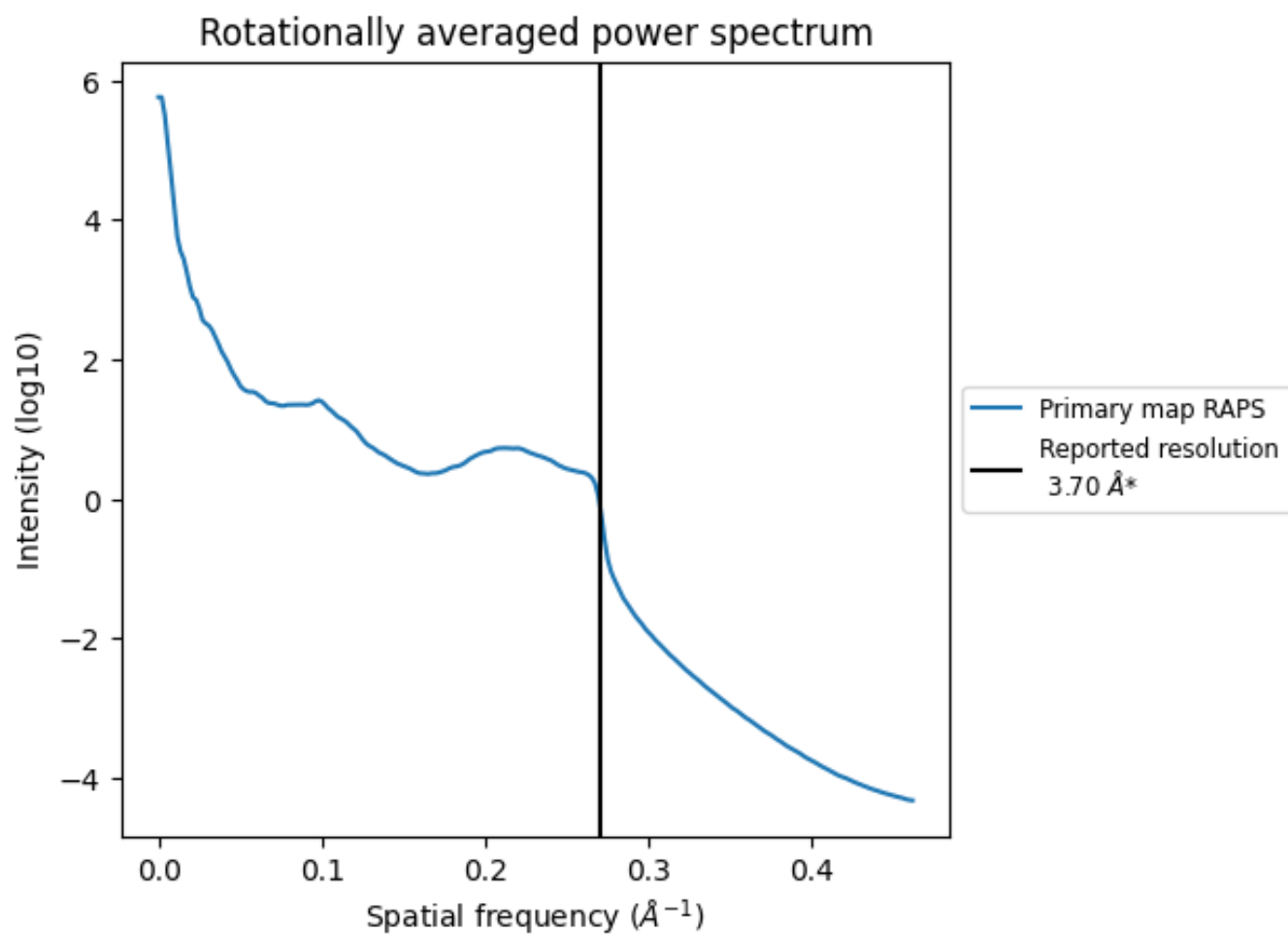
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 412 nm³; this corresponds to an approximate mass of 372 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.270\AA^{-1}

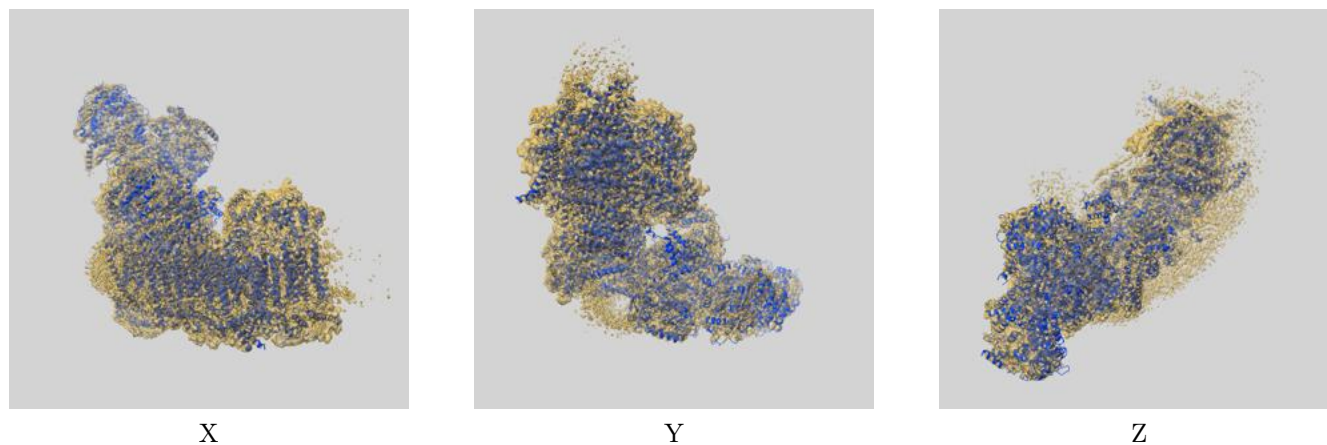
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

