



Full wwPDB EM Validation Report ⓘ

Jun 13, 2024 – 12:04 PM EDT

PDB ID : 8UEY
EMDB ID : EMD-42175
Title : In-situ complex I, Deactive class07
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:

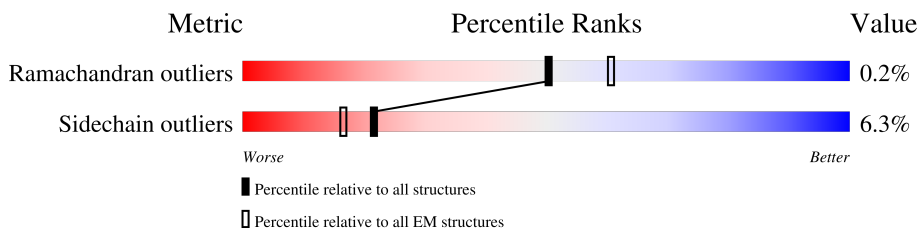
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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	
2	1B	255	
3	1C	264	
4	1D	476	
5	1E	249	
6	1F	464	
7	1G	727	
8	1H	318	
9	1I	239	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	1J	175	23% 92% 7%
11	1K	98	8% 92% 8%
12	1L	606	96% .
13	1M	459	98% .
14	1N	347	95% ..
15	1O	357	45% 85% 5% 10%
16	1P	377	58% 84% 6% 9%
17	1Q	175	46% 69% 5% 26%
18	1R	123	49% 71% 7% 22%
19	1S	99	80% 79% 9% 12%
20	1T	156	40% 47% 7% 46%
20	1U	156	7% 50% 5% 45%
21	1V	116	78% 93% 6%
22	1W	128	52% 80% 9% 10%
23	1X	172	22% 95% ..
24	1Y	141	96% ..
25	1Z	144	18% 93% 5%
26	1a	70	9% 90% 10%
27	1b	84	23% 92% 7%
28	1c	76	25% 61% 36%
29	1d	123	9% 91% 7%
30	1e	106	11% 89% 5% 7%
31	1f	135	14% 40% 58%
32	1g	154	13% 60% 5% 35%
33	1h	189	7% 69% 27%

Continued on next page...

Continued from previous page...

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 66812 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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1B	?	-	PRO	deletion	UNP A0A4X1VVS8
1B	?	-	SER	deletion	UNP A0A4X1VVS8
1B	?	-	SER	deletion	UNP A0A4X1VVS8

- 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	394	3189	2040	547	580	22	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	293	2316	1556	355	384	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
			Total	C	N	O	S		
18	1R	96	741	452	140	146	3	0	0

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

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

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

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

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

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

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

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

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

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

- 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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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	S		
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

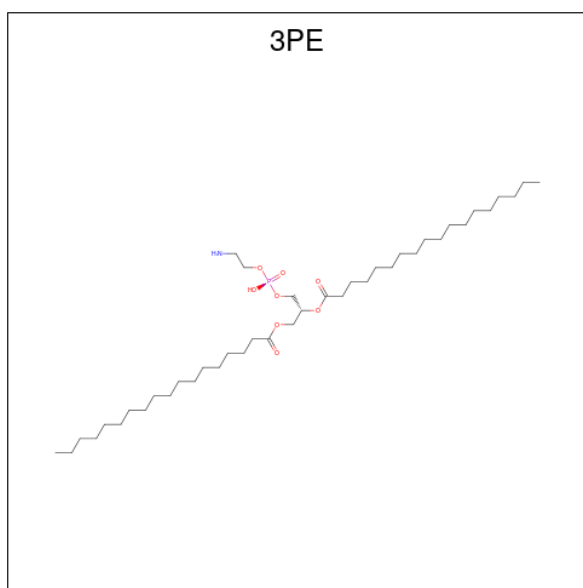
There is a discrepancy between the modelled and reference sequences:

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-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



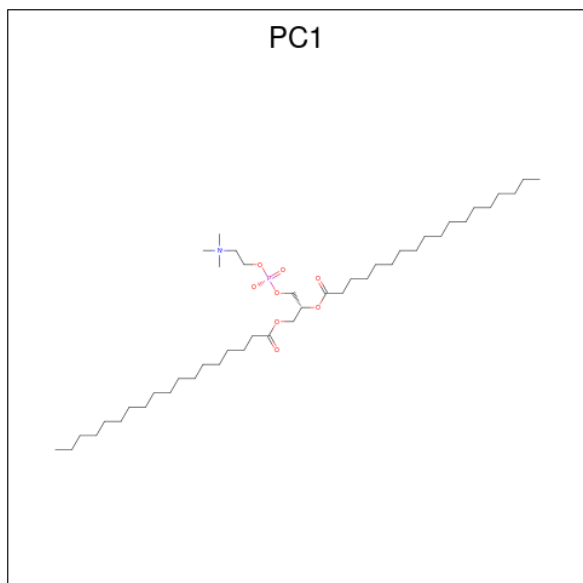
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	1A	1	47	37	1	8	1	0
45	1L	1	46	36	1	8	1	0
45	1L	1	42	32	1	8	1	0
45	1N	1	51	41	1	8	1	0

Continued on next page...

