



Full wwPDB EM Validation Report ⓘ

Jun 13, 2024 – 12:15 PM EDT

PDB ID : 8UEU
EMDB ID : EMD-42171
Title : In-situ complex I, Deactive class03
Authors : Zheng, W.; Zhu, J.; Zhang, K.
Deposited on : 2023-10-02
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

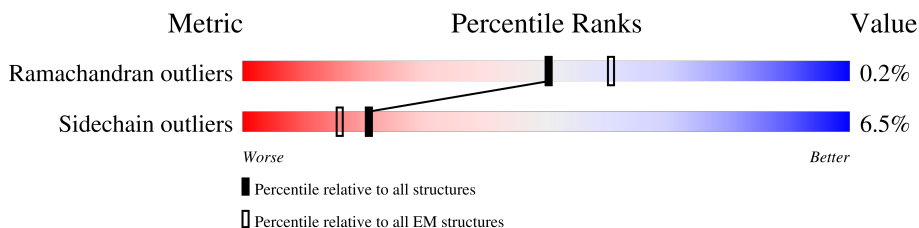
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

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 3.60 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	1A	115	17% (red), 70% (green), 7% (yellow), 23% (grey)
2	1B	258	17% (red), 54% (green), 6% (yellow), 40% (grey)
3	1C	264	43% (red), 76% (green), 21% (grey)
4	1D	476	30% (red), 85% (green), 5% (yellow), 10% (grey)
5	1E	249	85% (red), 80% (green), 6% (yellow), 14% (grey)
6	1F	464	91% (red), 88% (green), 5% (yellow), 7% (grey)
7	1G	727	68% (red), 91% (green), 5% (yellow), 16% (grey)
8	1H	318	20% (red), 95% (green), 5% (yellow)
9	1I	239	13% (red), 70% (green), 26% (grey)

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Mol	Chain	Length	Quality of chain
10	1J	175	23% 93% 7%
11	1K	98	10% 91% 9%
12	1L	606	96% .
13	1M	459	97% .
14	1N	347	96% .
15	1O	357	46% 84% 5% 10%
16	1P	377	62% 85% 5% 9%
17	1Q	175	50% 66% 8% 26%
18	1R	123	55% 73% 5% 22%
19	1S	99	84% 80% 8% 12%
20	1T	156	44% 47% 7% 46%
20	1U	156	7% 51% 45%
21	1V	116	83% 91% 9% .
22	1W	128	62% 77% 12% 10%
23	1X	172	23% 90% 10% .
24	1Y	141	8% 96% ..
25	1Z	144	22% 94% ..
26	1a	70	13% 96% .
27	1b	84	24% 92% 7% .
28	1c	76	18% 62% .. 36%
29	1d	123	9% 93% 5% .
30	1e	106	14% 81% 12% 7%
31	1f	135	15% 39% . 58%
32	1g	154	12% 58% 6% 35%
33	1h	189	9% 69% . 27%

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Mol	Chain	Length	Quality of chain
34	1i	128	
35	1j	105	
36	1k	98	
37	1l	186	
38	1m	129	
39	1n	179	
40	1o	137	
41	1p	176	
42	1q	145	
43	1r	114	
44	1s	471	

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 67263 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1A	88	707	484	101	117	5	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1B	155	1242	791	226	211	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	1C	209	1740	1125	297	316	2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1C	104	GLN	ARG	conflict	UNP A0A286ZNN4
1C	154	GLY	ASP	conflict	UNP A0A286ZNN4

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	1D	429	3452	2207	593	628	24	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1D	0	GLY	GLU	conflict	UNP A0A8D0QM68

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	1E	214	1658	1058	278	312	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	1F	432	3325	2100	592	613	20	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	1G	699	5362	3360	933	1029	40	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	1H	318	2504	1673	385	425	21	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	1I	176	1412	887	243	269	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	1J	175	1339	898	190	238	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	1K	98	750	494	113	129	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	1L	606	4818	3195	746	826	51	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	1M	459	3632	2411	572	610	39	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	1N	347	2712	1783	420	463	46	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	1O	320	2590	1649	440	491	10	0	0

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	1P	342	2751	1783	481	478	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	1Q	129	1047	659	186	199	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1R	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1S	87	Total	C	N	O	S	0	0
			700	440	131	127	2		

- Molecule 20 is a protein called NADH:ubiquinone oxidoreductase subunit AB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1T	85	Total	C	N	O	S	0	0
			689	445	101	138	5		
20	1U	86	Total	C	N	O	S	0	0
			694	448	102	139	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1V	115	Total	C	N	O	S	0	0
			927	599	157	168	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1W	115	Total	C	N	O	S	0	0
			971	619	179	168	5		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1X	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	1Y	139	1016	648	173	189	6	0	0

- Molecule 25 is a protein called NADH:ubiquinone oxidoreductase subunit A13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	1Z	141	1168	752	202	205	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	1a	70	562	361	101	94	6	0	0

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	1b	83	643	417	110	115	1	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	1c	49	417	276	71	70	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	1d	121	996	648	172	170	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1d	-2	ACE	-	acetylation	UNP A0A480JRW3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	1e	99	816	519	151	140	6	0	0

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa].

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	1f	57	487	316	89	80	2	0	0

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1f	-77	MET	-	initiating methionine	UNP A0A8D1IZ33
1f	-76	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-75	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-74	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-73	ILE	-	expression tag	UNP A0A8D1IZ33
1f	-72	LEU	-	expression tag	UNP A0A8D1IZ33
1f	-71	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-70	LEU	-	expression tag	UNP A0A8D1IZ33
1f	-69	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-68	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-67	THR	-	expression tag	UNP A0A8D1IZ33
1f	-66	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-65	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-64	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-63	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-62	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-61	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-60	CYS	-	expression tag	UNP A0A8D1IZ33
1f	-59	ASP	-	expression tag	UNP A0A8D1IZ33
1f	-58	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-57	ASN	-	expression tag	UNP A0A8D1IZ33
1f	-56	GLN	-	expression tag	UNP A0A8D1IZ33
1f	-55	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-54	VAL	-	expression tag	UNP A0A8D1IZ33
1f	-53	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-52	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-51	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-50	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-49	PHE	-	expression tag	UNP A0A8D1IZ33

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	1g	100	835	535	138	158	4	0	0

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	1h	138	1151	754	195	199	3	0	0

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	1i	127	1100	723	194	181	2	0	0

- Molecule 35 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	1j	71	601	394	99	107	1	0	0

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	1k	81	649	422	110	116	1	0	0

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	1l	156	1310	847	213	242	8	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		
38	1m	128	1062	691	182	189	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	1n	172	1495	956	273	258	8	0	0

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	1o	122	1045	650	198	187	10	0	0

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	1p	173	1449	908	263	270	8	0	0

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	1q	145	1212	775	219	213	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	1r	96	767	483	144	137	3	0	0

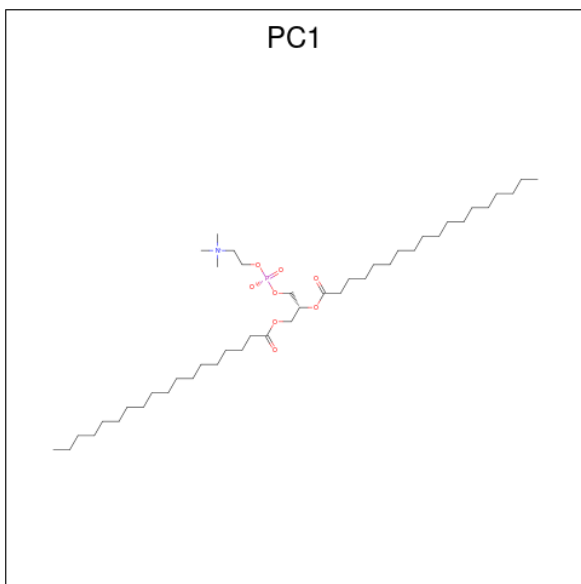
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1r	0	ACE	-	insertion	UNP A0A8W4F7N8

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	1s	45	382	238	70	73	1	0	0

- Molecule 45 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	1A	1	35	25	1	8	1	0
45	1H	1	44	34	1	8	1	0
45	1I	1	54	44	1	8	1	0
45	1M	1	46	36	1	8	1	0
45	1g	1	44	34	1	8	1	0

- Molecule 46 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



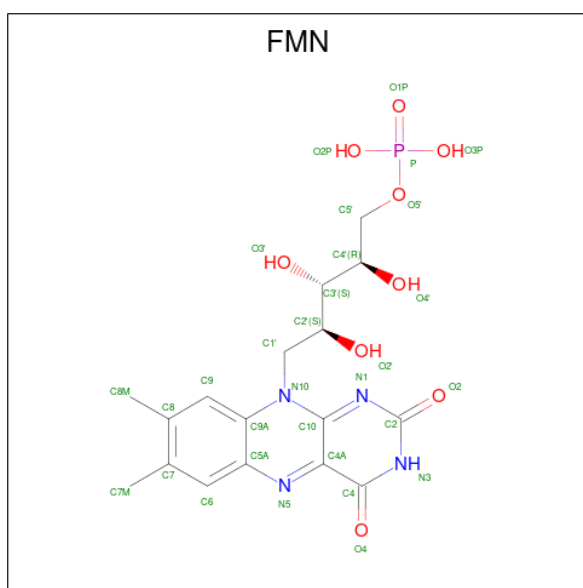
Mol	Chain	Residues	Atoms			AltConf
46	1B	1	Total	Fe	S	0
			8	4	4	
46	1F	1	Total	Fe	S	0
			8	4	4	
46	1G	1	Total	Fe	S	0
			8	4	4	
46	1G	1	Total	Fe	S	0
			8	4	4	
46	1I	1	Total	Fe	S	0
			8	4	4	
46	1I	1	Total	Fe	S	0
			8	4	4	

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



Mol	Chain	Residues	Atoms			AltConf
47	1E	1	Total	Fe	S	0
			4	2	2	
47	1G	1	Total	Fe	S	0
			4	2	2	

- Molecule 48 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).

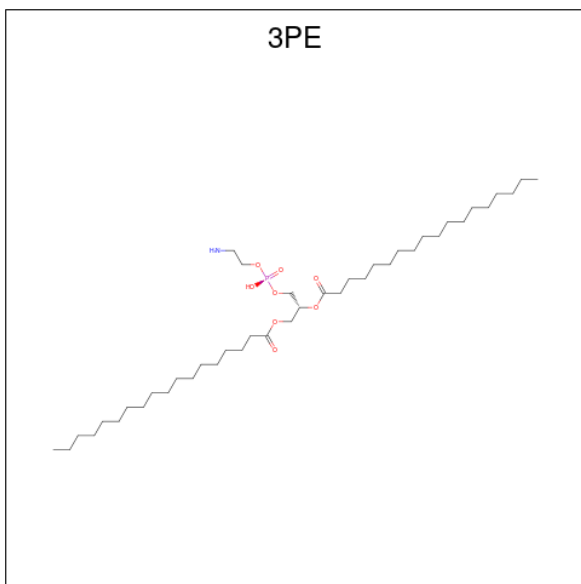


Mol	Chain	Residues	Atoms				AltConf	
48	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 49 is POTASSIUM ION (three-letter code: K) (formula: K).

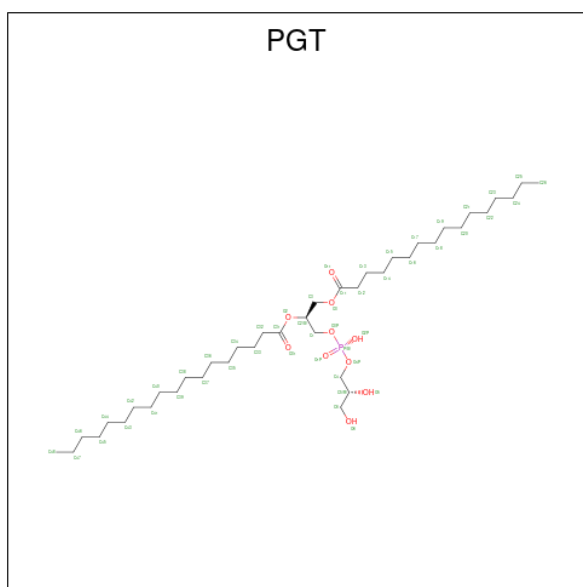
Mol	Chain	Residues	Atoms	AltConf
49	1G	1	Total K 1 1	0

- Molecule 50 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



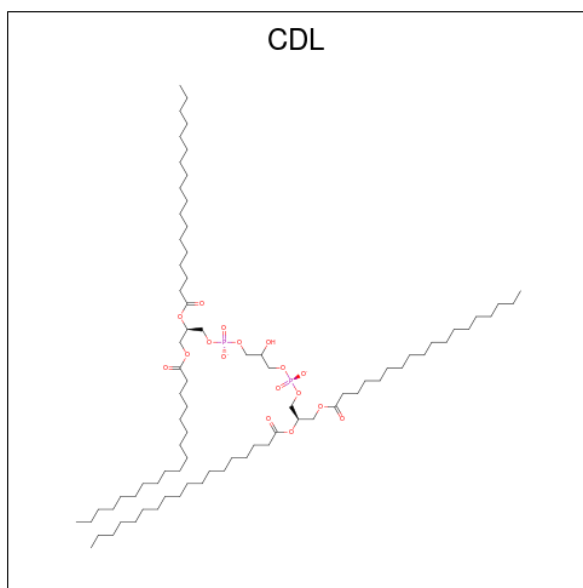
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
50	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
50	1L	1	Total	C	N	O	P	0
			42	32	1	8	1	
50	1N	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	1Y	1	Total	C	N	O	P	0
			31	21	1	8	1	
50	1Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	1b	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 51 is (1S)-2-[[[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: $C_{40}H_{79}O_{10}P$).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
51	1M	1	51	40	10	1	0

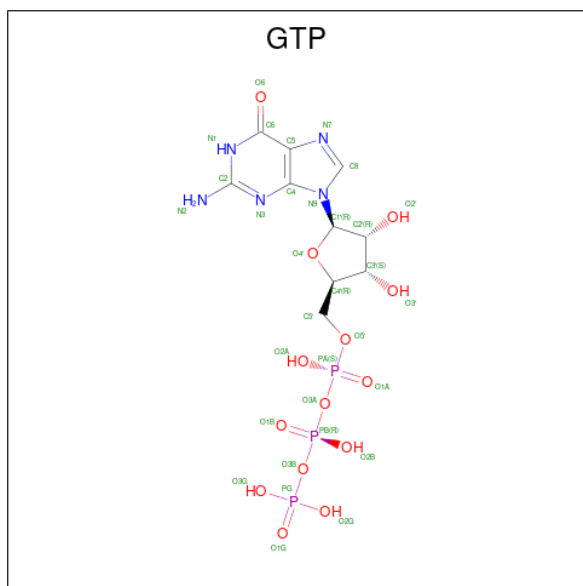
- Molecule 52 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
52	1N	1	77	58	17	2	0
52	1r	1	61	42	17	2	0

- Molecule 53 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:

$C_{10}H_{16}N_5O_{14}P_3$).

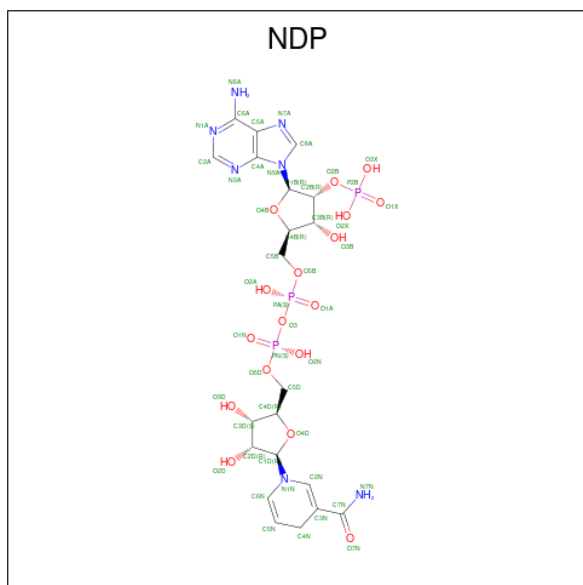


Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
53	10	1	32	10	5	14	3	0

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
54	10	1	1	1	0

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

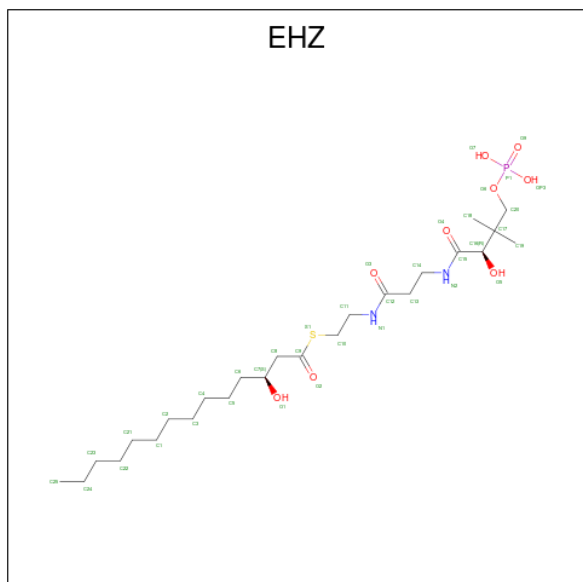


Mol	Chain	Residues	Atoms					AltConf
55	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

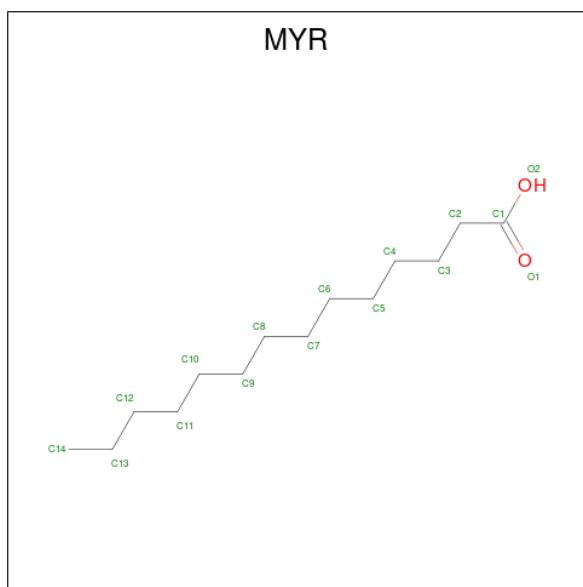
Mol	Chain	Residues	Atoms		AltConf
56	1R	1	Total	Zn	0
			1	1	

- Molecule 57 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonoxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: C₂₅H₄₉N₂O₉PS).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
57	1W	1	37	25	2	8	1	1	0
57	1n	1	37	25	2	8	1	1	0

- Molecule 58 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).

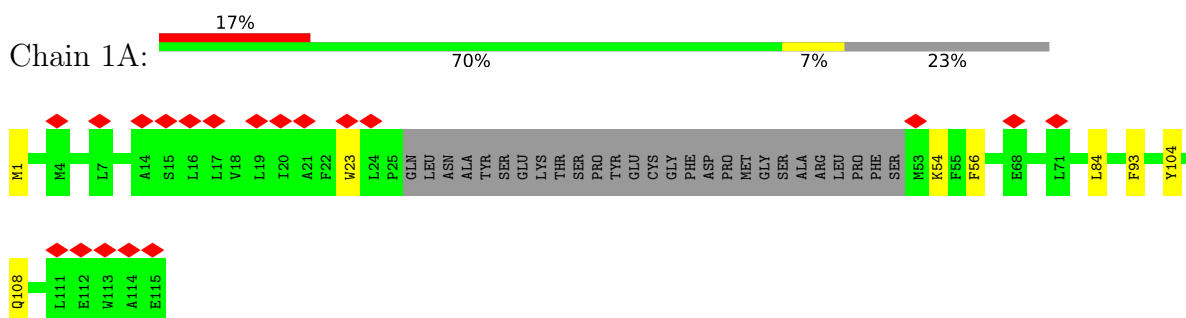


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
58	1l	1	15	14	1	0

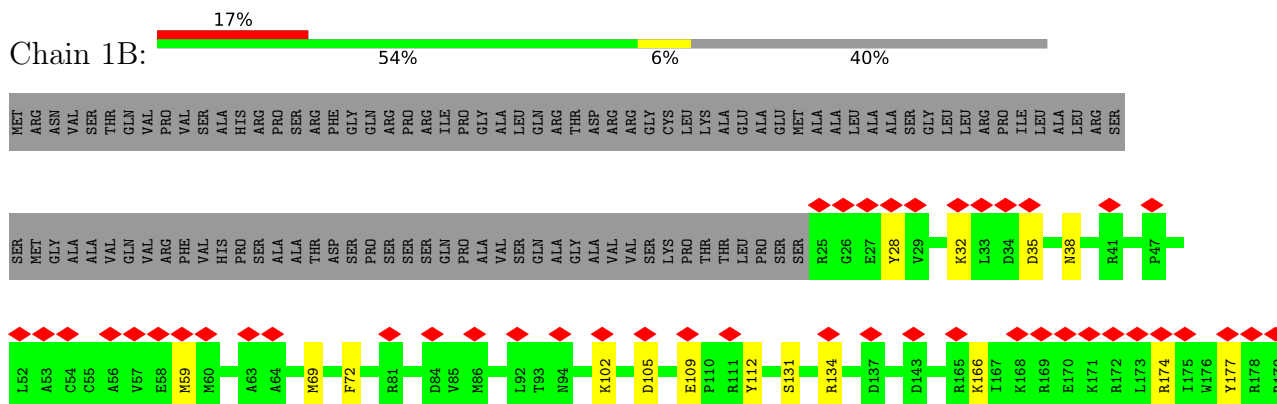
3 Residue-property plots [i](#)

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

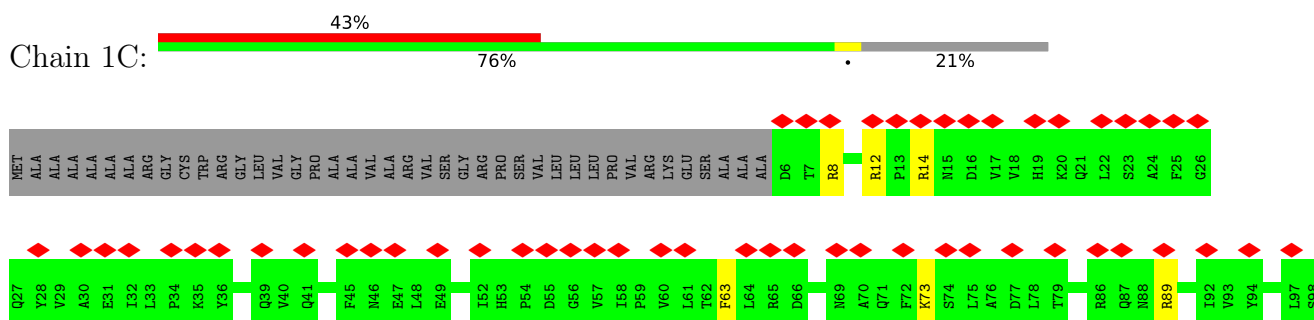
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