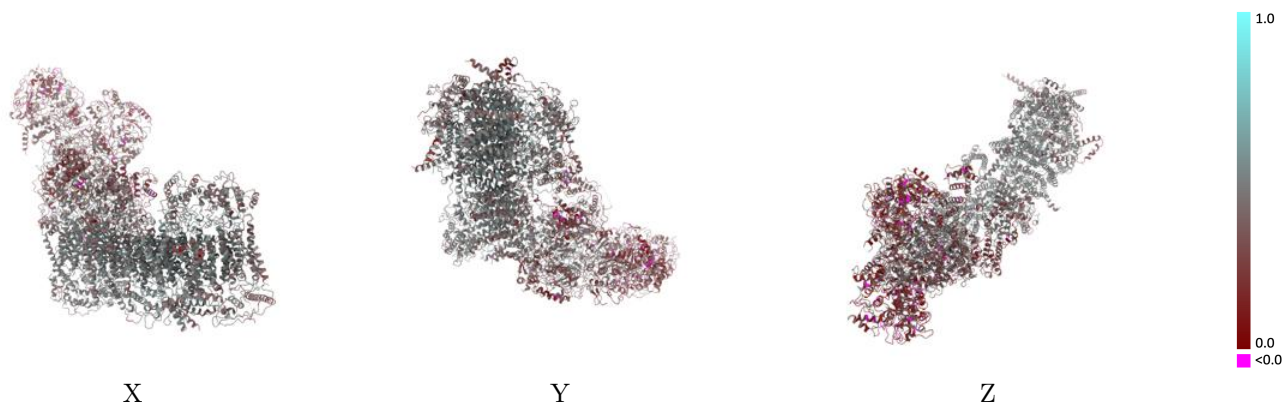
This section contains information regarding the fit between EMDB map EMD-6773 and PDB model 5XTD. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



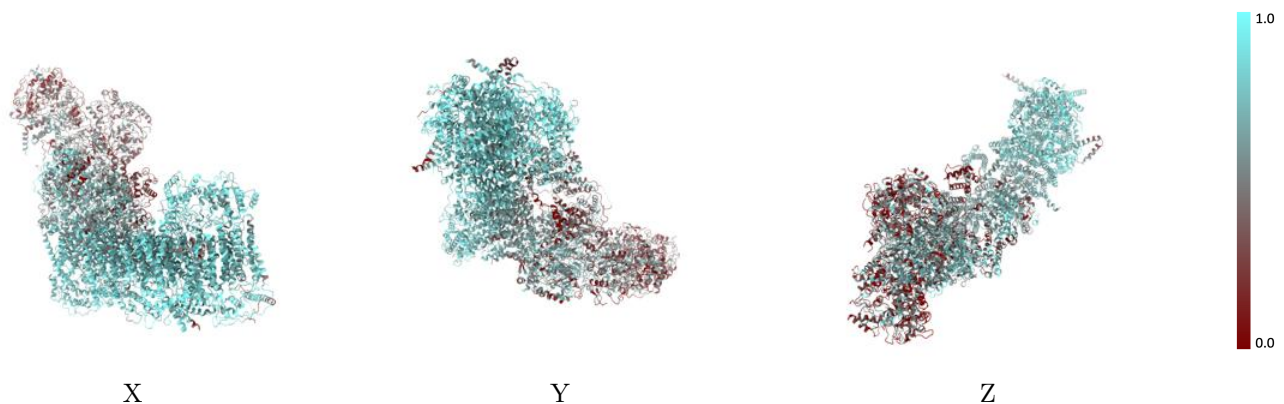
The images above show the 3D surface view of the map at the recommended contour level 0.0525 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