Continued from previous page...

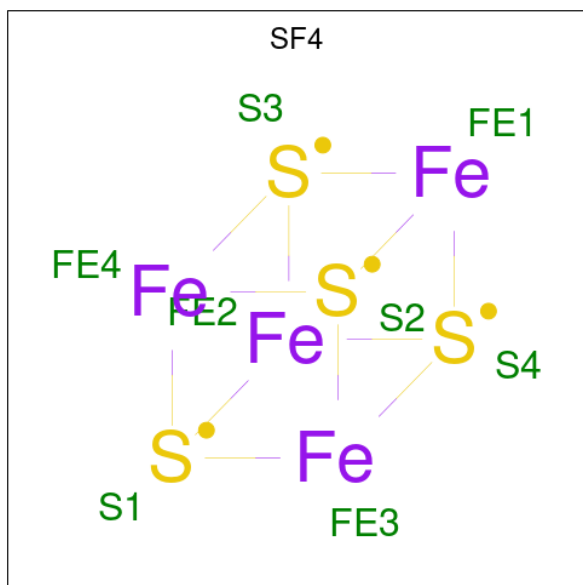
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	1Y	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	1Y	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



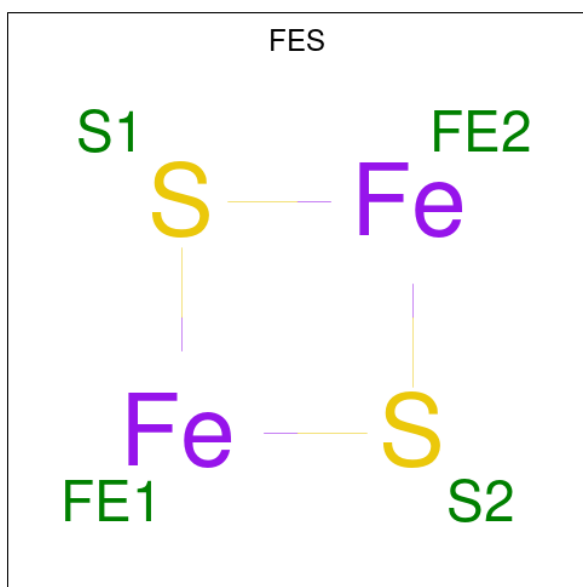
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	1A	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	1I	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	1I	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	1L	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	1f	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 47 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



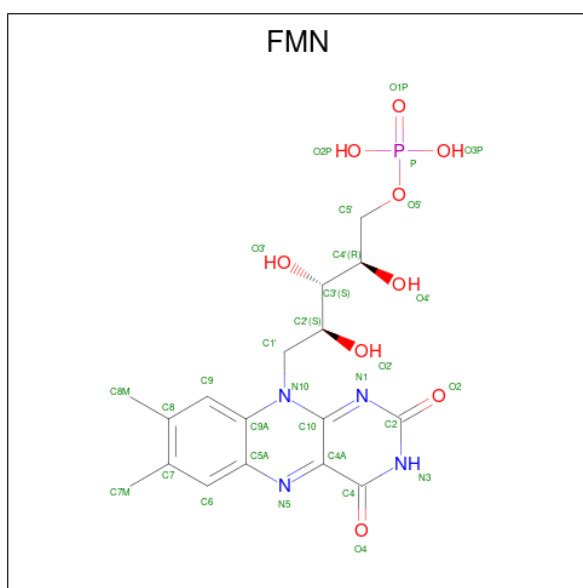
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	1B	1	8	4	4	0
47	1F	1	8	4	4	0
47	1G	1	8	4	4	0
47	1G	1	8	4	4	0
47	1I	1	8	4	4	0
47	1I	1	8	4	4	0

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
48	1E	1	4	2	2	0
48	1G	1	4	2	2	0