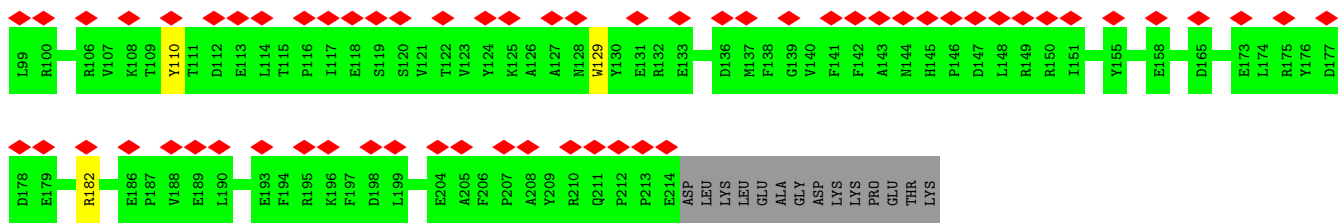


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

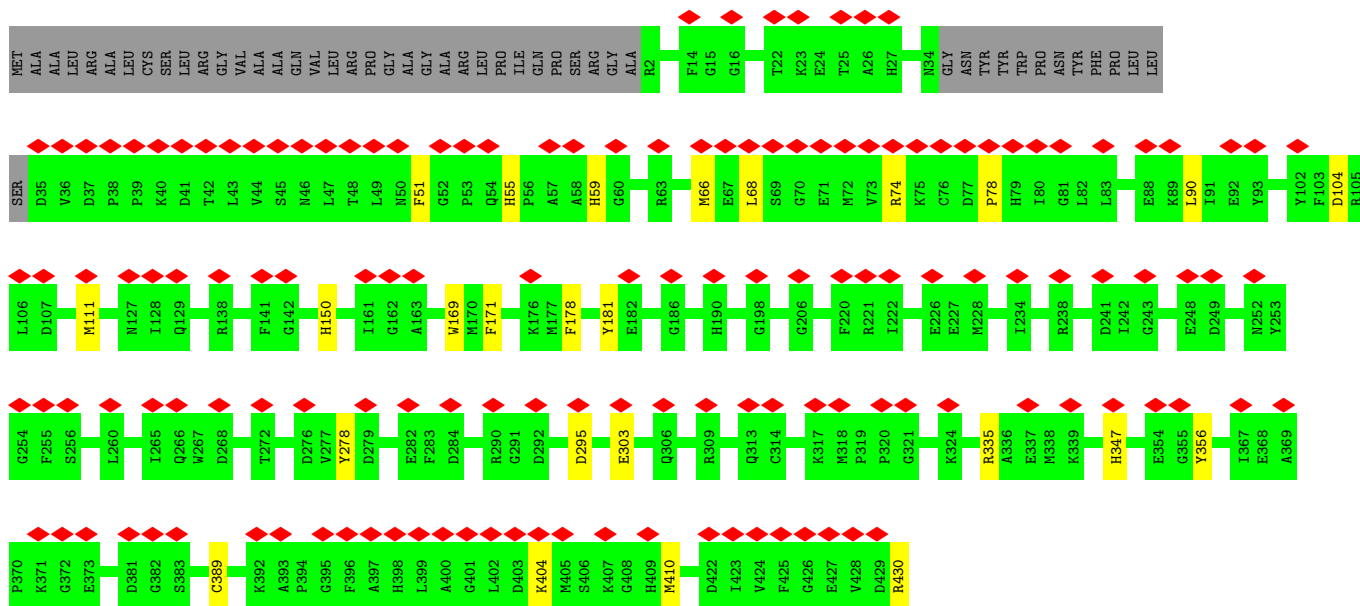
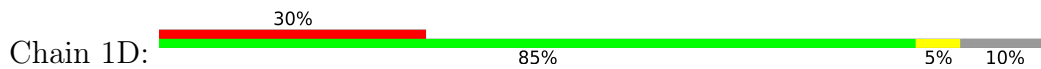


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

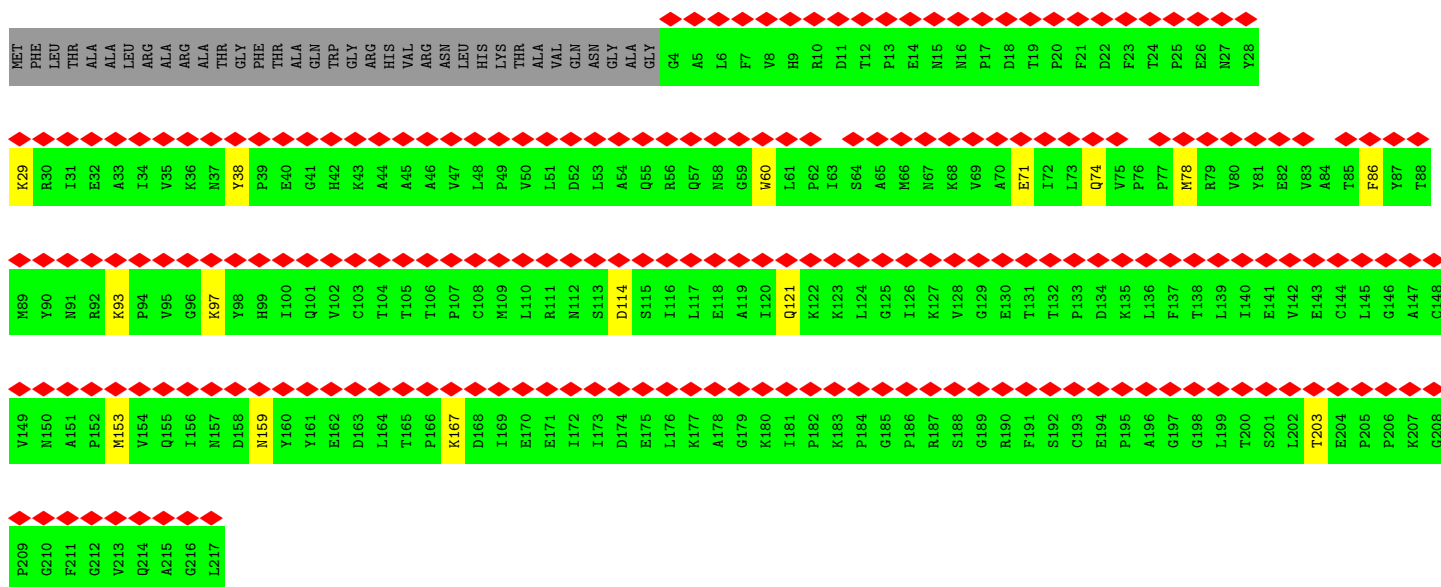
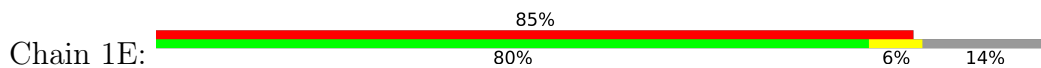




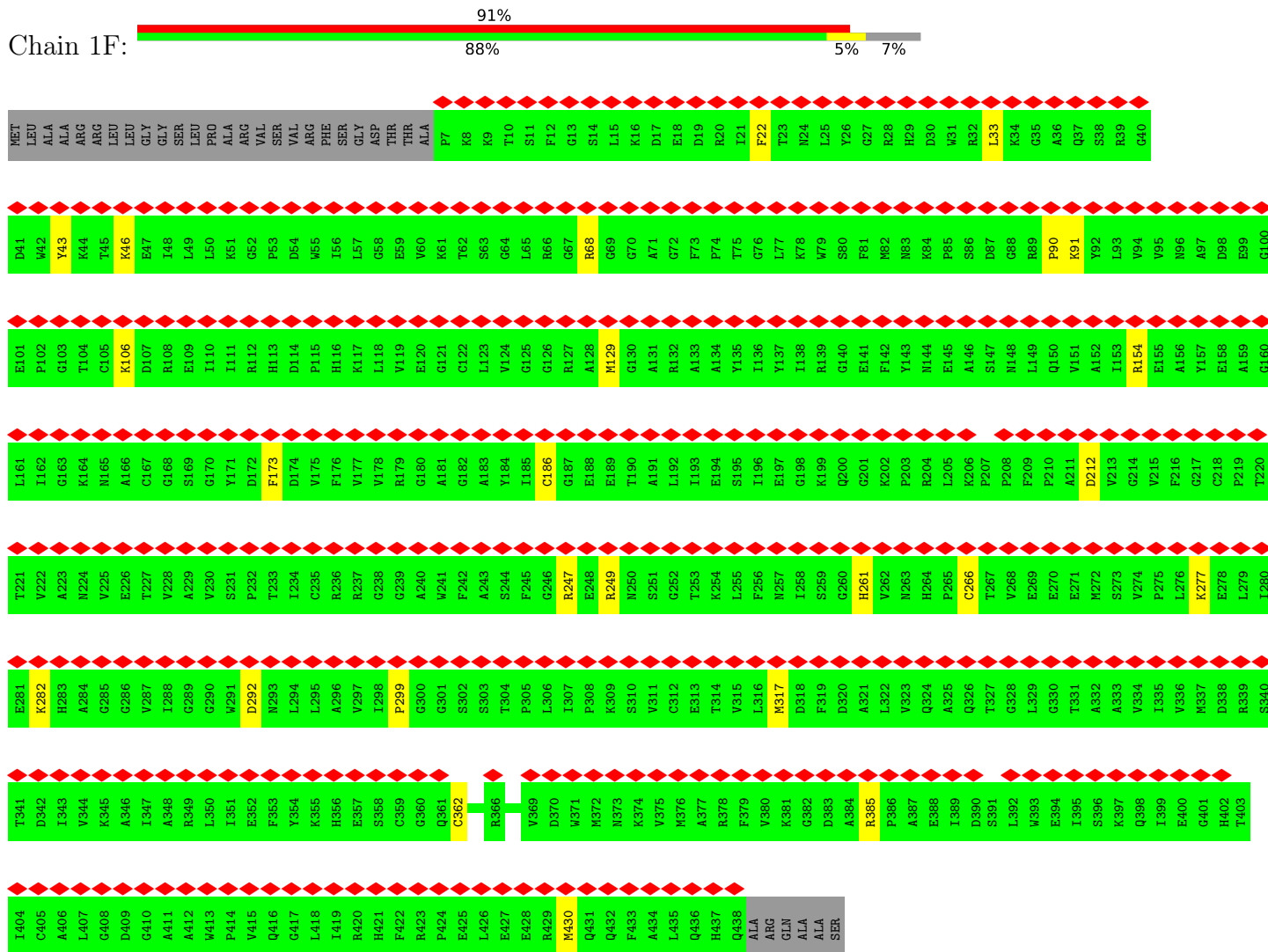
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



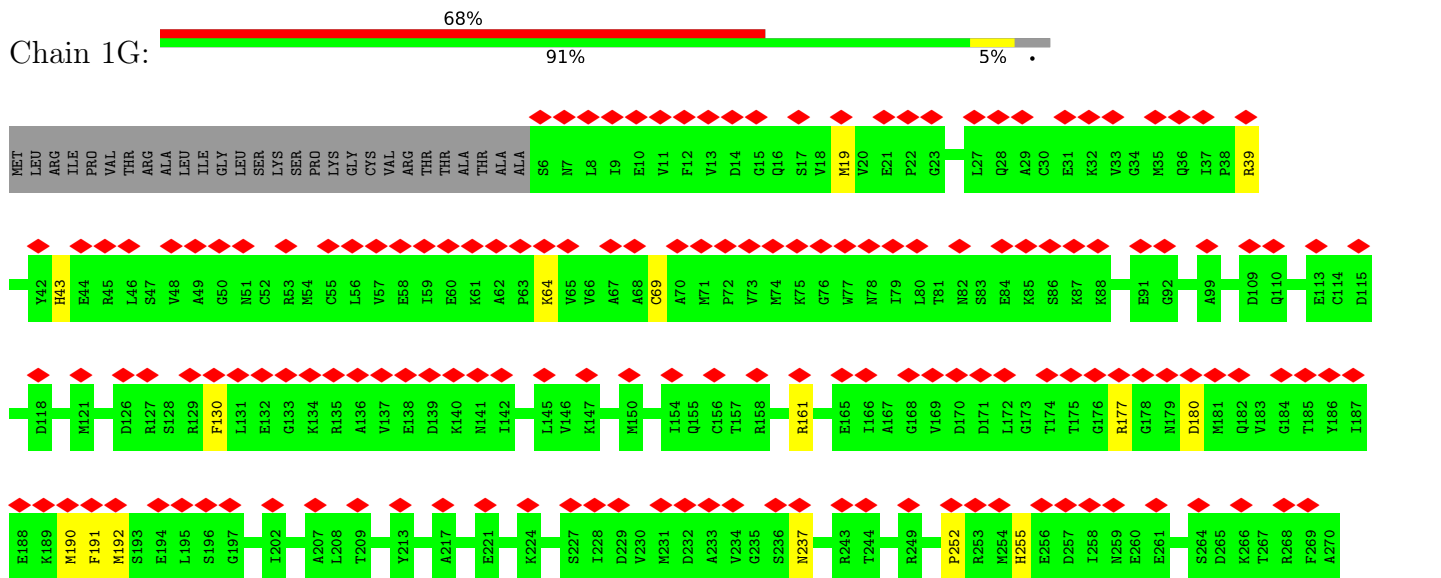
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

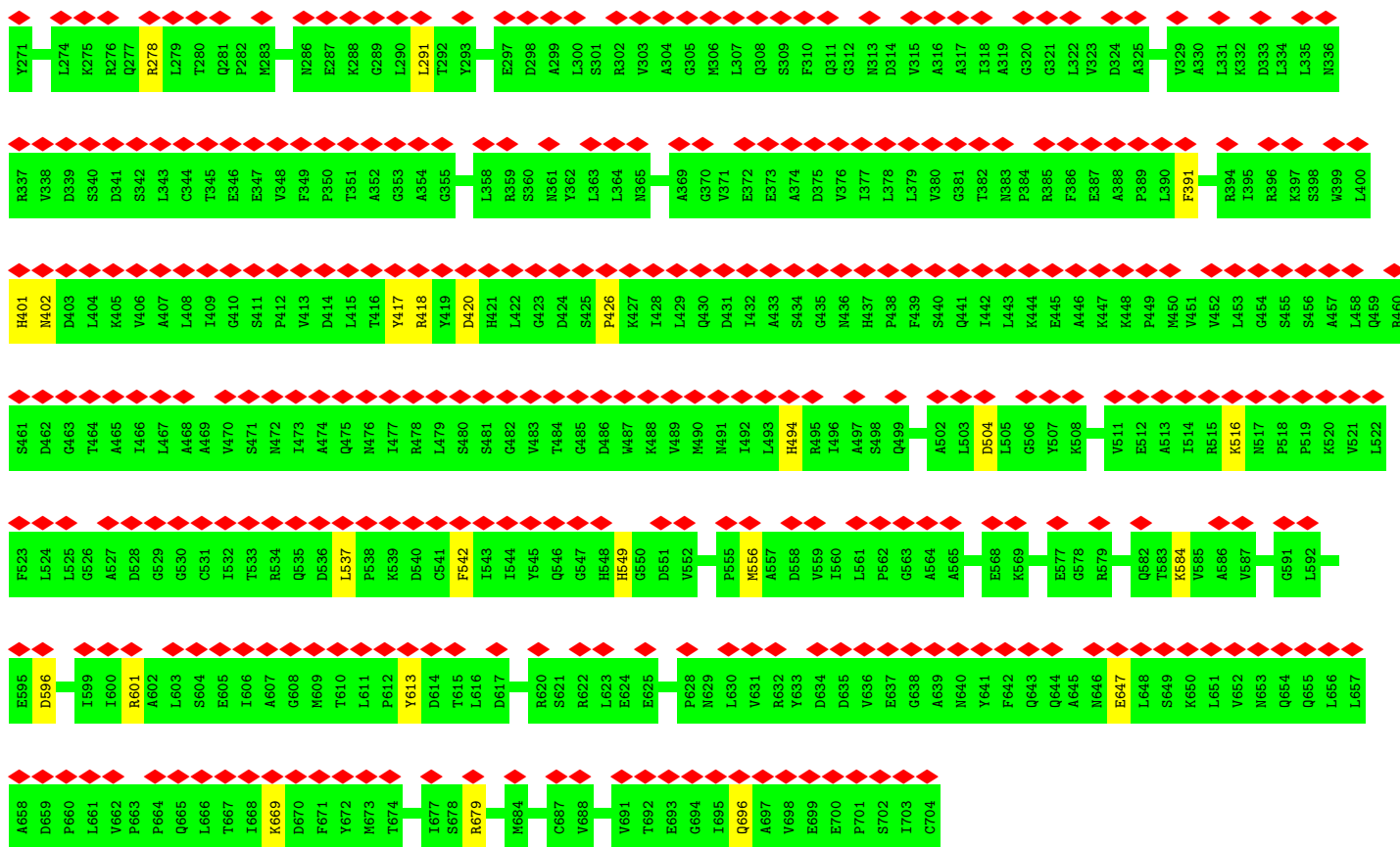


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

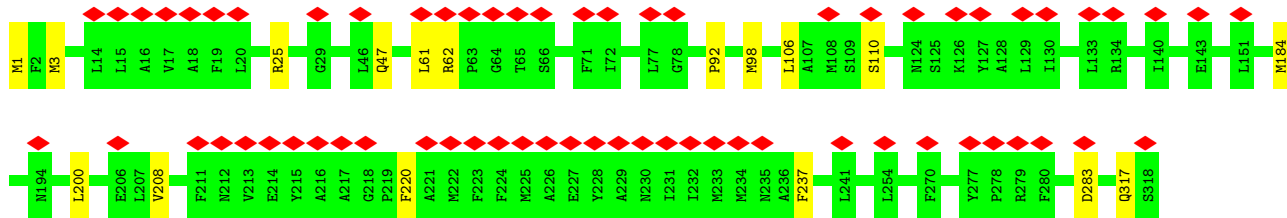


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

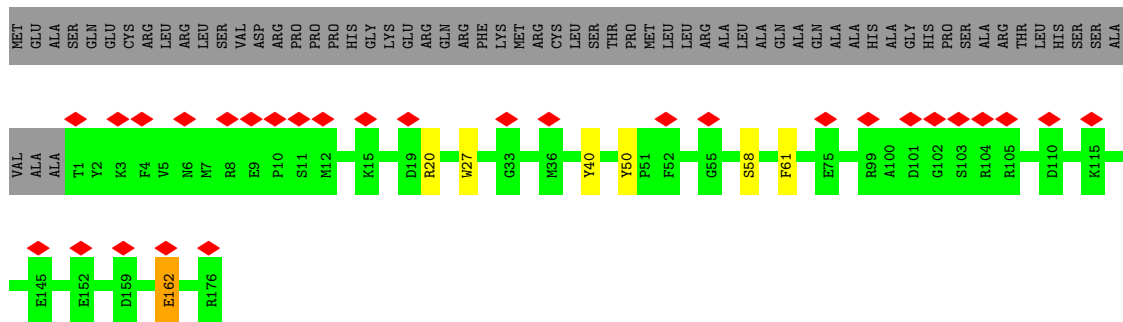




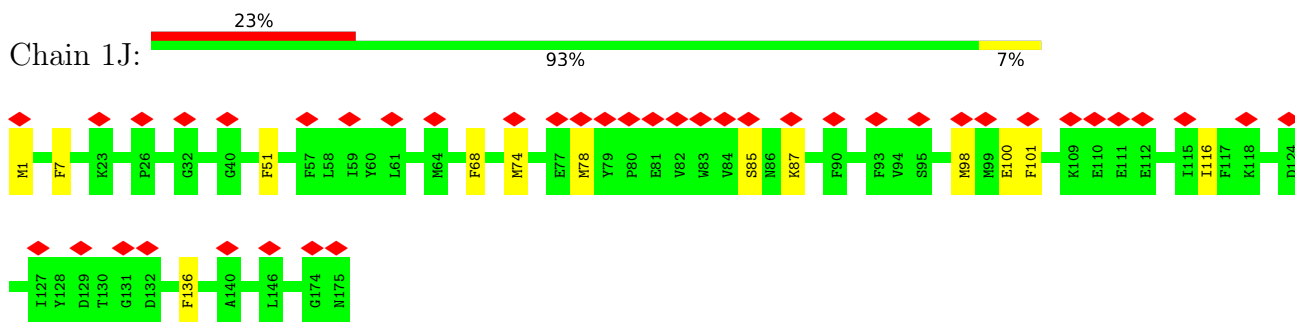
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



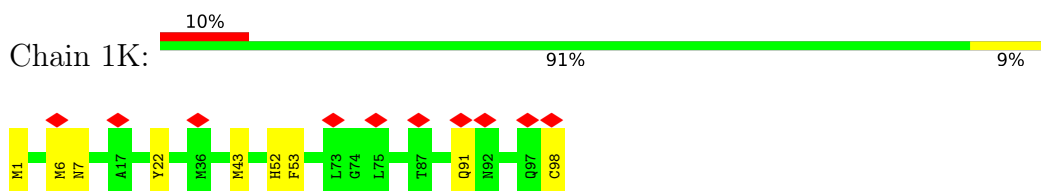
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



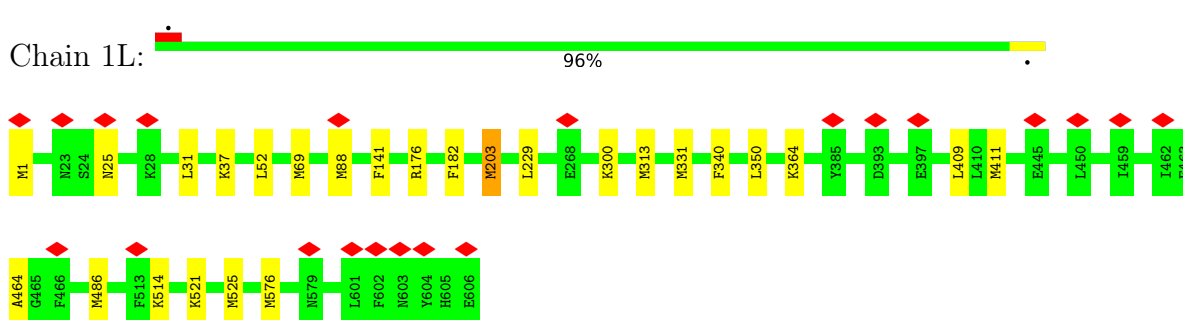
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



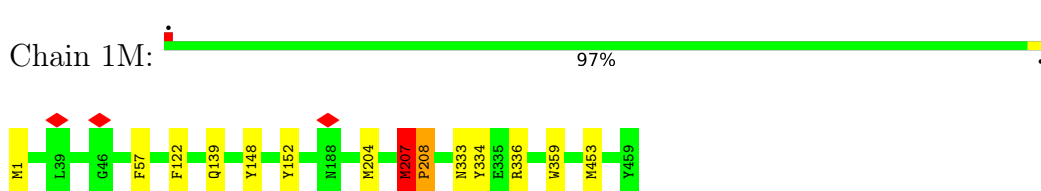
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



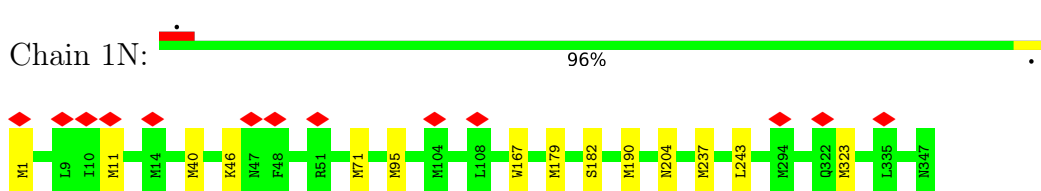
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5