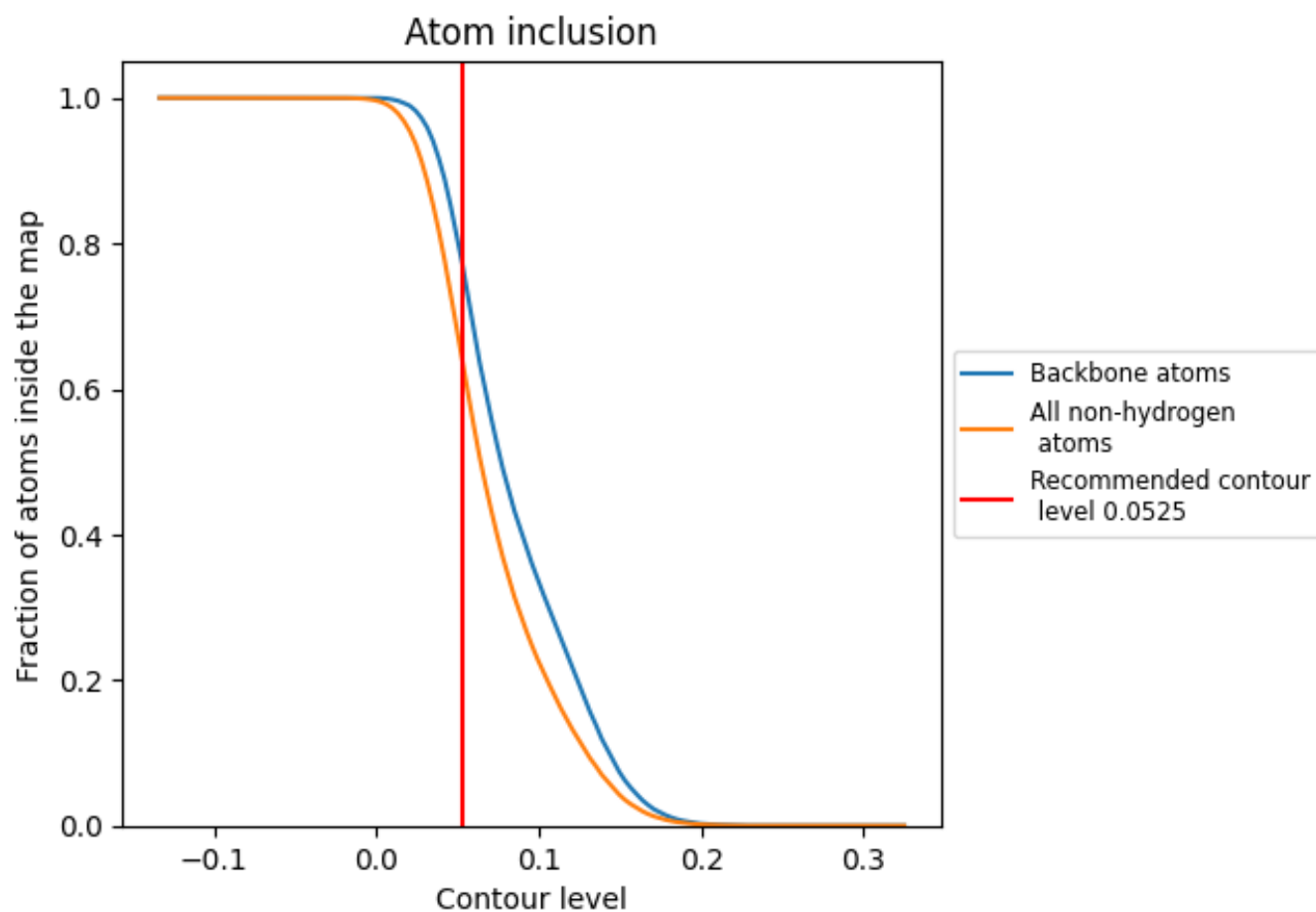
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0525).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 64% 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 (0.0525) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6415	 0.4010
A	 0.3441	 0.2340
B	 0.7528	 0.4320
C	 0.7907	 0.4590
E	 0.3912	 0.3140
F	 0.3687	 0.2200
G	 0.1291	 0.2310
H	 0.4365	 0.2870
I	 0.4067	 0.3250
J	 0.5258	 0.3290
K	 0.3022	 0.2340
L	 0.3507	 0.2970
M	 0.4033	 0.2840
N	 0.5340	 0.3760
O	 0.3385	 0.2460
P	 0.5333	 0.3350
Q	 0.6233	 0.3820
S	 0.8200	 0.4740
T	 0.4144	 0.3560
U	 0.7866	 0.4510
V	 0.6179	 0.4430
W	 0.8033	 0.4550
X	 0.7882	 0.4390
Y	 0.8359	 0.4350
Z	 0.7599	 0.4170
a	 0.8663	 0.5000
b	 0.7051	 0.3980
c	 0.8315	 0.4840
d	 0.8263	 0.4620
e	 0.7658	 0.4730
f	 0.6675	 0.3950
g	 0.7956	 0.4890
h	 0.8172	 0.4660
i	 0.7812	 0.5020
j	 0.6044	 0.4120



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Chain	Atom inclusion	Q-score
k	 0.7112	 0.4750
l	 0.7562	 0.4770
m	 0.7010	 0.4490
n	 0.7366	 0.4510
o	 0.7889	 0.4710
p	 0.8178	 0.4600
r	 0.8292	 0.5080
s	 0.7679	 0.4740
u	 0.8406	 0.4560
v	 0.7172	 0.3930
w	 0.6343	 0.3910