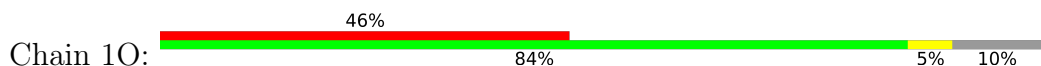
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

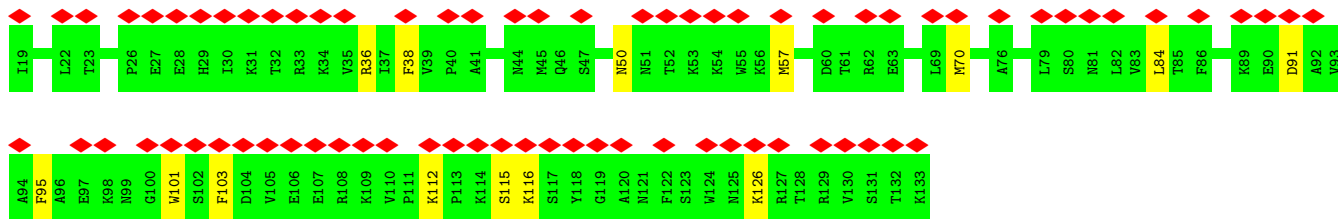


- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

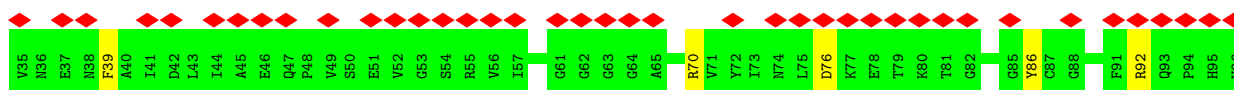
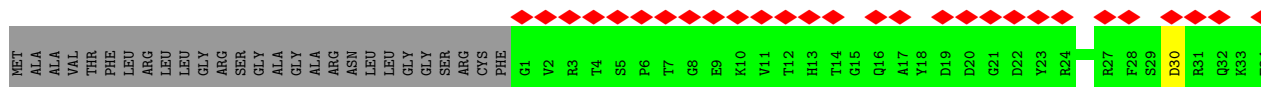
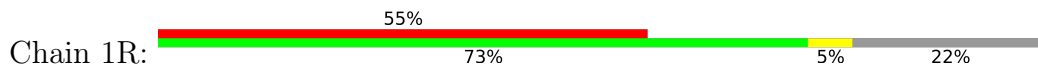


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

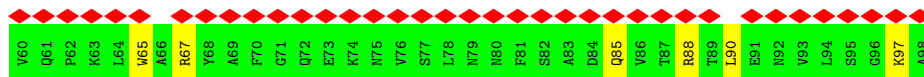
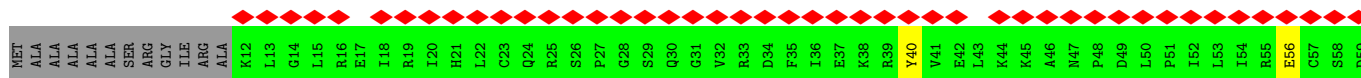
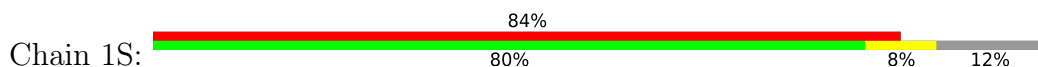




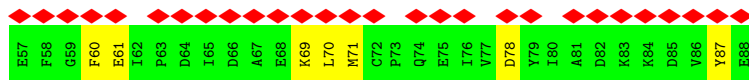
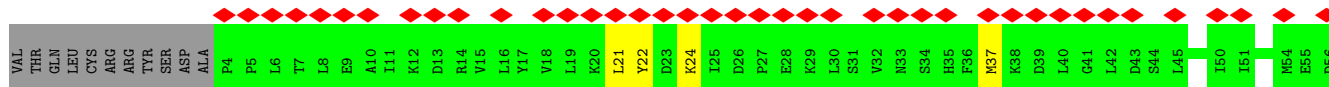
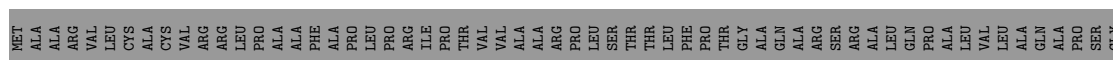
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

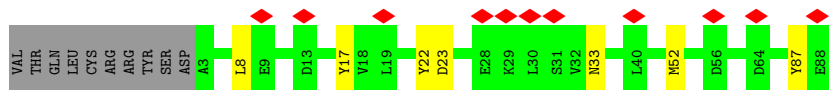


• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

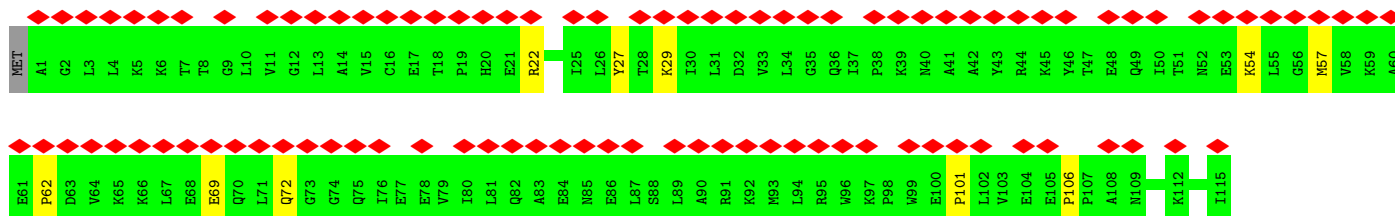
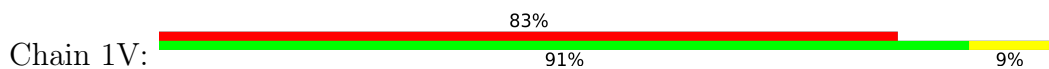


• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

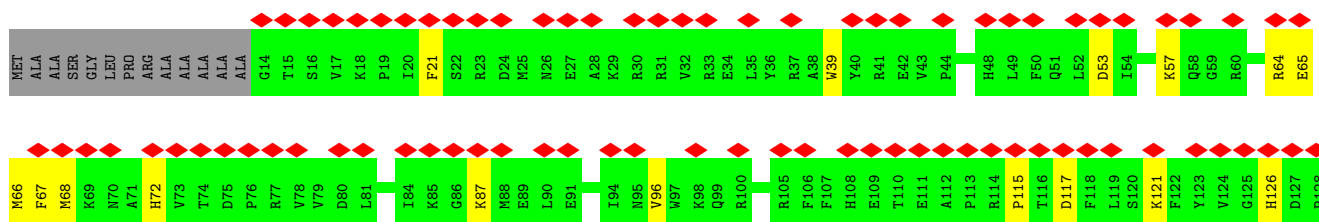
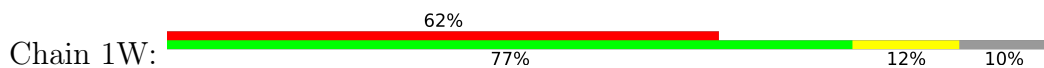




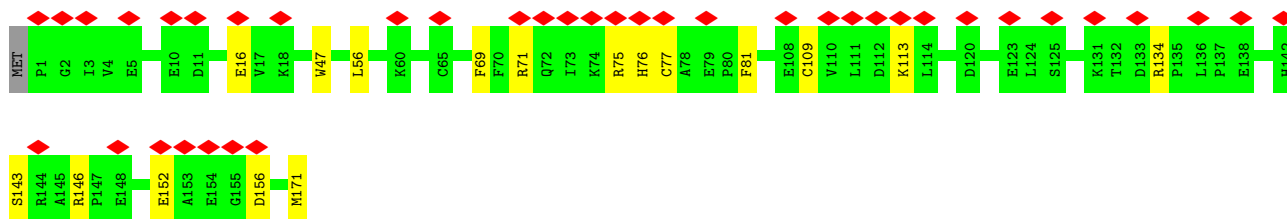
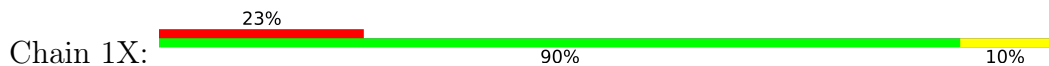
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



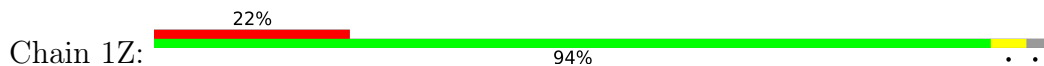
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

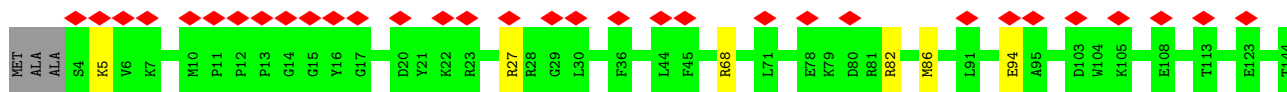


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

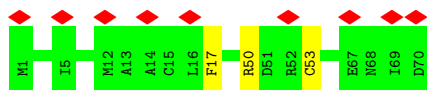


- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

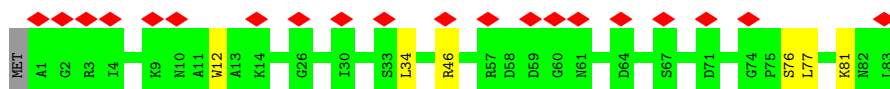




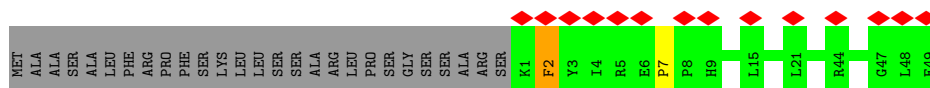
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



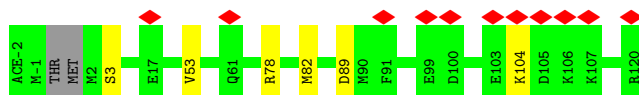
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



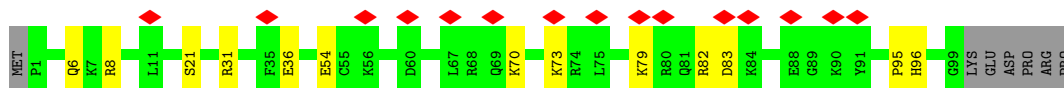
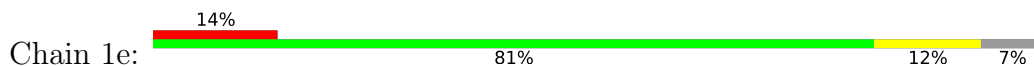
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



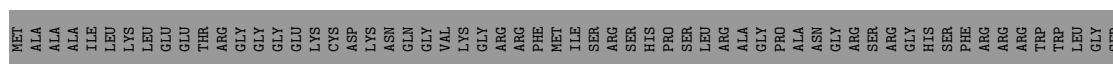
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



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



- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]



VAL	VAL	PRO	PRO
ALA	ALA	ALA	ALA
GLU	GLU	ALA	ALA
ALA	ALA	ALA	ALA
LYS	LYS	ALA	ALA
GLY	GLY	E31	E31
GLU	GLU	P32	P32
LEU	LEU	F33	F33
GLY	GLY	D34	D34
GLY	GLY	N35	N35
ARG	ARG	S36	S36
PRO	PRO	T37	T37
LEU	LEU	Y38	Y38
VAL	VAL	R39	R39
GLN	GLN	M40	M40
GLY	GLY	L41	L41
PRO	PRO	Q42	Q42
LYS	LYS	H43	H43
ALA	ALA	H44	H44
VAL	VAL	E45	E45
ASP	ASP	Y46	Y46
GLY	GLY	S47	S47
GLN	GLN	T48	T48
ASP	ASP	Y49	Y49
GLU	GLU	T50	T50
GLY	GLY	F51	F51
ALA	ALA	L52	L52
LYS	LYS	D63	D63
LYS	LYS	L54	L54
LYS	LYS	N56	N56
ALA	ALA	V56	V56
GLY	GLY	E57	E57
ILE	ILE	L58	L58
ALA	ALA	S59	S59
GLY	GLY	K60	K60
ASP	ASP	F61	F61
ALA	ALA	R62	R62
ALA	ALA	M63	M63
PRO	PRO	P64	P64
GLY	GLY	Q66	Q66
THR	THR	P66	P66
ALA	ALA	S67	S67
GLY	GLY	S68	S68
ARG	ARG	G69	G69
ASP	ASP	R70	R70
ALA	ALA	Q71	Q71
PRO	PRO	S72	S72
THR	THR	P73	P73
GLU	GLU	R74	R74
PRO	PRO	H75	H75
THR	THR		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.941	Depositor
Minimum map value	-0.401	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	425.6, 425.6, 425.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, ZN, FME, K, SF4, PC1, GTP, EHZ, CDL, SAC, PGT, FMN, MG, ACE, MYR, 3PE, FES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1A	0.26	0/713	0.53	0/975
2	1B	0.29	0/1273	0.61	0/1722
3	1C	0.30	0/1791	0.58	0/2439
4	1D	0.28	0/3545	0.53	0/4806
5	1E	0.27	0/1698	0.56	0/2311
6	1F	0.36	2/3401 (0.1%)	0.66	5/4595 (0.1%)
7	1G	0.28	0/5451	0.59	2/7387 (0.0%)
8	1H	0.27	0/2566	0.52	0/3509
9	1I	0.29	0/1443	0.57	0/1952
10	1J	0.28	0/1364	0.51	0/1850
11	1K	0.25	0/751	0.54	0/1018
12	1L	0.26	0/4939	0.51	2/6718 (0.0%)
13	1M	0.25	0/3713	0.53	2/5063 (0.0%)
14	1N	0.26	0/2765	0.55	1/3758 (0.0%)
15	1O	0.26	0/2650	0.51	0/3588
16	1P	0.27	0/2828	0.55	0/3834
17	1Q	0.26	0/1070	0.57	0/1446
18	1R	0.27	0/755	0.67	2/1018 (0.2%)
19	1S	0.27	0/711	0.67	0/956
20	1T	0.28	0/701	0.59	0/946
20	1U	0.29	0/706	0.58	0/954
21	1V	0.36	0/946	0.75	3/1281 (0.2%)
22	1W	1.19	3/995 (0.3%)	1.18	4/1340 (0.3%)
23	1X	0.26	0/1436	0.56	1/1938 (0.1%)
24	1Y	0.25	0/1037	0.49	0/1404
25	1Z	0.27	0/1199	0.55	0/1617
26	1a	0.27	0/577	0.49	0/777
27	1b	0.27	0/664	0.53	0/912
28	1c	0.35	0/430	0.70	2/581 (0.3%)
29	1d	0.28	0/1024	0.54	0/1383
30	1e	0.26	0/836	0.57	1/1118 (0.1%)
31	1f	0.26	0/499	0.57	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	1g	0.27	0/858	0.54	0/1165
33	1h	0.27	0/1184	0.52	0/1603
34	1i	0.25	0/1131	0.50	0/1541
35	1j	0.24	0/627	0.51	0/858
36	1k	0.28	0/668	0.52	0/903
37	1l	0.26	0/1365	0.49	0/1867
38	1m	0.26	0/1092	0.54	0/1481
39	1n	0.24	0/1549	0.50	0/2098
40	1o	0.25	0/1069	0.57	1/1430 (0.1%)
41	1p	0.26	0/1481	0.51	0/1997
42	1q	0.29	0/1253	0.60	1/1704 (0.1%)
43	1r	0.27	0/782	0.61	0/1057
44	1s	0.27	0/394	0.57	0/533
All	All	0.31	5/67930 (0.0%)	0.57	27/92106 (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
13	1M	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1W	115	PRO	CG-CD	-34.13	0.38	1.50
6	1F	299	PRO	CG-CD	-11.17	1.13	1.50
22	1W	115	PRO	N-CD	8.98	1.60	1.47
22	1W	115	PRO	CB-CG	7.62	1.88	1.50
6	1F	299	PRO	N-CD	6.46	1.56	1.47

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1W	115	PRO	N-CD-CG	-30.04	58.15	103.20
22	1W	115	PRO	CA-CB-CG	-12.79	79.70	104.00
6	1F	299	PRO	N-CD-CG	-12.54	84.40	103.20
6	1F	90	PRO	CA-N-CD	-12.25	94.35	111.50
6	1F	299	PRO	CA-N-CD	-11.89	94.85	111.50
7	1G	426	PRO	CA-N-CD	-11.34	95.62	111.50
22	1W	115	PRO	CA-N-CD	-10.76	96.43	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1c	7	PRO	CA-N-CD	-9.99	97.51	111.50
13	1M	207	MET	C-N-CD	-9.45	99.82	120.60
21	1V	106	PRO	CA-N-CD	-9.22	98.60	111.50
21	1V	62	PRO	CA-N-CD	-8.99	98.92	111.50
18	1R	92	ARG	C-N-CA	7.96	141.61	121.70
7	1G	426	PRO	N-CD-CG	-7.66	91.71	103.20
12	1L	350	LEU	CA-CB-CG	7.48	132.51	115.30
6	1F	90	PRO	N-CD-CG	-7.34	92.18	103.20
6	1F	299	PRO	CA-CB-CG	-6.97	90.75	104.00
13	1M	208	PRO	CA-N-CD	-6.43	102.50	111.50
22	1W	115	PRO	N-CA-CB	-6.37	95.59	102.60
18	1R	30	ASP	CB-CG-OD2	6.19	123.87	118.30
14	1N	11	MET	CA-CB-CG	6.16	123.78	113.30
21	1V	101	PRO	CA-N-CD	-5.85	103.31	111.50
42	1q	72	ASP	CB-CG-OD2	5.75	123.47	118.30
40	1o	47	ASP	CB-CG-OD1	5.55	123.29	118.30
12	1L	203	MET	CB-CG-SD	5.40	128.60	112.40
30	1e	95	PRO	CA-N-CD	-5.37	103.98	111.50
23	1X	109	CYS	CA-CB-SG	5.15	123.27	114.00
28	1c	7	PRO	N-CD-CG	-5.08	95.58	103.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	1M	207	MET	Peptide
13	1M	208	PRO	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	1A	84/115 (73%)	81 (96%)	3 (4%)	0	100	100
2	1B	153/258 (59%)	142 (93%)	11 (7%)	0	100	100
3	1C	207/264 (78%)	191 (92%)	16 (8%)	0	100	100
4	1D	427/476 (90%)	396 (93%)	31 (7%)	0	100	100
5	1E	212/249 (85%)	184 (87%)	28 (13%)	0	100	100
6	1F	430/464 (93%)	392 (91%)	37 (9%)	1 (0%)	47	79
7	1G	697/727 (96%)	637 (91%)	59 (8%)	1 (0%)	51	83
8	1H	316/318 (99%)	298 (94%)	15 (5%)	3 (1%)	17	57
9	1I	174/239 (73%)	159 (91%)	14 (8%)	1 (1%)	25	64
10	1J	173/175 (99%)	159 (92%)	12 (7%)	2 (1%)	13	51
11	1K	96/98 (98%)	87 (91%)	8 (8%)	1 (1%)	15	55
12	1L	604/606 (100%)	556 (92%)	47 (8%)	1 (0%)	47	79
13	1M	457/459 (100%)	444 (97%)	12 (3%)	1 (0%)	47	79
14	1N	345/347 (99%)	325 (94%)	20 (6%)	0	100	100
15	1O	318/357 (89%)	295 (93%)	23 (7%)	0	100	100
16	1P	340/377 (90%)	311 (92%)	29 (8%)	0	100	100
17	1Q	127/175 (73%)	113 (89%)	13 (10%)	1 (1%)	19	59
18	1R	94/123 (76%)	89 (95%)	5 (5%)	0	100	100
19	1S	85/99 (86%)	77 (91%)	8 (9%)	0	100	100
20	1T	83/156 (53%)	77 (93%)	6 (7%)	0	100	100
20	1U	84/156 (54%)	74 (88%)	10 (12%)	0	100	100
21	1V	113/116 (97%)	102 (90%)	11 (10%)	0	100	100
22	1W	113/128 (88%)	108 (96%)	4 (4%)	1 (1%)	17	57
23	1X	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
24	1Y	137/141 (97%)	132 (96%)	5 (4%)	0	100	100
25	1Z	139/144 (96%)	128 (92%)	11 (8%)	0	100	100
26	1a	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
27	1b	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
28	1c	47/76 (62%)	45 (96%)	1 (2%)	1 (2%)	7	40
29	1d	117/123 (95%)	109 (93%)	6 (5%)	2 (2%)	9	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	1e	97/106 (92%)	89 (92%)	8 (8%)	0	100	100
31	1f	55/135 (41%)	48 (87%)	7 (13%)	0	100	100
32	1g	98/154 (64%)	91 (93%)	6 (6%)	1 (1%)	15	55
33	1h	136/189 (72%)	130 (96%)	6 (4%)	0	100	100
34	1i	124/128 (97%)	119 (96%)	5 (4%)	0	100	100
35	1j	69/105 (66%)	68 (99%)	1 (1%)	0	100	100
36	1k	79/98 (81%)	72 (91%)	7 (9%)	0	100	100
37	1l	154/186 (83%)	142 (92%)	12 (8%)	0	100	100
38	1m	126/129 (98%)	117 (93%)	9 (7%)	0	100	100
39	1n	170/179 (95%)	161 (95%)	9 (5%)	0	100	100
40	1o	120/137 (88%)	115 (96%)	5 (4%)	0	100	100
41	1p	171/176 (97%)	166 (97%)	5 (3%)	0	100	100
42	1q	143/145 (99%)	131 (92%)	11 (8%)	1 (1%)	22	61
43	1r	90/114 (79%)	83 (92%)	7 (8%)	0	100	100
44	1s	43/471 (9%)	39 (91%)	4 (9%)	0	100	100
All	All	8165/9744 (84%)	7582 (93%)	565 (7%)	18 (0%)	50	79

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	1H	92	PRO
9	1I	162	GLU
10	1J	85	SER
12	1L	464	ALA
13	1M	207	MET
29	1d	3	SER
29	1d	53	VAL
42	1q	142	THR
6	1F	249	ARG
8	1H	208	VAL
10	1J	116	ILE
28	1c	2	PHE
11	1K	22	TYR
7	1G	696	GLN
8	1H	200	LEU
17	1Q	70	MET
22	1W	96	VAL

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Mol	Chain	Res	Type
32	1g	24	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1A	76/99 (77%)	69 (91%)	7 (9%)	9 39
2	1B	131/212 (62%)	115 (88%)	16 (12%)	5 26
3	1C	190/227 (84%)	181 (95%)	9 (5%)	26 61
4	1D	371/405 (92%)	346 (93%)	25 (7%)	16 50
5	1E	183/207 (88%)	168 (92%)	15 (8%)	11 42
6	1F	346/368 (94%)	324 (94%)	22 (6%)	17 52
7	1G	588/610 (96%)	551 (94%)	37 (6%)	18 53
8	1H	274/274 (100%)	261 (95%)	13 (5%)	26 61
9	1I	151/201 (75%)	142 (94%)	9 (6%)	19 54
10	1J	140/140 (100%)	130 (93%)	10 (7%)	14 48
11	1K	84/84 (100%)	77 (92%)	7 (8%)	11 42
12	1L	539/539 (100%)	516 (96%)	23 (4%)	29 63
13	1M	408/408 (100%)	396 (97%)	12 (3%)	42 72
14	1N	310/310 (100%)	298 (96%)	12 (4%)	32 65
15	1O	283/307 (92%)	264 (93%)	19 (7%)	16 50
16	1P	296/323 (92%)	276 (93%)	20 (7%)	16 50
17	1Q	117/152 (77%)	104 (89%)	13 (11%)	6 31
18	1R	79/97 (81%)	75 (95%)	4 (5%)	24 58
19	1S	77/82 (94%)	69 (90%)	8 (10%)	7 33
20	1T	79/133 (59%)	68 (86%)	11 (14%)	3 22
20	1U	79/133 (59%)	72 (91%)	7 (9%)	9 40
21	1V	100/101 (99%)	93 (93%)	7 (7%)	15 48
22	1W	107/112 (96%)	93 (87%)	14 (13%)	4 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	1X	153/154 (99%)	137 (90%)	16 (10%)	7	33
24	1Y	101/102 (99%)	97 (96%)	4 (4%)	31	65
25	1Z	123/124 (99%)	117 (95%)	6 (5%)	25	59
26	1a	58/58 (100%)	55 (95%)	3 (5%)	23	58
27	1b	69/70 (99%)	63 (91%)	6 (9%)	10	41
28	1c	45/66 (68%)	44 (98%)	1 (2%)	52	77
29	1d	107/109 (98%)	103 (96%)	4 (4%)	34	66
30	1e	87/94 (93%)	75 (86%)	12 (14%)	3	22
31	1f	54/113 (48%)	49 (91%)	5 (9%)	9	38
32	1g	92/129 (71%)	83 (90%)	9 (10%)	8	36
33	1h	121/158 (77%)	113 (93%)	8 (7%)	16	51
34	1i	119/120 (99%)	116 (98%)	3 (2%)	47	75
35	1j	62/84 (74%)	58 (94%)	4 (6%)	17	51
36	1k	63/76 (83%)	56 (89%)	7 (11%)	6	31
37	1l	141/161 (88%)	138 (98%)	3 (2%)	53	78
38	1m	113/114 (99%)	105 (93%)	8 (7%)	14	48
39	1n	156/160 (98%)	150 (96%)	6 (4%)	33	66
40	1o	110/120 (92%)	103 (94%)	7 (6%)	17	52
41	1p	154/156 (99%)	141 (92%)	13 (8%)	11	42
42	1q	131/131 (100%)	122 (93%)	9 (7%)	15	49
43	1r	85/98 (87%)	79 (93%)	6 (7%)	14	48
44	1s	44/351 (12%)	39 (89%)	5 (11%)	5	29
All	All	7196/8272 (87%)	6731 (94%)	465 (6%)	21	51

All (465) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	23	TRP
1	1A	54	LYS
1	1A	56	PHE
1	1A	84	LEU
1	1A	93	PHE
1	1A	104	TYR
1	1A	108	GLN

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Mol	Chain	Res	Type
2	1B	28	TYR
2	1B	32	LYS
2	1B	35	ASP
2	1B	38	ASN
2	1B	59	MET
2	1B	69	MET
2	1B	72	PHE
2	1B	102	LYS
2	1B	105	ASP
2	1B	109	GLU
2	1B	112	TYR
2	1B	131	SER
2	1B	134	ARG
2	1B	166	LYS
2	1B	174	ARG
2	1B	177	TYR
3	1C	8	ARG
3	1C	12	ARG
3	1C	14	ARG
3	1C	63	PHE
3	1C	73	LYS
3	1C	89	ARG
3	1C	110	TYR
3	1C	129	TRP
3	1C	182	ARG
4	1D	51	PHE
4	1D	55	HIS
4	1D	59	HIS
4	1D	66	MET
4	1D	68	LEU
4	1D	74	ARG
4	1D	78	PRO
4	1D	90	LEU
4	1D	104	ASP
4	1D	111	MET
4	1D	150	HIS
4	1D	169	TRP
4	1D	171	PHE
4	1D	178	PHE
4	1D	181	TYR
4	1D	278	TYR
4	1D	295	ASP

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Mol	Chain	Res	Type
4	1D	303	GLU
4	1D	335	ARG
4	1D	347	HIS
4	1D	356	TYR
4	1D	389	CYS
4	1D	404	LYS
4	1D	410	MET
4	1D	430	ARG
5	1E	29	LYS
5	1E	38	TYR
5	1E	60	TRP
5	1E	71	GLU
5	1E	74	GLN
5	1E	78	MET
5	1E	86	PHE
5	1E	93	LYS
5	1E	97	LYS
5	1E	114	ASP
5	1E	121	GLN
5	1E	153	MET
5	1E	159	ASN
5	1E	167	LYS
5	1E	203	THR
6	1F	22	PHE
6	1F	33	LEU
6	1F	43	TYR
6	1F	46	LYS
6	1F	68	ARG
6	1F	91	LYS
6	1F	106	LYS
6	1F	129	MET
6	1F	154	ARG
6	1F	173	PHE
6	1F	186	CYS
6	1F	212	ASP
6	1F	247	ARG
6	1F	261	HIS
6	1F	266	CYS
6	1F	277	LYS
6	1F	282	LYS
6	1F	292	ASP
6	1F	317	MET

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Mol	Chain	Res	Type
6	1F	362	CYS
6	1F	385	ARG
6	1F	430	MET
7	1G	19	MET
7	1G	39	ARG
7	1G	43	HIS
7	1G	64	LYS
7	1G	69	CYS
7	1G	130	PHE
7	1G	161	ARG
7	1G	177	ARG
7	1G	180	ASP
7	1G	190	MET
7	1G	191	PHE
7	1G	192	MET
7	1G	237	ASN
7	1G	252	PRO
7	1G	255	HIS
7	1G	278	ARG
7	1G	291	LEU
7	1G	391	PHE
7	1G	401	HIS
7	1G	402	ASN
7	1G	417	TYR
7	1G	418	ARG
7	1G	420	ASP
7	1G	494	HIS
7	1G	504	ASP
7	1G	516	LYS
7	1G	537	LEU
7	1G	542	PHE
7	1G	549	HIS
7	1G	556	MET
7	1G	584	LYS
7	1G	596	ASP
7	1G	601	ARG
7	1G	613	TYR
7	1G	647	GLU
7	1G	669	LYS
7	1G	679	ARG
8	1H	3	MET
8	1H	25	ARG

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Mol	Chain	Res	Type
8	1H	47	GLN
8	1H	61	LEU
8	1H	62	ARG
8	1H	98	MET
8	1H	106	LEU
8	1H	110	SER
8	1H	184	MET
8	1H	220	PHE
8	1H	237	PHE
8	1H	283	ASP
8	1H	317	GLN
9	1I	20	ARG
9	1I	27	TRP
9	1I	40	TYR
9	1I	50	TYR
9	1I	58	SER
9	1I	61	PHE
9	1I	123	GLN
9	1I	140	SER
9	1I	162	GLU
10	1J	7	PHE
10	1J	51	PHE
10	1J	68	PHE
10	1J	74	MET
10	1J	78	MET
10	1J	87	LYS
10	1J	98	MET
10	1J	100	GLU
10	1J	101	PHE
10	1J	136	PHE
11	1K	6	MET
11	1K	7	ASN
11	1K	43	MET
11	1K	52	HIS
11	1K	53	PHE
11	1K	91	GLN
11	1K	98	CYS
12	1L	25	ASN
12	1L	31	LEU
12	1L	37	LYS
12	1L	52	LEU
12	1L	69	MET

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Mol	Chain	Res	Type
12	1L	88	MET
12	1L	141	PHE
12	1L	176	ARG
12	1L	182	PHE
12	1L	203	MET
12	1L	229	LEU
12	1L	300	LYS
12	1L	313	MET
12	1L	331	MET
12	1L	340	PHE
12	1L	364	LYS
12	1L	409	LEU
12	1L	411	MET
12	1L	486	MET
12	1L	514	LYS
12	1L	521	LYS
12	1L	525	MET
12	1L	576	MET
13	1M	57	PHE
13	1M	122	PHE
13	1M	139	GLN
13	1M	148	TYR
13	1M	152	TYR
13	1M	204	MET
13	1M	207	MET
13	1M	333	ASN
13	1M	334	TYR
13	1M	336	ARG
13	1M	359	TRP
13	1M	453	MET
14	1N	40	MET
14	1N	46	LYS
14	1N	71	MET
14	1N	95	MET
14	1N	167	TRP
14	1N	179	MET
14	1N	182	SER
14	1N	190	MET
14	1N	204	ASN
14	1N	237	MET
14	1N	243	LEU
14	1N	323	MET

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Mol	Chain	Res	Type
15	1O	28	ASP
15	1O	40	ARG
15	1O	67	LYS
15	1O	90	ASP
15	1O	138	MET
15	1O	145	ARG
15	1O	146	LYS
15	1O	157	LYS
15	1O	161	CYS
15	1O	190	HIS
15	1O	206	TYR
15	1O	208	LYS
15	1O	211	LEU
15	1O	223	TYR
15	1O	226	ARG
15	1O	236	GLU
15	1O	242	LYS
15	1O	248	TRP
15	1O	318	TRP
16	1P	13	ARG
16	1P	29	PHE
16	1P	50	ARG
16	1P	82	ARG
16	1P	83	LYS
16	1P	145	TYR
16	1P	154	LYS
16	1P	177	ARG
16	1P	181	TYR
16	1P	186	ARG
16	1P	193	LEU
16	1P	206	TYR
16	1P	235	ARG
16	1P	243	GLN
16	1P	253	PHE
16	1P	263	TYR
16	1P	265	TRP
16	1P	288	HIS
16	1P	300	LEU
16	1P	335	LYS
17	1Q	36	ARG
17	1Q	38	PHE
17	1Q	50	ASN

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Mol	Chain	Res	Type
17	1Q	57	MET
17	1Q	84	LEU
17	1Q	91	ASP
17	1Q	95	PHE
17	1Q	101	TRP
17	1Q	103	PHE
17	1Q	112	LYS
17	1Q	115	SER
17	1Q	116	LYS
17	1Q	126	LYS
18	1R	39	PHE
18	1R	70	ARG
18	1R	76	ASP
18	1R	86	TYR
19	1S	40	TYR
19	1S	56	GLU
19	1S	65	TRP
19	1S	67	ARG
19	1S	85	GLN
19	1S	88	ARG
19	1S	90	LEU
19	1S	97	LYS
20	1T	21	LEU
20	1T	22	TYR
20	1T	24	LYS
20	1T	37	MET
20	1T	60	PHE
20	1T	61	GLU
20	1T	69	LYS
20	1T	70	LEU
20	1T	71	MET
20	1T	78	ASP
20	1T	87	TYR
20	1U	8	LEU
20	1U	17	TYR
20	1U	22	TYR
20	1U	23	ASP
20	1U	33	ASN
20	1U	52	MET
20	1U	87	TYR
21	1V	22	ARG
21	1V	27	TYR

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Mol	Chain	Res	Type
21	1V	29	LYS
21	1V	54	LYS
21	1V	57	MET
21	1V	69	GLU
21	1V	72	GLN
22	1W	21	PHE
22	1W	39	TRP
22	1W	53	ASP
22	1W	57	LYS
22	1W	64	ARG
22	1W	65	GLU
22	1W	66	MET
22	1W	67	PHE
22	1W	68	MET
22	1W	72	HIS
22	1W	87	LYS
22	1W	117	ASP
22	1W	121	LYS
22	1W	126	HIS
23	1X	16	GLU
23	1X	47	TRP
23	1X	56	LEU
23	1X	69	PHE
23	1X	71	ARG
23	1X	75	ARG
23	1X	76	HIS
23	1X	77	CYS
23	1X	81	PHE
23	1X	113	LYS
23	1X	134	ARG
23	1X	143	SER
23	1X	146	ARG
23	1X	152	GLU
23	1X	156	ASP
23	1X	171	MET
24	1Y	57	ARG
24	1Y	60	PHE
24	1Y	90	PHE
24	1Y	126	MET
25	1Z	5	LYS
25	1Z	27	ARG
25	1Z	68	ARG

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Mol	Chain	Res	Type
25	1Z	82	ARG
25	1Z	86	MET
25	1Z	94	GLU
26	1a	17	PHE
26	1a	50	ARG
26	1a	53	CYS
27	1b	12	TRP
27	1b	34	LEU
27	1b	46	ARG
27	1b	76	SER
27	1b	77	LEU
27	1b	81	LYS
28	1c	2	PHE
29	1d	78	ARG
29	1d	82	MET
29	1d	89	ASP
29	1d	104	LYS
30	1e	6	GLN
30	1e	8	ARG
30	1e	21	SER
30	1e	31	ARG
30	1e	36	GLU
30	1e	54	GLU
30	1e	70	LYS
30	1e	73	LYS
30	1e	79	LYS
30	1e	82	ARG
30	1e	83	ASP
30	1e	96	HIS
31	1f	15	LEU
31	1f	22	PHE
31	1f	24	CYS
31	1f	28	ARG
31	1f	29	ARG
32	1g	29	ASP
32	1g	43	ASP
32	1g	63	PHE
32	1g	79	TYR
32	1g	99	TYR
32	1g	103	ASN
32	1g	105	LEU
32	1g	112	CYS

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Mol	Chain	Res	Type
32	1g	122	GLU
33	1h	7	ARG
33	1h	27	PHE
33	1h	46	PHE
33	1h	59	TYR
33	1h	111	ARG
33	1h	122	TRP
33	1h	123	TYR
33	1h	130	LYS
34	1i	16	GLU
34	1i	37	ARG
34	1i	56	TRP
35	1j	13	GLN
35	1j	40	PHE
35	1j	50	HIS
35	1j	59	TRP
36	1k	22	LYS
36	1k	34	LYS
36	1k	46	ARG
36	1k	58	ASN
36	1k	59	ASN
36	1k	74	PHE
36	1k	86	TYR
37	1l	71	LEU
37	1l	82	ASP
37	1l	124	SER
38	1m	4	LYS
38	1m	30	LYS
38	1m	45	GLU
38	1m	55	ARG
38	1m	61	ASP
38	1m	69	TYR
38	1m	80	ARG
38	1m	113	LYS
39	1n	47	PHE
39	1n	48	ASP
39	1n	116	ASP
39	1n	126	ARG
39	1n	134	ARG
39	1n	172	ARG
40	1o	21	MET
40	1o	30	PHE

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Mol	Chain	Res	Type
40	1o	38	MET
40	1o	53	GLN
40	1o	93	ASP
40	1o	94	TYR
40	1o	110	ARG
41	1p	14	ARG
41	1p	25	LEU
41	1p	49	GLU
41	1p	53	GLN
41	1p	54	GLN
41	1p	62	TYR
41	1p	63	TYR
41	1p	92	ARG
41	1p	95	TYR
41	1p	126	LYS
41	1p	136	LYS
41	1p	159	LYS
41	1p	170	LYS
42	1q	52	ASN
42	1q	68	MET
42	1q	72	ASP
42	1q	81	MET
42	1q	87	HIS
42	1q	96	ASP
42	1q	106	ARG
42	1q	108	TYR
42	1q	115	PHE
43	1r	2	SER
43	1r	19	LEU
43	1r	59	ARG
43	1r	63	MET
43	1r	101	LYS
43	1r	106	SER
44	1s	38	TYR
44	1s	51	PHE
44	1s	62	ARG
44	1s	70	ARG
44	1s	74	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	10	ASN
2	1B	121	ASN
2	1B	162	GLN
3	1C	39	GLN
3	1C	88	ASN
3	1C	160	HIS
4	1D	316	ASN
5	1E	9	HIS
5	1E	91	ASN
6	1F	116	HIS
6	1F	148	ASN
6	1F	150	GLN
6	1F	257	ASN
6	1F	373	ASN
7	1G	383	ASN
7	1G	491	ASN
8	1H	212	ASN
12	1L	139	GLN
12	1L	295	GLN
12	1L	506	ASN
13	1M	48	ASN
14	1N	174	GLN
16	1P	216	ASN
17	1Q	44	ASN
22	1W	102	HIS
25	1Z	90	ASN
27	1b	10	ASN
27	1b	45	ASN
30	1e	6	GLN
30	1e	20	GLN
32	1g	86	GLN
36	1k	59	ASN
40	1o	3	HIS
41	1p	103	ASN
41	1p	122	GLN
42	1q	46	ASN
42	1q	87	HIS
42	1q	116	ASN
44	1s	40	ASN
44	1s	42	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](#)

8 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
14	FME	1N	1	14	8,9,10	0.50	0	7,9,11	0.97	1 (14%)
10	FME	1J	1	10	8,9,10	0.53	0	7,9,11	0.98	1 (14%)
1	FME	1A	1	1	8,9,10	0.52	0	7,9,11	1.04	1 (14%)
11	FME	1K	1	11	8,9,10	0.51	0	7,9,11	1.15	1 (14%)
8	FME	1H	1	8	8,9,10	0.50	0	7,9,11	1.01	1 (14%)
34	SAC	1i	1	-	7,8,9	0.54	0	8,9,11	1.07	1 (12%)
13	FME	1M	1	13	8,9,10	0.51	0	7,9,11	1.00	1 (14%)
12	FME	1L	1	12	8,9,10	0.50	0	7,9,11	0.97	1 (14%)

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
14	FME	1N	1	14	-	0/7/9/11	-
10	FME	1J	1	10	-	2/7/9/11	-
1	FME	1A	1	1	-	1/7/9/11	-
11	FME	1K	1	11	-	1/7/9/11	-
8	FME	1H	1	8	-	1/7/9/11	-
34	SAC	1i	1	-	-	0/7/8/10	-
13	FME	1M	1	13	-	2/7/9/11	-
12	FME	1L	1	12	-	0/7/9/11	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1i	1	SAC	O-C-CA	-2.91	117.14	124.78
1	1A	1	FME	O-C-CA	-2.54	118.13	124.78
10	1J	1	FME	O-C-CA	-2.53	118.15	124.78
11	1K	1	FME	O-C-CA	-2.51	118.19	124.78
13	1M	1	FME	O-C-CA	-2.49	118.25	124.78
8	1H	1	FME	O-C-CA	-2.49	118.25	124.78
12	1L	1	FME	O-C-CA	-2.38	118.53	124.78
14	1N	1	FME	O-C-CA	-2.32	118.70	124.78

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	1H	1	FME	O-C-CA-CB
10	1J	1	FME	O-C-CA-CB
13	1M	1	FME	O1-CN-N-CA
10	1J	1	FME	N-CA-CB-CG
11	1K	1	FME	C-CA-CB-CG
1	1A	1	FME	CB-CG-SD-CE
13	1M	1	FME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 3 are monoatomic - leaving 28 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
55	NDP	1P	501	-	45,52,52	0.61	0	53,80,80	0.74	2 (3%)
57	EHZ	1n	201	-	29,36,37	0.16	0	35,44,47	1.32	1 (2%)
50	3PE	1L	702	-	41,41,50	0.30	0	44,46,55	1.24	5 (11%)
45	PC1	1A	201	-	34,34,53	0.32	0	40,42,61	0.41	0
50	3PE	1N	401	-	50,50,50	0.27	0	53,55,55	0.40	0
46	SF4	1B	201	2	0,12,12	-	-	-	-	-
52	CDL	1r	201	-	60,60,99	0.33	0	66,72,111	0.41	0
46	SF4	1G	802	7	0,12,12	-	-	-	-	-
50	3PE	1b	101	-	46,46,50	0.27	0	49,51,55	0.34	0
46	SF4	1G	801	7	0,12,12	-	-	-	-	-
50	3PE	1Y	202	-	50,50,50	0.26	0	53,55,55	0.39	0
46	SF4	1I	201	9	0,12,12	-	-	-	-	-
58	MYR	1l	201	-	14,14,15	0.34	0	13,13,15	0.38	0
47	FES	1G	803	7	0,4,4	-	-	-	-	-
45	PC1	1H	401	-	43,43,53	0.29	0	49,51,61	0.33	0
52	CDL	1N	402	-	76,76,99	0.30	0	82,88,111	0.36	0
45	PC1	1M	502	-	45,45,53	0.28	0	51,53,61	0.34	0
46	SF4	1I	202	9	0,12,12	-	-	-	-	-
45	PC1	1I	203	-	53,53,53	0.26	0	59,61,61	0.30	0
45	PC1	1g	201	-	43,43,53	0.29	0	49,51,61	0.36	0
53	GTP	1O	401	54	26,34,34	0.96	2 (7%)	32,54,54	0.87	1 (3%)
46	SF4	1F	502	6	0,12,12	-	-	-	-	-
50	3PE	1L	701	-	45,45,50	0.28	0	48,50,55	0.32	0
57	EHZ	1W	201	-	29,36,37	0.17	0	35,44,47	1.26	1 (2%)
51	PGT	1M	501	-	50,50,50	0.49	0	53,56,56	0.49	0
48	FMN	1F	501	-	33,33,33	0.57	0	48,50,50	0.67	1 (2%)
47	FES	1E	301	5	0,4,4	-	-	-	-	-
50	3PE	1Y	201	-	30,30,50	0.34	0	33,35,55	0.65	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
57	EHZ	1n	201	-	-	2/42/44/45	-
50	3PE	1L	702	-	-	6/45/45/54	-
45	PC1	1A	201	-	-	5/38/38/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	3PE	1N	401	-	-	11/54/54/54	-
46	SF4	1B	201	2	-	-	0/6/5/5
52	CDL	1r	201	-	-	13/71/71/110	-
50	3PE	1b	101	-	-	4/50/50/54	-
46	SF4	1G	802	7	-	-	0/6/5/5
46	SF4	1G	801	7	-	-	0/6/5/5
50	3PE	1Y	202	-	-	9/54/54/54	-
46	SF4	1I	201	9	-	-	0/6/5/5
58	MYR	1l	201	-	-	0/11/12/13	-
47	FES	1E	301	5	-	-	0/1/1/1
47	FES	1G	803	7	-	-	0/1/1/1
45	PC1	1H	401	-	-	8/47/47/57	-
52	CDL	1N	402	-	-	6/87/87/110	-
45	PC1	1M	502	-	-	6/49/49/57	-
46	SF4	1I	202	9	-	-	0/6/5/5
45	PC1	1I	203	-	-	3/57/57/57	-
45	PC1	1g	201	-	-	6/47/47/57	-
53	GTP	1O	401	54	-	1/18/38/38	0/3/3/3
46	SF4	1F	502	6	-	-	0/6/5/5
50	3PE	1L	701	-	-	8/49/49/54	-
57	EHZ	1W	201	-	-	4/42/44/45	-
51	PGT	1M	501	-	-	23/55/55/55	-
48	FMN	1F	501	-	-	3/18/18/18	0/3/3/3
55	NDP	1P	501	-	-	5/30/77/77	0/5/5/5
50	3PE	1Y	201	-	-	6/34/34/54	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	1O	401	GTP	C5-C6	-2.63	1.42	1.47
53	1O	401	GTP	C8-N7	-2.07	1.31	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1n	201	EHZ	C10-S1-C9	7.31	124.62	101.87
57	1W	201	EHZ	C10-S1-C9	6.73	122.83	101.87
50	1L	702	3PE	O21-C21-C22	6.08	124.60	111.50
53	1O	401	GTP	O4'-C1'-C2'	-2.80	102.83	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	1L	702	3PE	O21-C21-O22	-2.62	117.38	123.70
55	1P	501	NDP	O4D-C1D-C2D	-2.50	101.19	106.64
50	1L	702	3PE	C2-O21-C21	2.48	123.90	117.79
50	1Y	201	3PE	O21-C21-C22	2.47	116.82	111.50
50	1L	702	3PE	O21-C2-C3	2.23	116.48	108.40
55	1P	501	NDP	C5A-C6A-N6A	2.23	123.74	120.35
50	1L	702	3PE	O21-C2-C1	2.11	116.05	108.40
48	1F	501	FMN	C4-N3-C2	-2.02	121.91	125.64

There are no chirality outliers.

All (129) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	1H	401	PC1	C11-O13-P-O12
45	1I	203	PC1	C1-O11-P-O14
45	1M	502	PC1	O32-C31-O31-C3
45	1M	502	PC1	C32-C31-O31-C3
45	1g	201	PC1	C1-O11-P-O14
48	1F	501	FMN	C1'-C2'-C3'-C4'
50	1L	701	3PE	C1-O11-P-O12
50	1L	702	3PE	O22-C21-O21-C2
50	1L	702	3PE	C22-C21-O21-C2
50	1Y	201	3PE	C1-O11-P-O14
50	1Y	201	3PE	O32-C31-O31-C3
50	1Y	201	3PE	C32-C31-O31-C3
50	1Y	201	3PE	O22-C21-O21-C2
50	1Y	201	3PE	C22-C21-O21-C2
50	1Y	202	3PE	C1-O11-P-O14
50	1Y	202	3PE	C2-C1-O11-P
51	1M	501	PGT	O31-C31-O2-C2
51	1M	501	PGT	C1-O3P-P-O1P
51	1M	501	PGT	C1-O3P-P-O4P
51	1M	501	PGT	C4-O4P-P-O1P
52	1r	201	CDL	CA3-OA5-PA1-OA3
52	1r	201	CDL	CB2-OB2-PB2-OB3
52	1r	201	CDL	CB4-CB3-OB5-PB2
57	1W	201	EHZ	O2-C9-S1-C10
57	1W	201	EHZ	C8-C9-S1-C10
57	1n	201	EHZ	O2-C9-S1-C10
57	1n	201	EHZ	C8-C9-S1-C10
51	1M	501	PGT	O11-C11-O3-C3
51	1M	501	PGT	C12-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
51	1M	501	PGT	C32-C31-O2-C2
57	1W	201	EHZ	C13-C12-N1-C11
57	1W	201	EHZ	O3-C12-N1-C11
45	1H	401	PC1	C31-C32-C33-C34
45	1A	201	PC1	C1-O11-P-O13
51	1M	501	PGT	C4-O4P-P-O3P
55	1P	501	NDP	C2D-C1D-N1N-C2N
55	1P	501	NDP	C2D-C1D-N1N-C6N
51	1M	501	PGT	C14-C15-C16-C17
51	1M	501	PGT	C40-C41-C42-C43
45	1I	203	PC1	C24-C25-C26-C27
51	1M	501	PGT	C15-C16-C17-C18
51	1M	501	PGT	C34-C35-C36-C37
48	1F	501	FMN	O2'-C2'-C3'-C4'
51	1M	501	PGT	C5-C4-O4P-P
50	1Y	202	3PE	C3C-C3D-C3E-C3F
45	1H	401	PC1	C11-O13-P-O11
50	1L	701	3PE	C1-O11-P-O13
50	1L	701	3PE	C38-C39-C3A-C3B
51	1M	501	PGT	C21-C22-C23-C24
50	1L	702	3PE	O11-C1-C2-O21
50	1N	401	3PE	O31-C31-C32-C33
50	1b	101	3PE	O21-C2-C3-O31
52	1N	402	CDL	OA6-CA4-CA6-OA8
52	1r	201	CDL	CA4-CA3-OA5-PA1
52	1N	402	CDL	C76-C77-C78-C79
52	1N	402	CDL	CA3-CA4-CA6-OA8
51	1M	501	PGT	C22-C23-C24-C25
50	1Y	202	3PE	C35-C36-C37-C38
50	1Y	202	3PE	O11-C1-C2-O21
45	1I	203	PC1	O31-C31-C32-C33
51	1M	501	PGT	C33-C34-C35-C36
45	1M	502	PC1	C2-C1-O11-P
50	1N	401	3PE	C2-C1-O11-P
48	1F	501	FMN	O2'-C2'-C3'-O3'
55	1P	501	NDP	O4D-C1D-N1N-C6N
50	1N	401	3PE	C34-C35-C36-C37
51	1M	501	PGT	C45-C46-C47-C48
50	1b	101	3PE	C1-C2-C3-O31
50	1N	401	3PE	C2-C3-O31-C31
52	1r	201	CDL	OB6-CB4-CB6-OB8
50	1Y	201	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
50	1Y	202	3PE	C1-O11-P-O13
52	1r	201	CDL	CB2-OB2-PB2-OB5
55	1P	501	NDP	O4D-C1D-N1N-C2N
45	1A	201	PC1	C1-O11-P-O14
45	1H	401	PC1	C11-O13-P-O14
50	1L	701	3PE	C1-O11-P-O14
52	1r	201	CDL	CB3-OB5-PB2-OB3
50	1Y	202	3PE	C12-C11-O13-P
50	1b	101	3PE	C12-C11-O13-P
51	1M	501	PGT	C32-C33-C34-C35
45	1A	201	PC1	O13-C11-C12-N
50	1L	702	3PE	C1-C2-C3-O31
52	1r	201	CDL	C52-C51-CB5-OB6
50	1b	101	3PE	C33-C34-C35-C36
50	1L	701	3PE	C36-C37-C38-C39
50	1N	401	3PE	C39-C3A-C3B-C3C
50	1N	401	3PE	O21-C2-C3-O31
45	1M	502	PC1	C11-O13-P-O11
50	1N	401	3PE	C1-O11-P-O13
52	1r	201	CDL	CA3-OA5-PA1-OA2
51	1M	501	PGT	C4-C5-C6-O6
51	1M	501	PGT	C2-C1-O3P-P
52	1N	402	CDL	C55-C56-C57-C58
50	1L	702	3PE	C1-C2-O21-C21
50	1N	401	3PE	C3A-C3B-C3C-C3D
45	1g	201	PC1	C1-O11-P-O13
50	1N	401	3PE	O11-C1-C2-O21
45	1g	201	PC1	O11-C1-C2-C3
50	1Y	202	3PE	O11-C1-C2-C3
52	1r	201	CDL	CB3-CB4-CB6-OB8
45	1M	502	PC1	C35-C36-C37-C38
51	1M	501	PGT	C39-C40-C41-C42
52	1N	402	CDL	C53-C54-C55-C56
51	1M	501	PGT	C41-C42-C43-C44
45	1g	201	PC1	O31-C31-C32-C33
45	1A	201	PC1	O21-C2-C3-O31
45	1H	401	PC1	O21-C2-C3-O31
50	1L	701	3PE	O31-C31-C32-C33
50	1Y	202	3PE	C3F-C3G-C3H-C3I
52	1r	201	CDL	C12-C13-C14-C15
50	1L	701	3PE	C39-C3A-C3B-C3C
45	1H	401	PC1	C22-C23-C24-C25

Continued on next page...

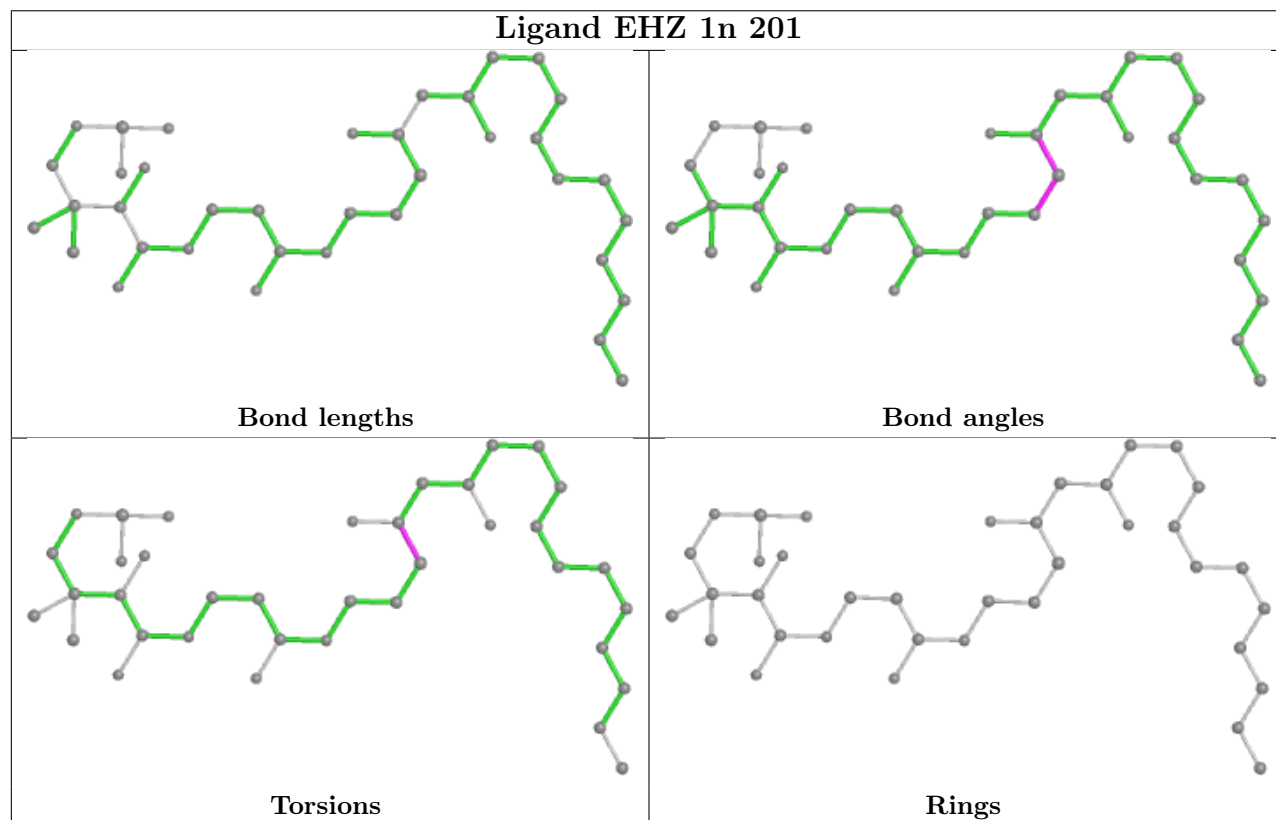
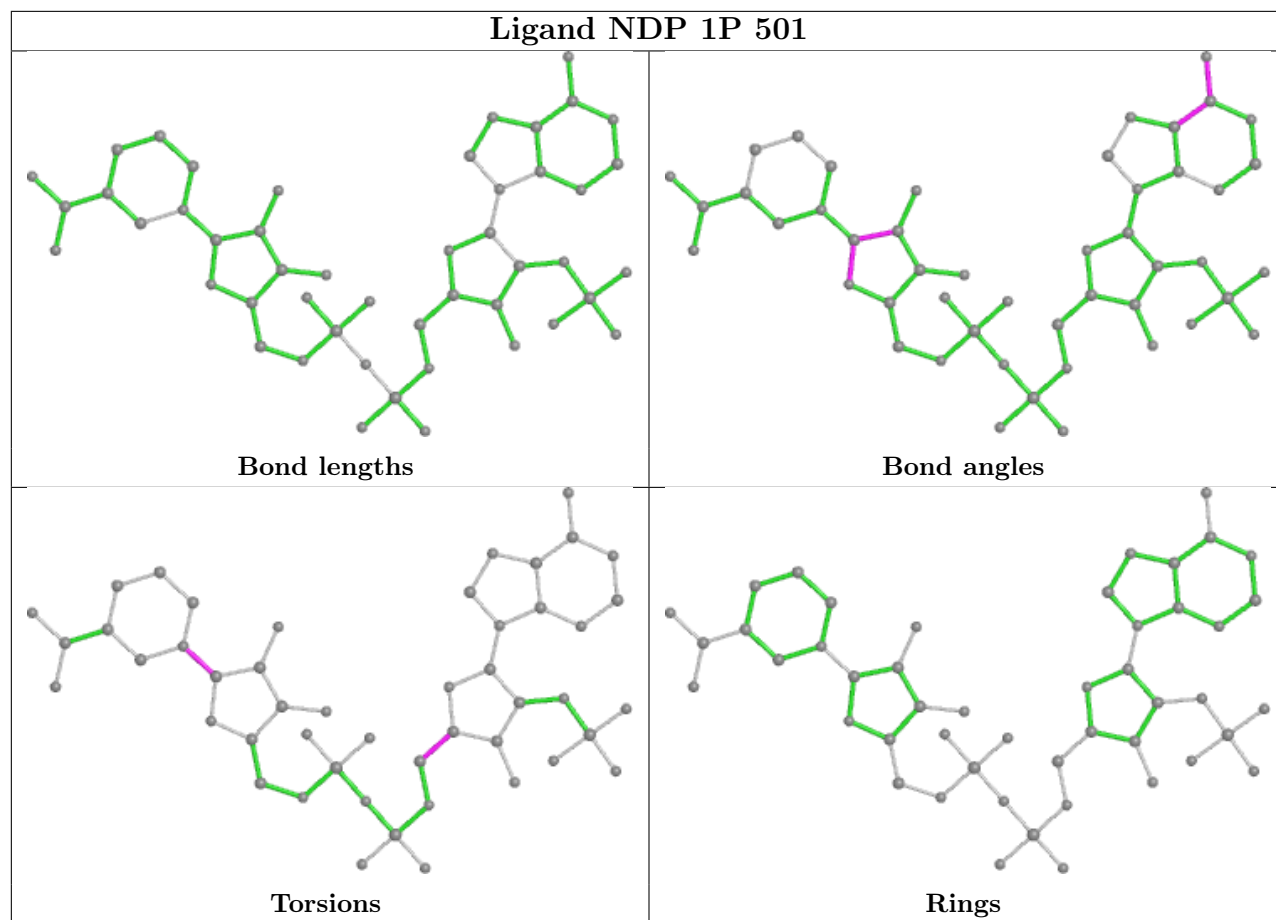
Continued from previous page...

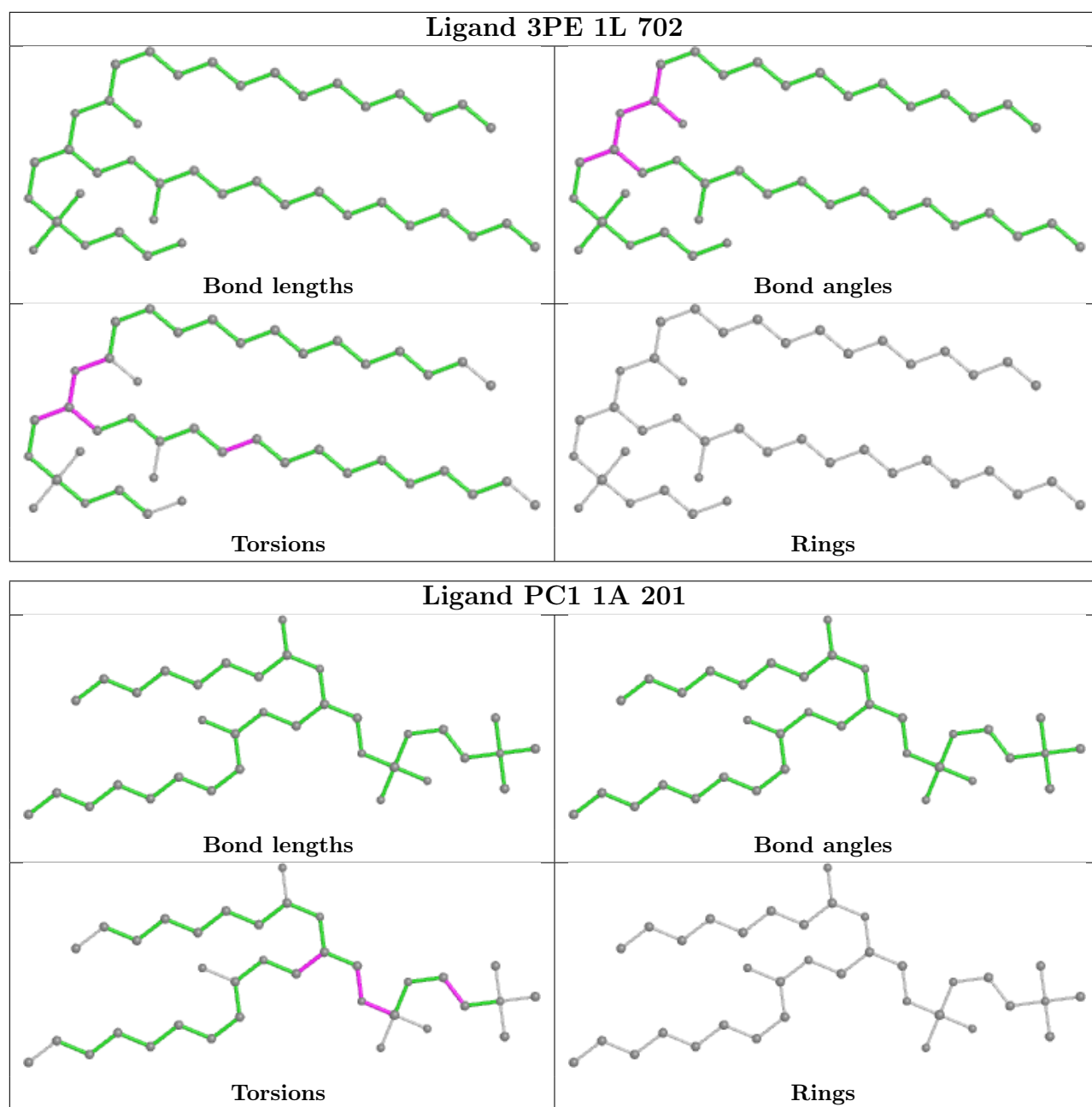
Mol	Chain	Res	Type	Atoms
45	1A	201	PC1	C2-C1-O11-P
53	1O	401	GTP	C4'-C5'-O5'-PA
50	1L	702	3PE	C32-C33-C34-C35
45	1M	502	PC1	C11-O13-P-O14
50	1N	401	3PE	C1-O11-P-O14
51	1M	501	PGT	C4-O4P-P-O2P
55	1P	501	NDP	O4B-C4B-C5B-O5B
45	1H	401	PC1	C32-C33-C34-C35
50	1N	401	3PE	O32-C31-C32-C33
45	1g	201	PC1	O32-C31-C32-C33
45	1g	201	PC1	O21-C21-C22-C23
52	1r	201	CDL	C32-C31-CA7-OA8
52	1N	402	CDL	C37-C38-C39-C40
50	1L	701	3PE	O32-C31-C32-C33
45	1H	401	PC1	O31-C31-C32-C33
52	1r	201	CDL	C12-C11-CA5-OA6

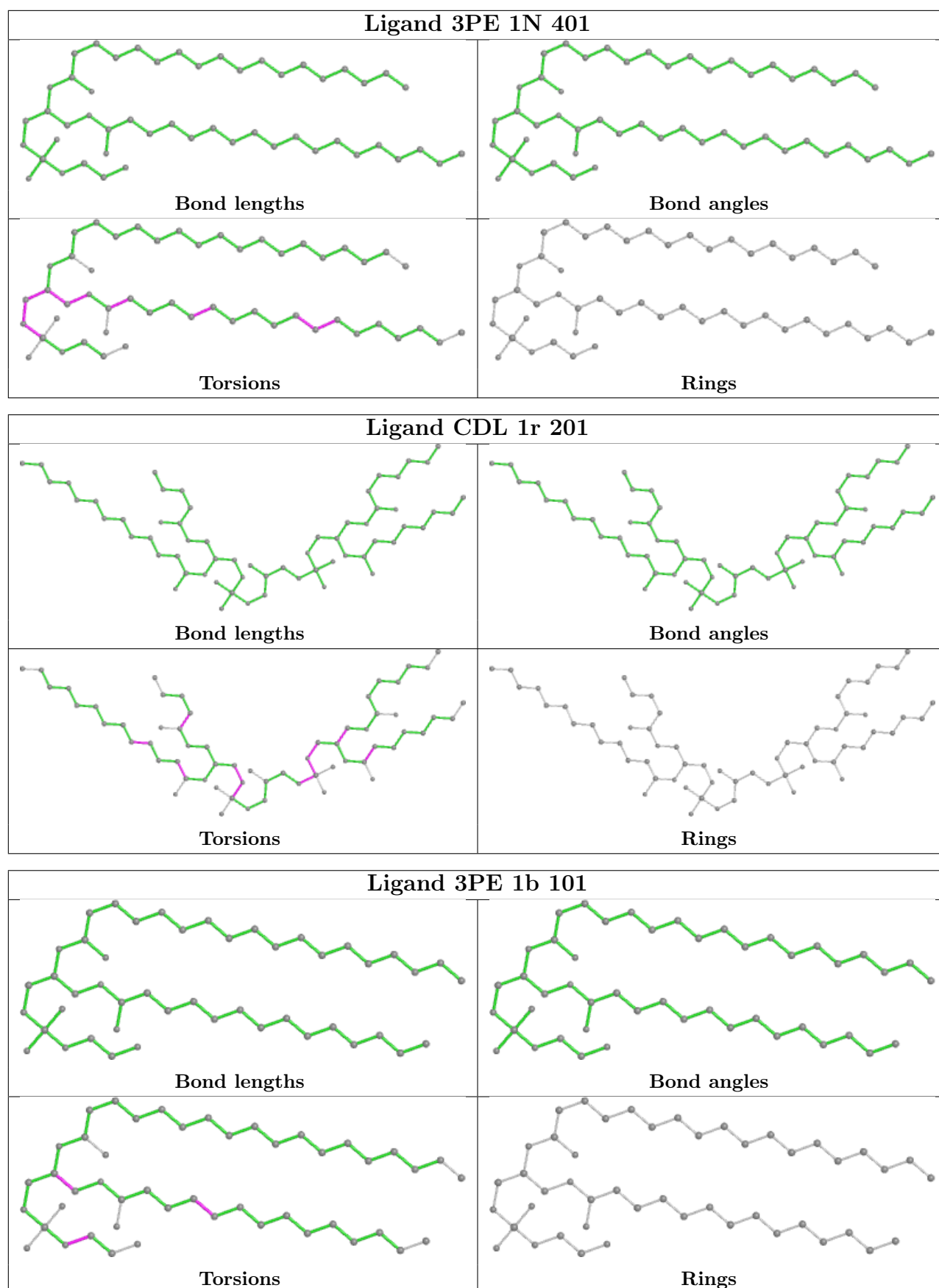
There are no ring outliers.

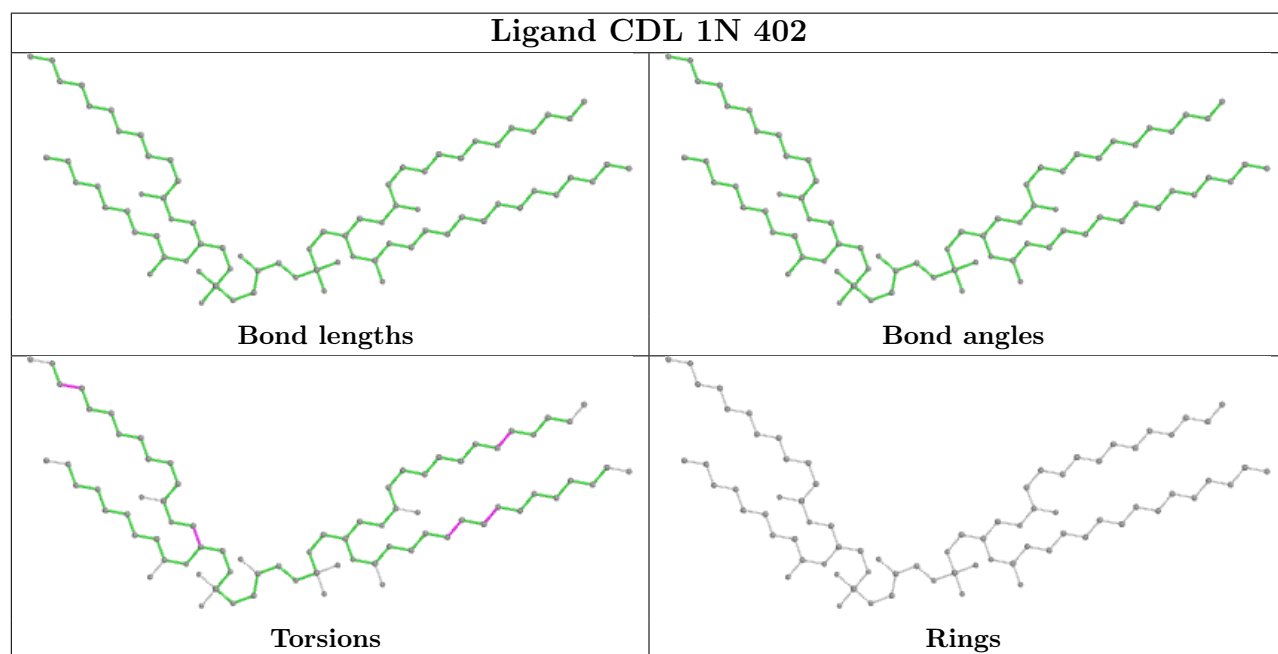
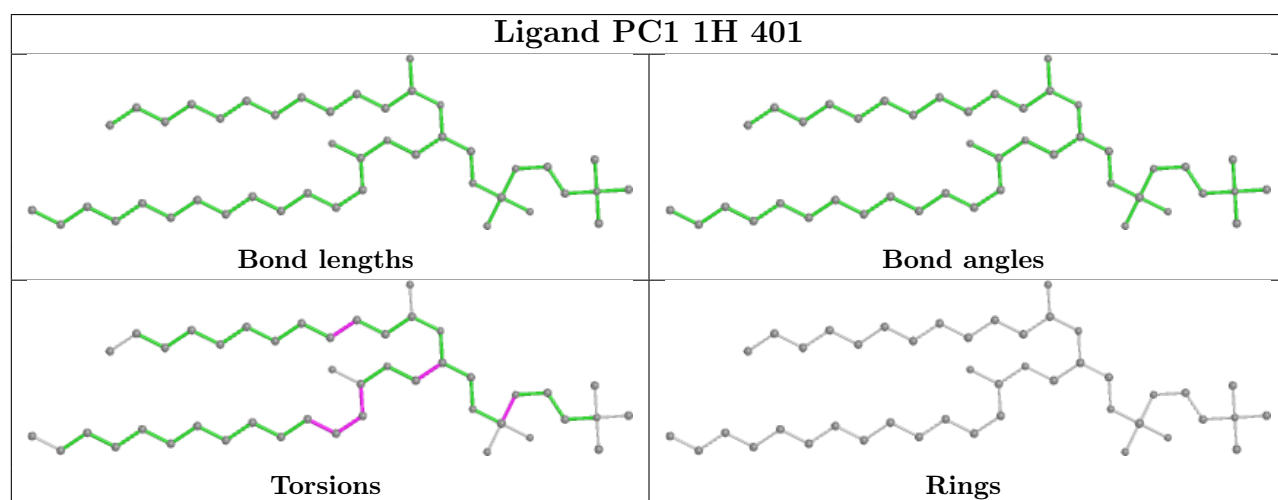
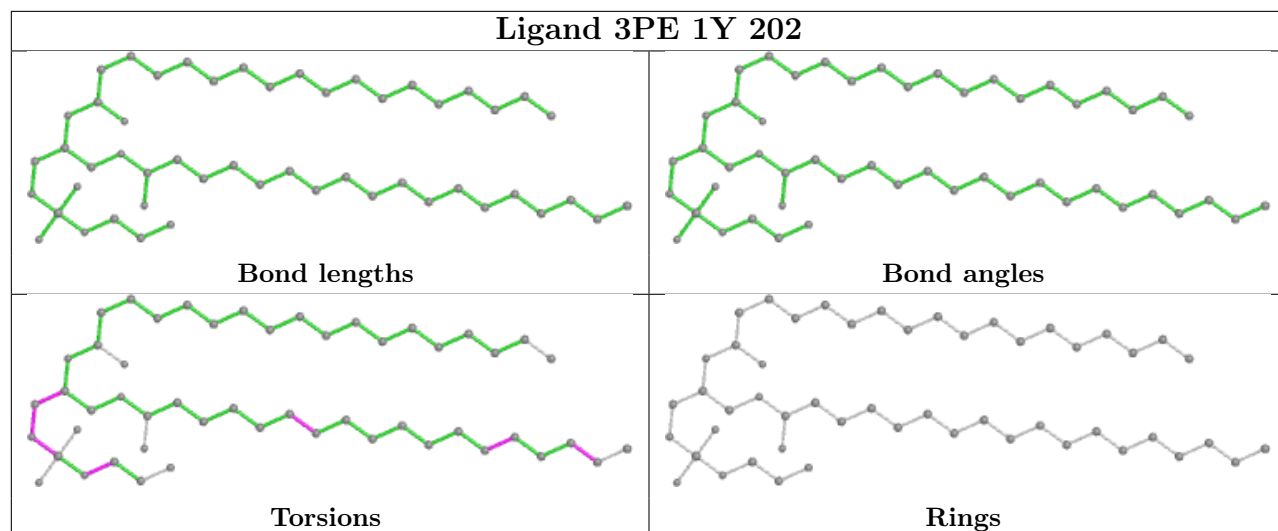
No monomer is involved in short contacts.

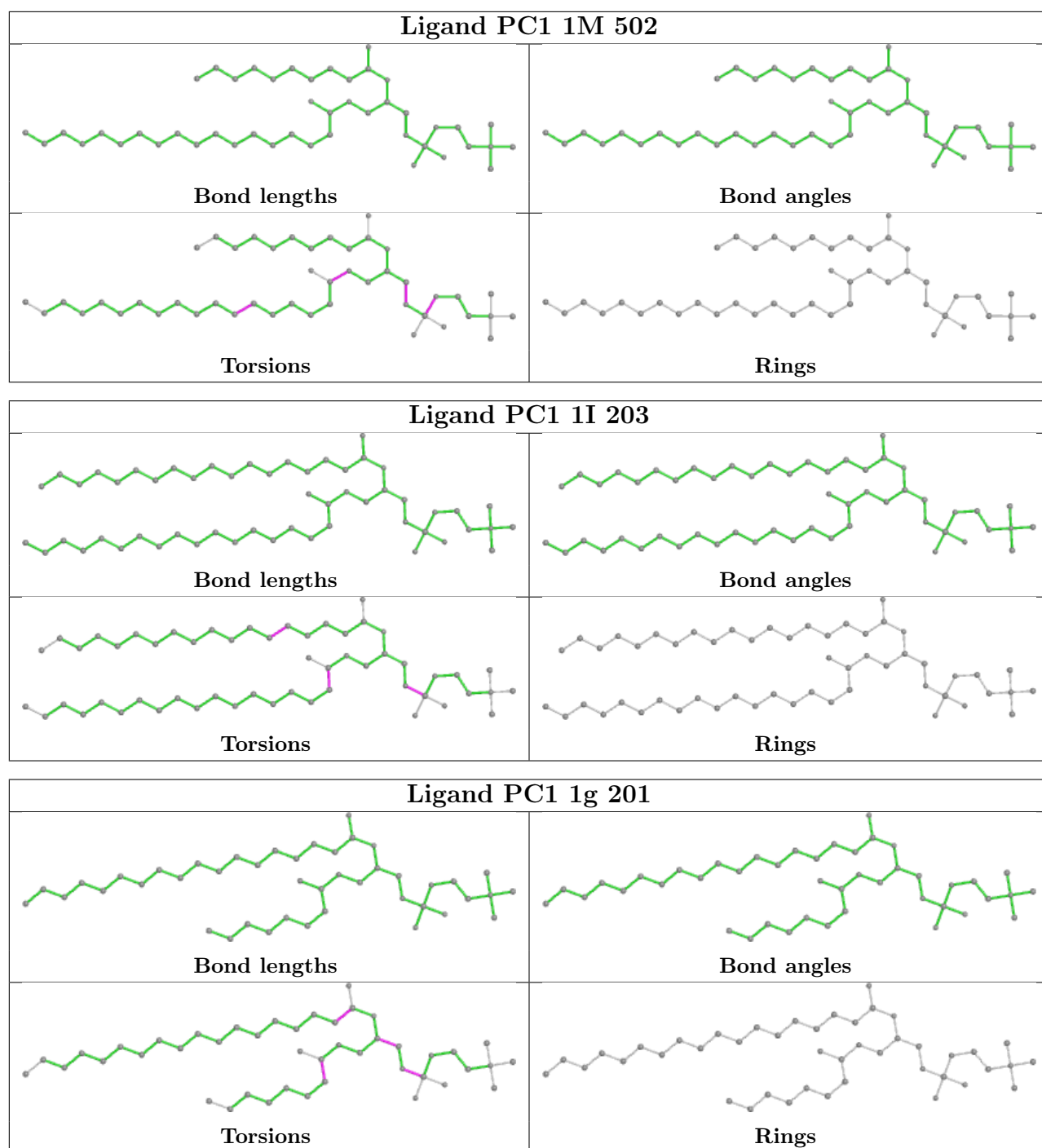
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

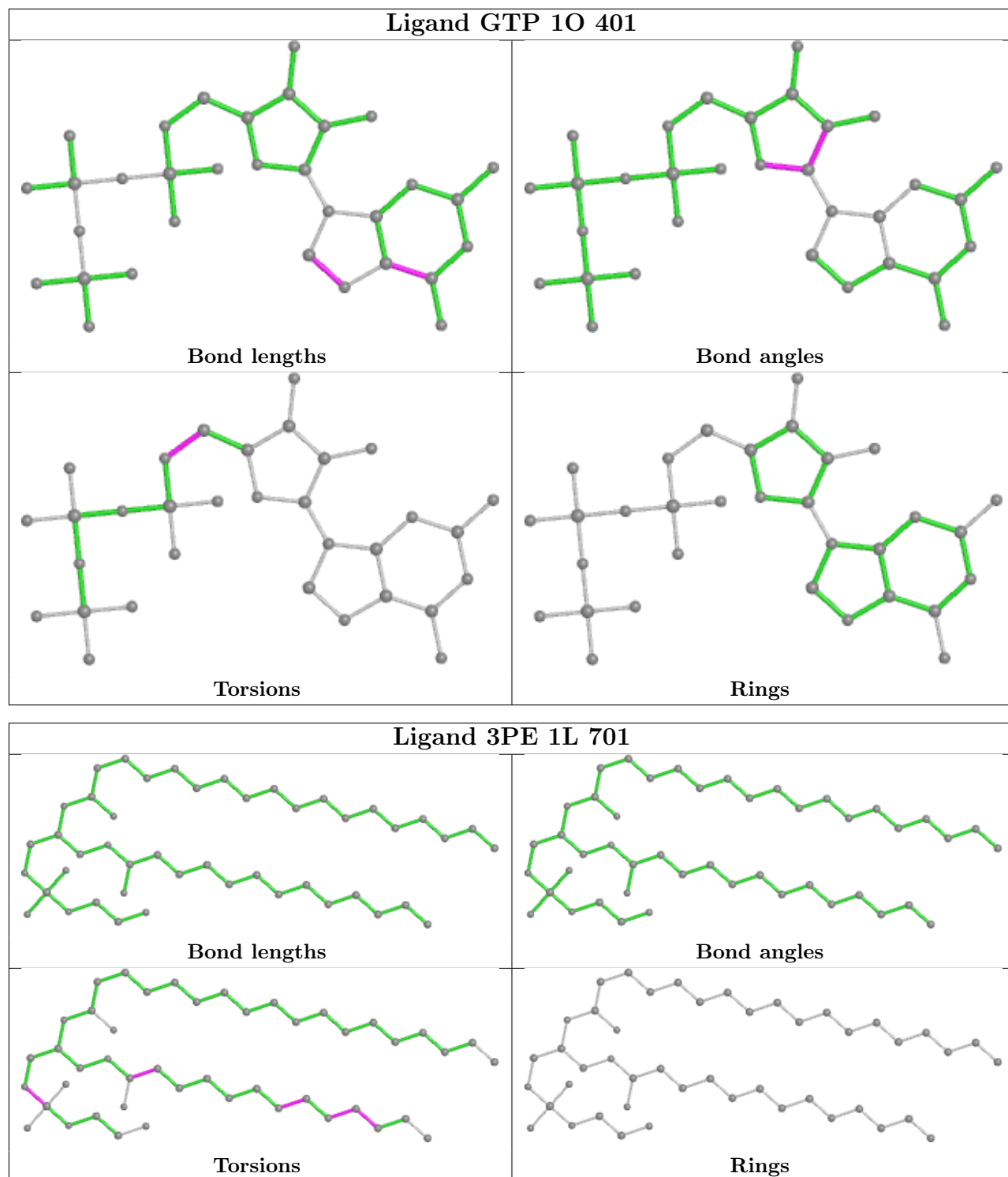


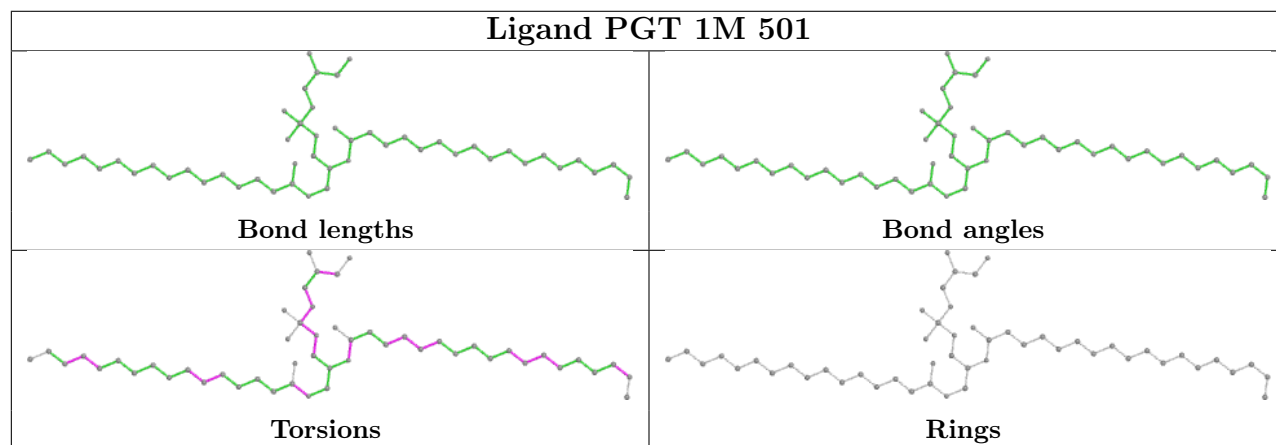
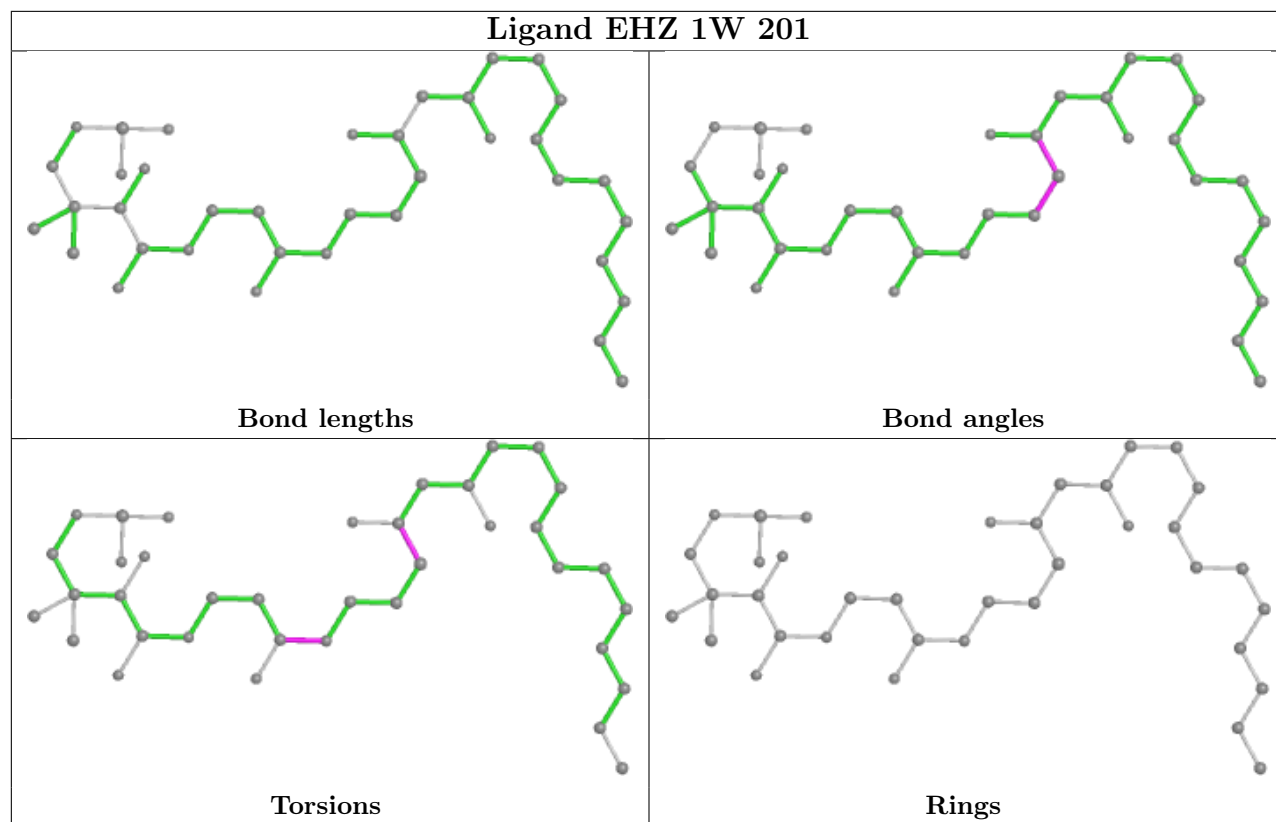


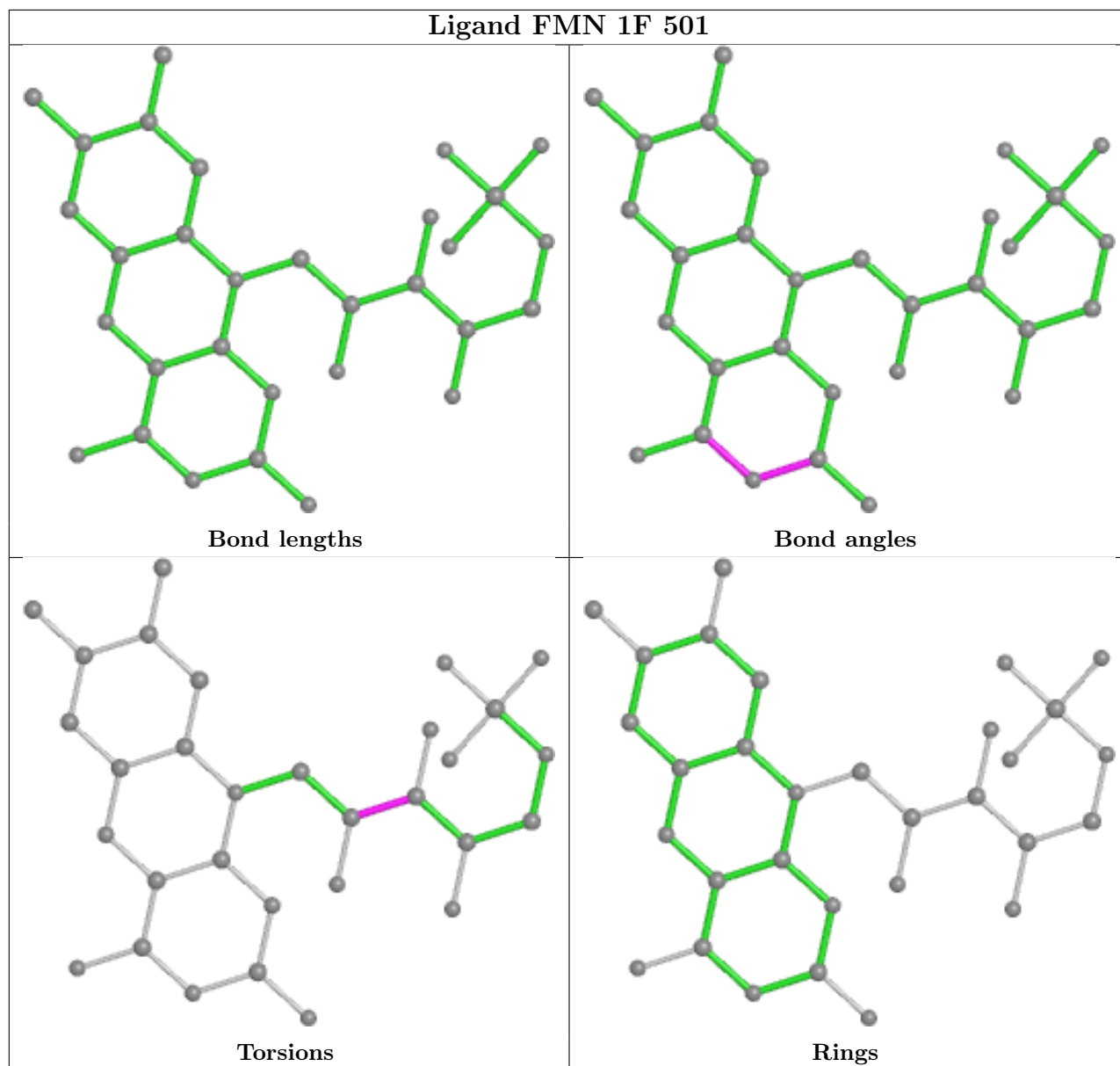


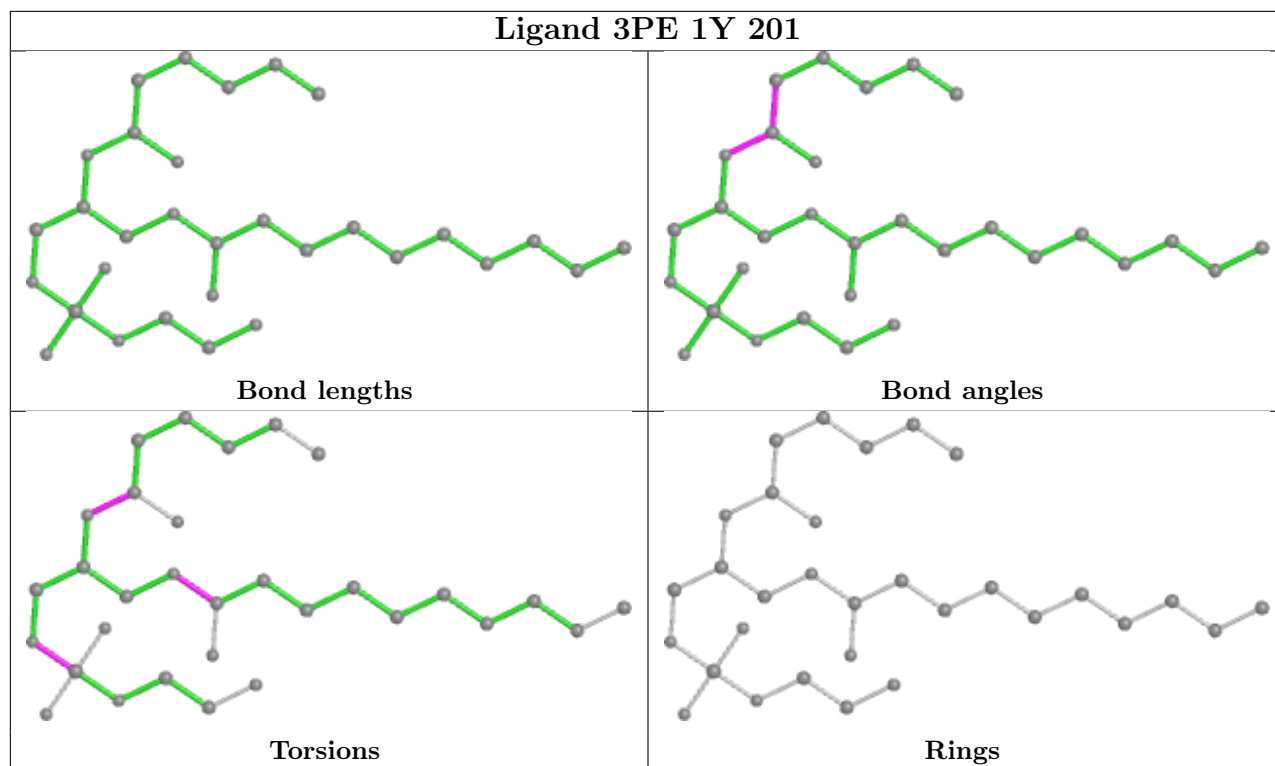












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	1i	1
43	1r	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1i	1:SAC	C	2:GLY	N	3.85
1	1r	1:ALA	C	2:SER	N	3.14

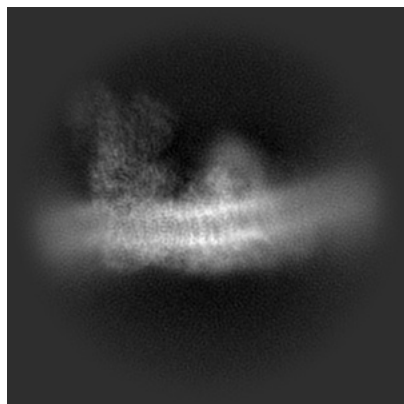
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42171. These allow visual inspection of the internal detail of the map and identification of artifacts.

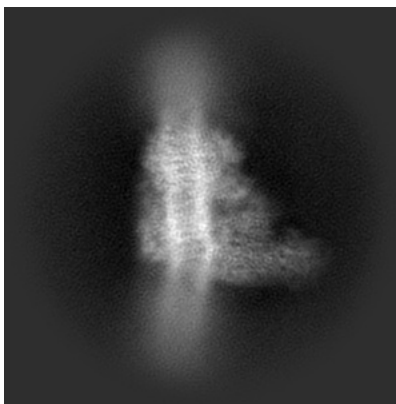
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

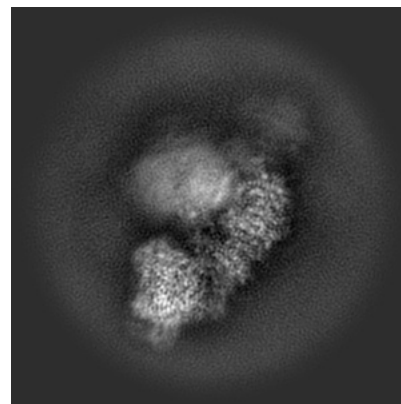
6.1.1 Primary map



X

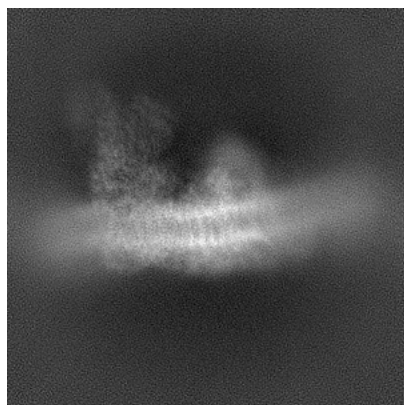


Y

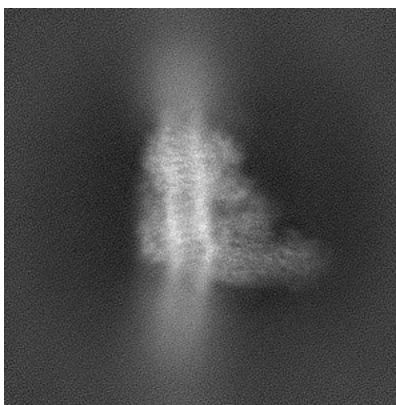


Z

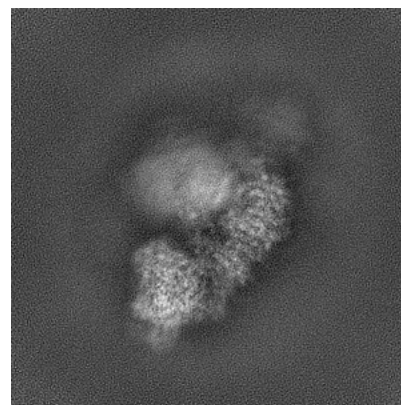
6.1.2 Raw map



X



Y

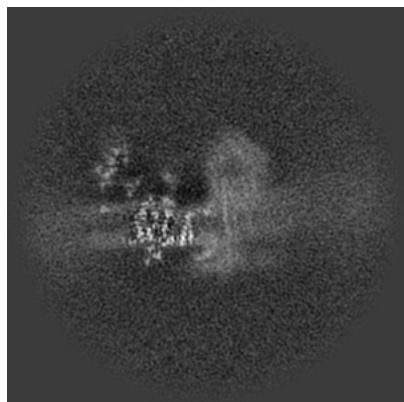


Z

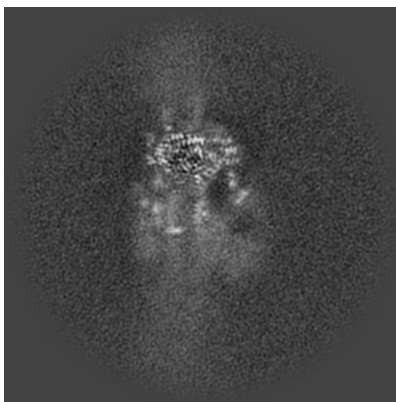
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

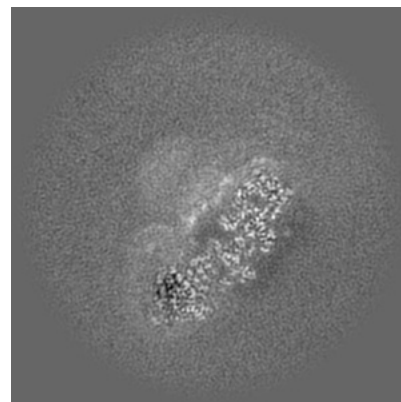
6.2.1 Primary map



X Index: 160



Y Index: 160

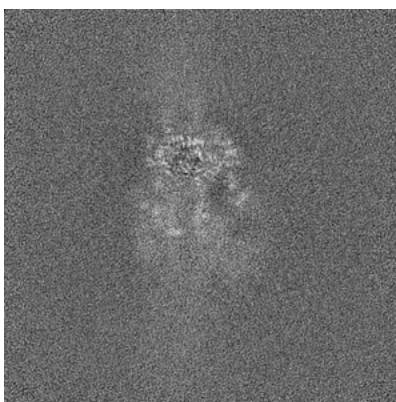


Z Index: 160

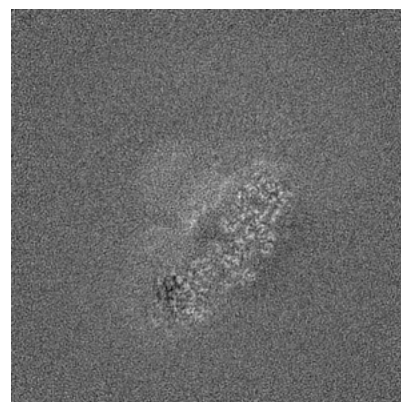
6.2.2 Raw map



X Index: 160



Y Index: 160

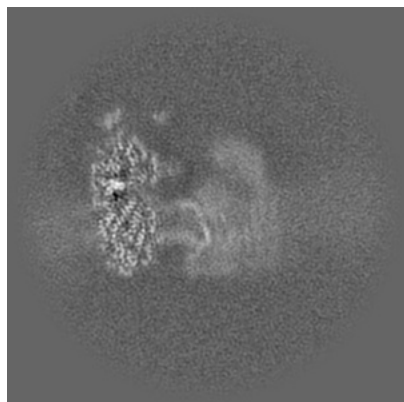


Z Index: 160

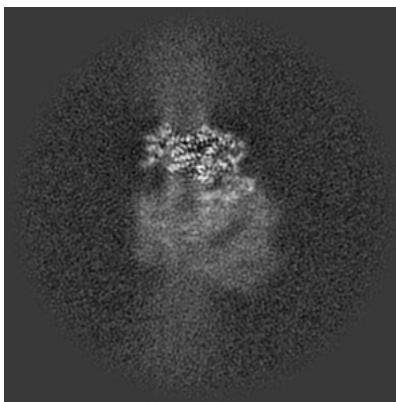
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

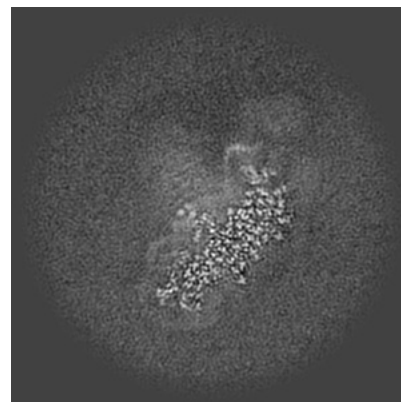
6.3.1 Primary map



X Index: 140

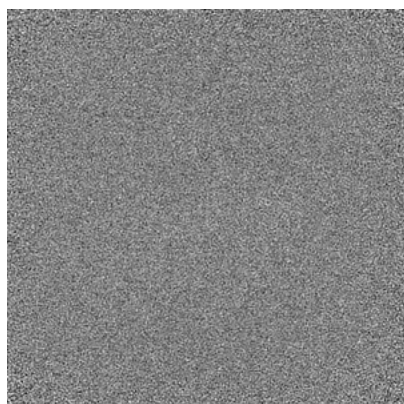


Y Index: 171

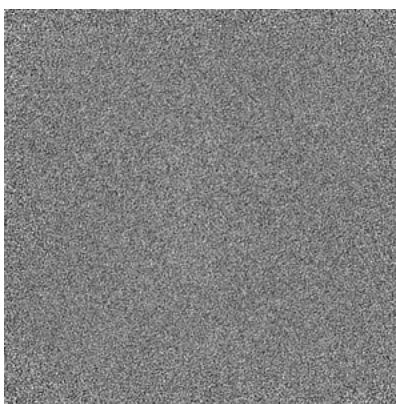


Z Index: 134

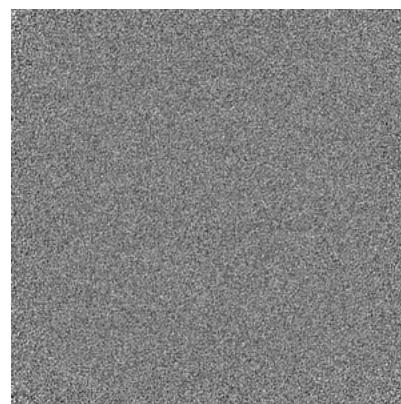
6.3.2 Raw map



X Index: 0



Y Index: 0

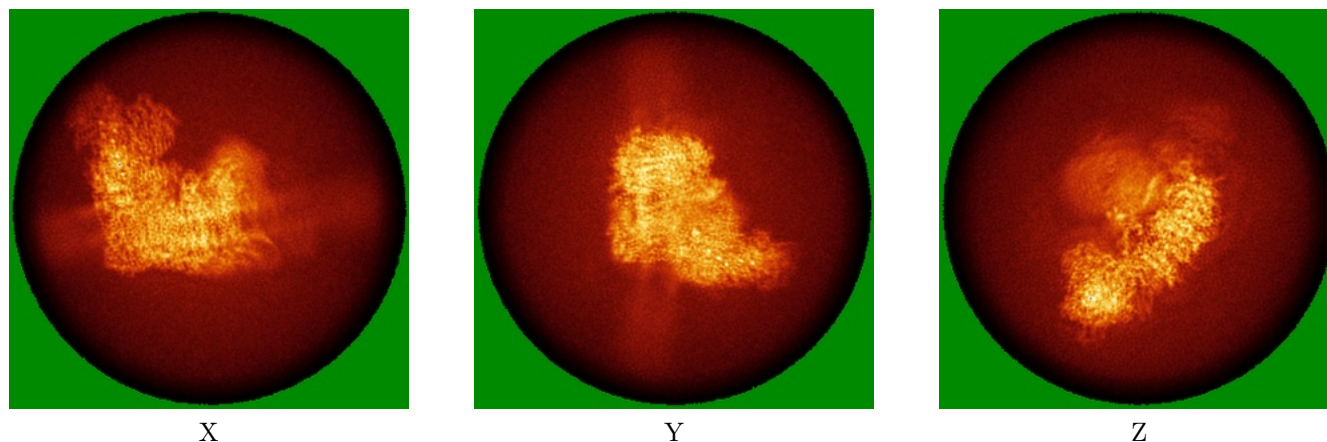


Z Index: 0

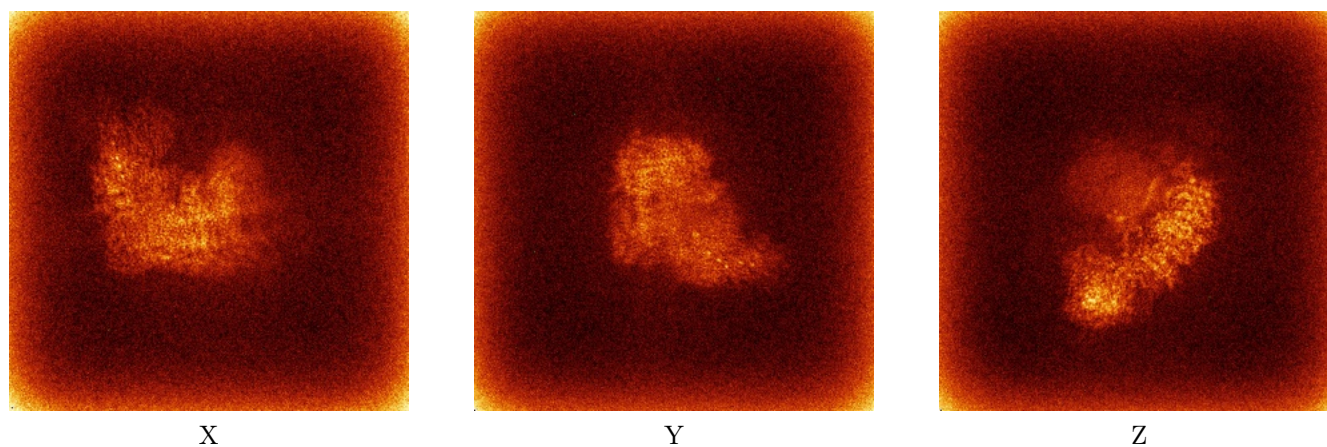
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



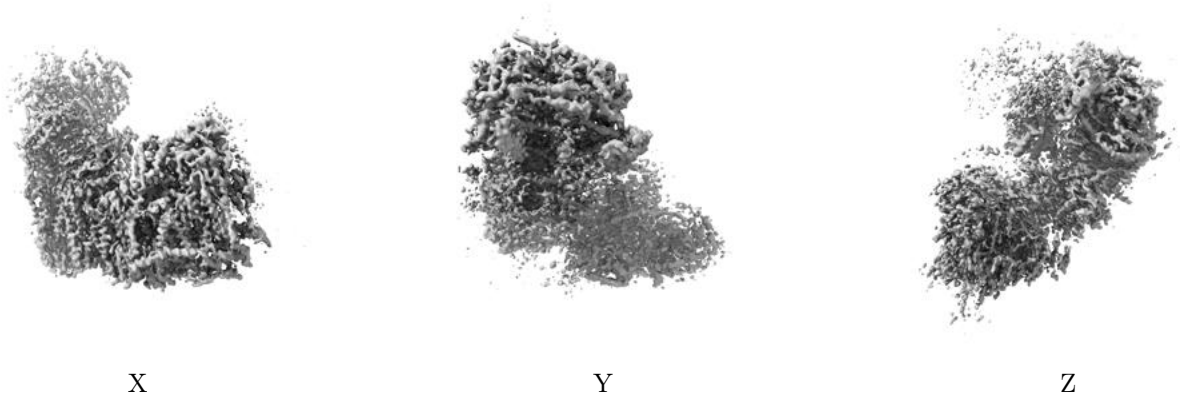
6.4.2 Raw map



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.

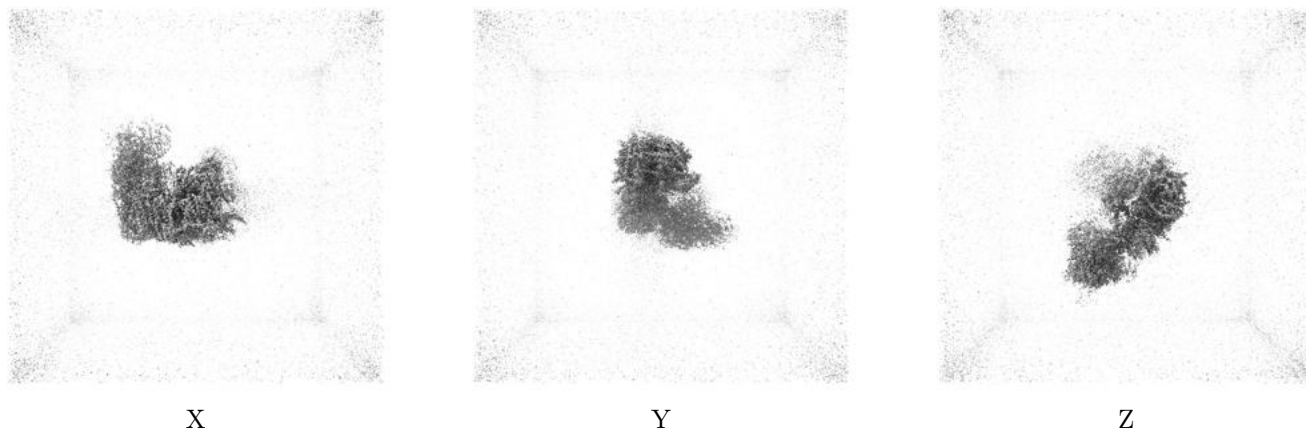
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

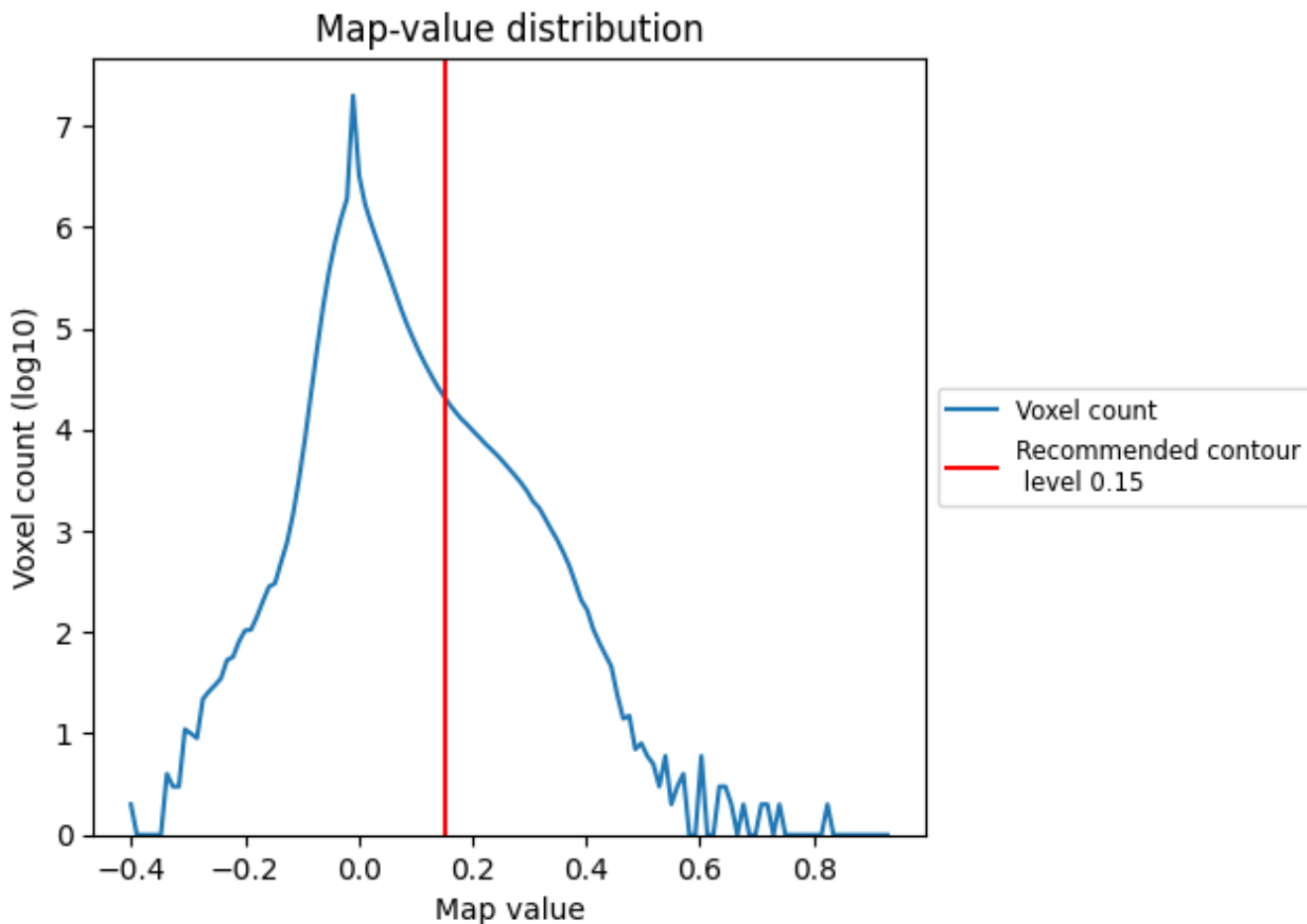
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

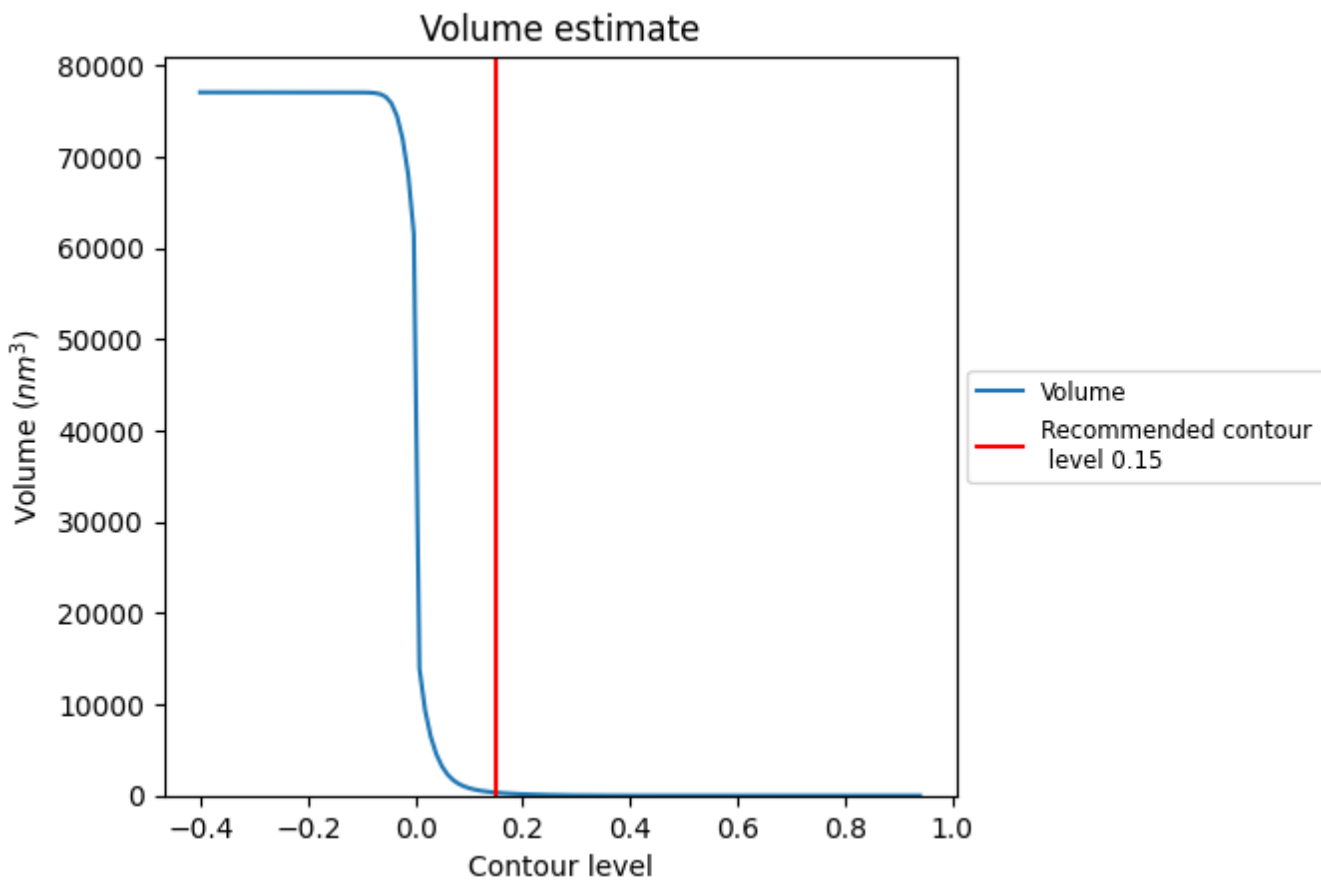
This section contains the results of statistical analysis of the map.

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.

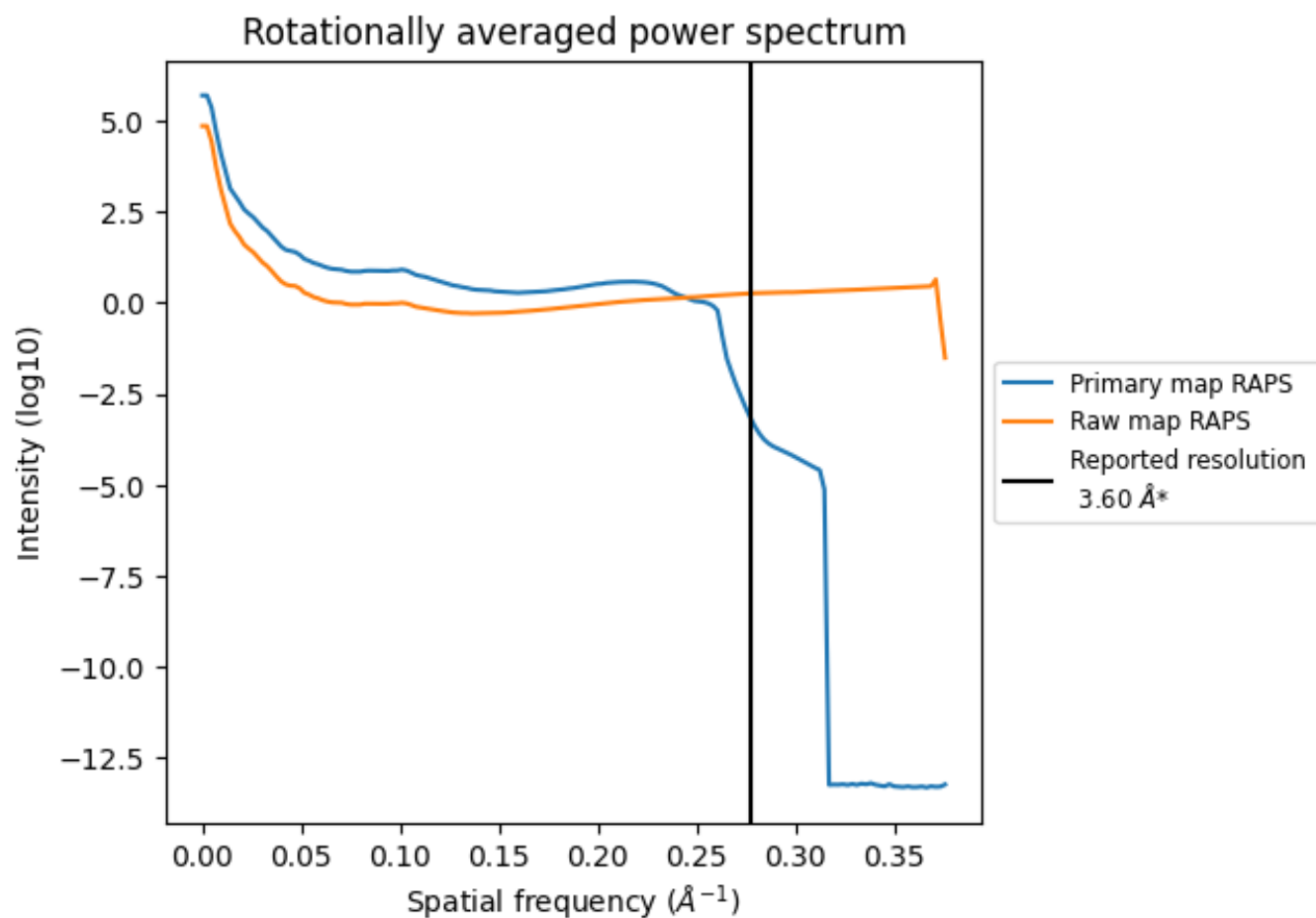
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 329 nm³; this corresponds to an approximate mass of 297 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](#)

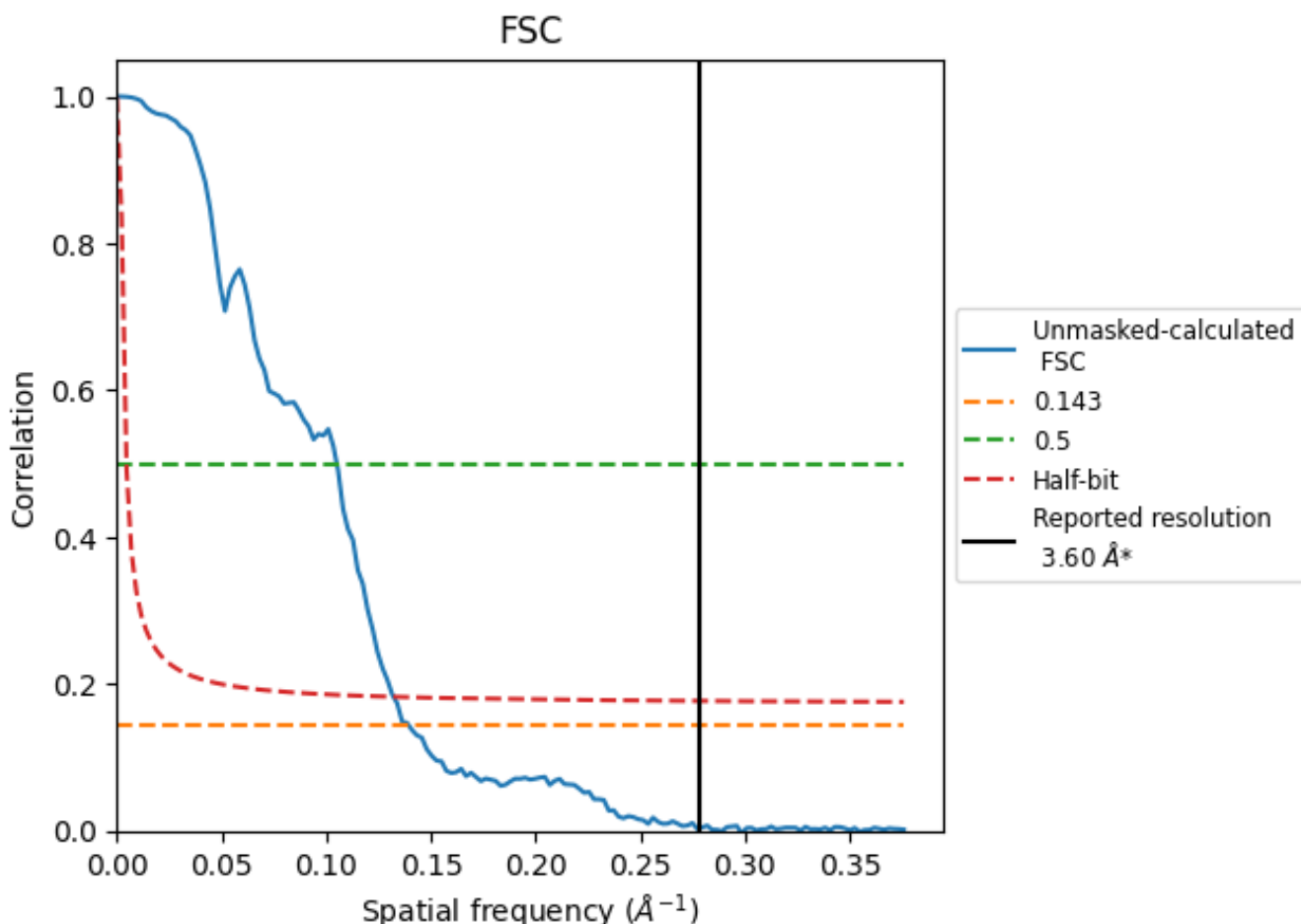


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

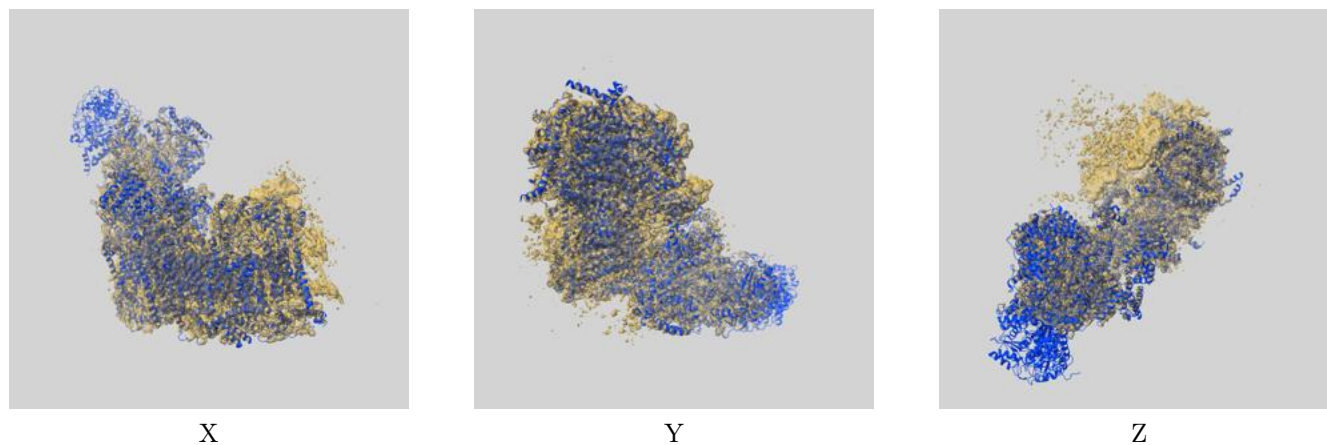
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.17	9.51	7.56

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.17 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

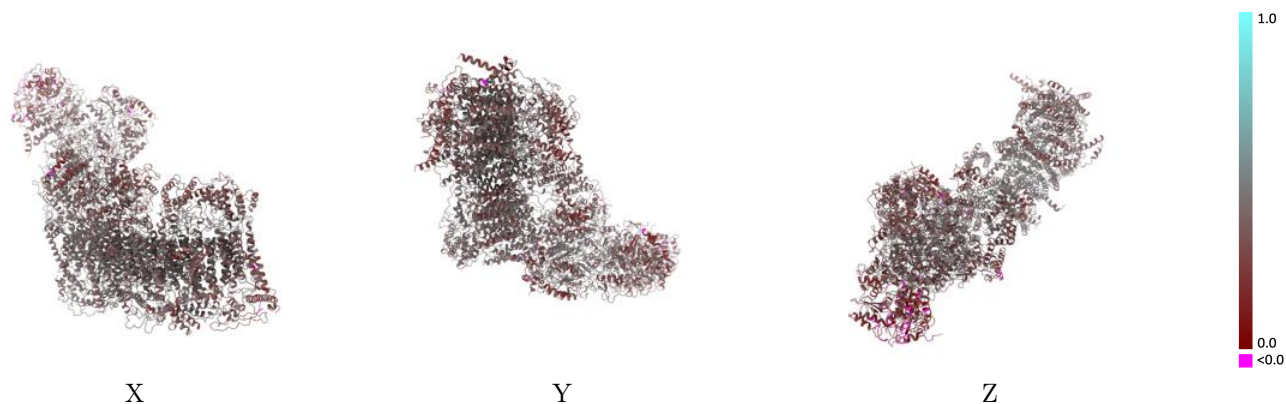
This section contains information regarding the fit between EMDB map EMD-42171 and PDB model 8UEU. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



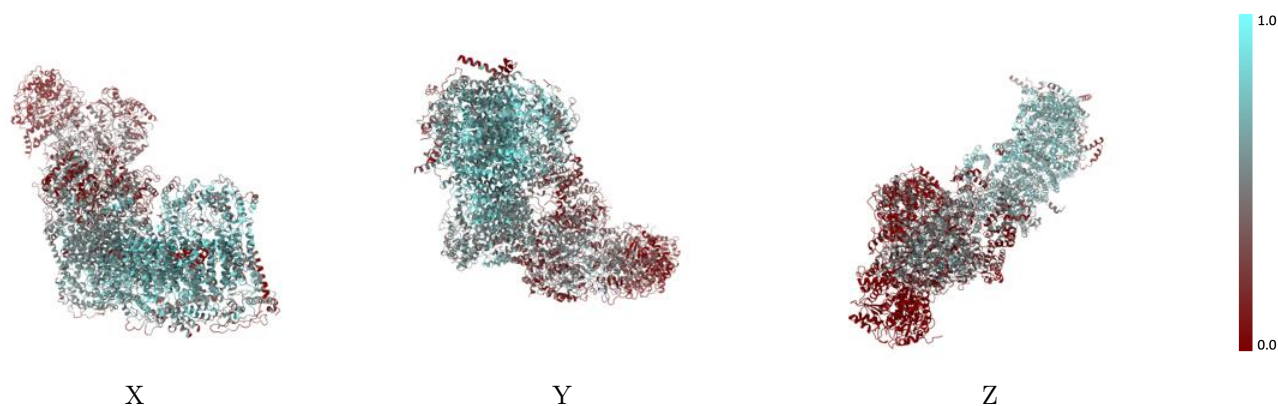
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



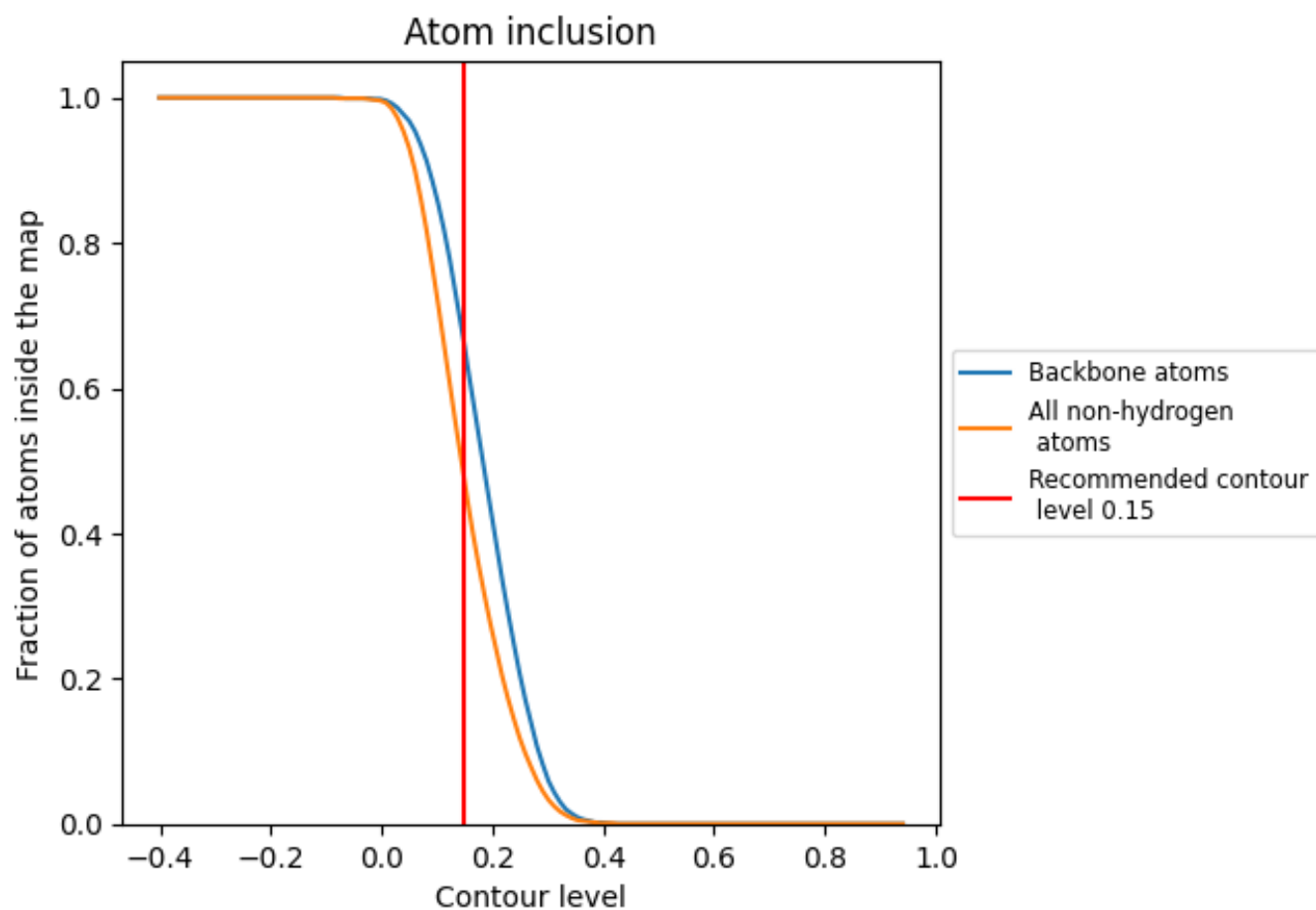
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 47% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4700	 0.3710
1A	 0.5100	 0.3940
1B	 0.5440	 0.4170
1C	 0.3790	 0.4030
1D	 0.4830	 0.3910
1E	 0.0210	 0.2640
1F	 0.0350	 0.2430
1G	 0.2770	 0.3550
1H	 0.5430	 0.3880
1I	 0.5620	 0.4180
1J	 0.5150	 0.3800
1K	 0.6090	 0.3970
1L	 0.7040	 0.3990
1M	 0.7470	 0.4300
1N	 0.6630	 0.4130
1O	 0.3890	 0.3580
1P	 0.2930	 0.3360
1Q	 0.2960	 0.3780
1R	 0.2880	 0.3890
1S	 0.1230	 0.2940
1T	 0.2060	 0.2870
1U	 0.6160	 0.3480
1V	 0.2130	 0.3310
1W	 0.3100	 0.3290
1X	 0.5310	 0.3960
1Y	 0.6440	 0.3680
1Z	 0.5490	 0.4110
1a	 0.6250	 0.4080
1b	 0.5050	 0.3990
1c	 0.4900	 0.3790
1d	 0.6760	 0.4140
1e	 0.5830	 0.4140
1f	 0.4830	 0.3910
1g	 0.5860	 0.3820
1h	 0.6600	 0.4040



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Chain	Atom inclusion	Q-score
1i	 0.4100	 0.3420
1j	 0.5120	 0.3480
1k	 0.4910	 0.3600
1l	 0.6450	 0.3910
1m	 0.7020	 0.3750
1n	 0.6520	 0.3640
1o	 0.5250	 0.3160
1p	 0.6040	 0.3850
1q	 0.4360	 0.4070
1r	 0.3620	 0.4010
1s	 0.0000	 0.2000