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

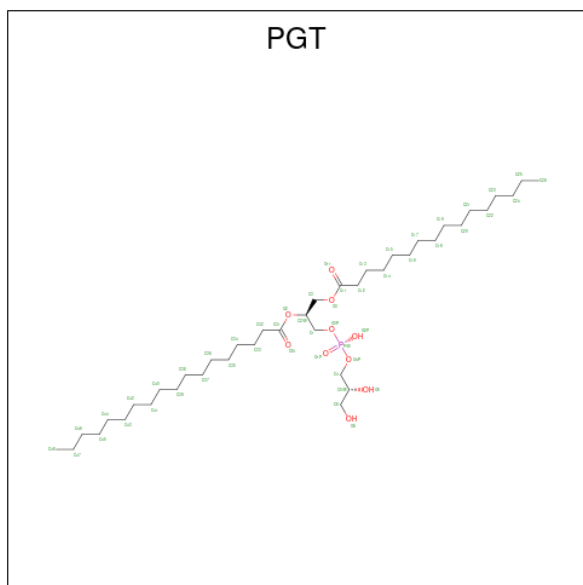


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	1F	1	31	17	4	9	1	0

- Molecule 50 is POTASSIUM ION (three-letter code: K) (formula: K).

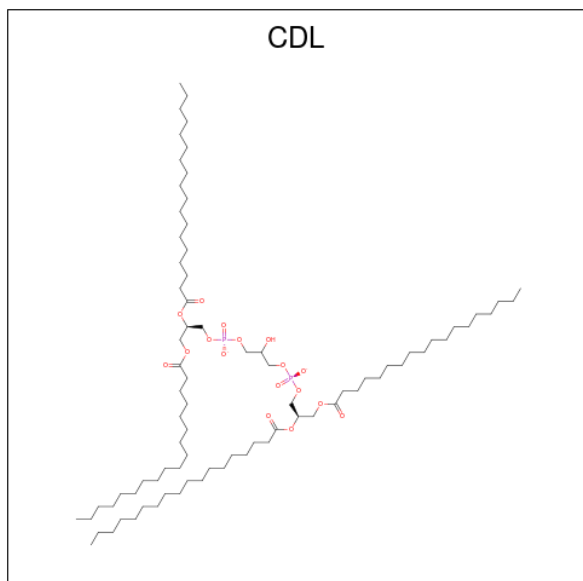
Mol	Chain	Residues	Atoms		AltConf
50	1G	1	Total	K	0
			1	1	

- Molecule 51 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: C₄₀H₇₉O₁₀P).



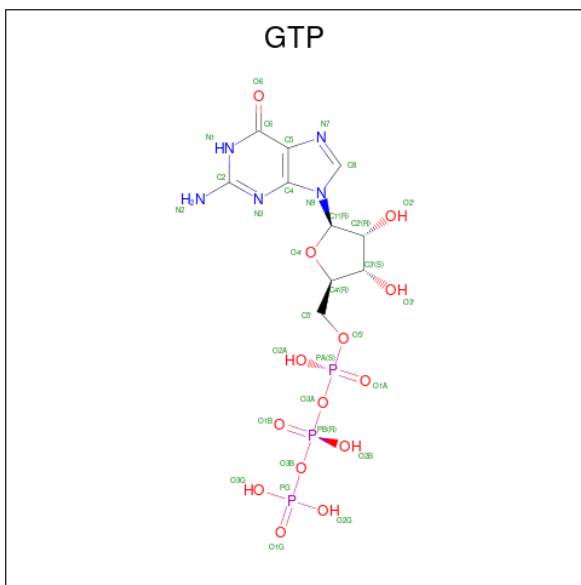
Mol	Chain	Residues	Atoms			AltConf	
51	1M	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 52 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

- Molecule 53 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

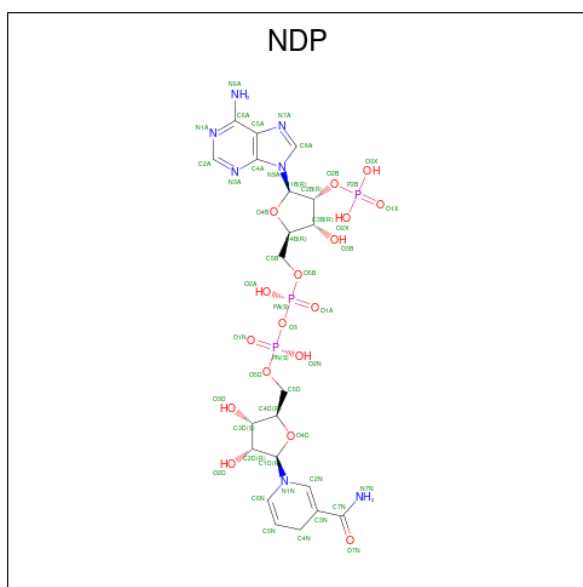


Mol	Chain	Residues	Atoms					AltConf
53	1O	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

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

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

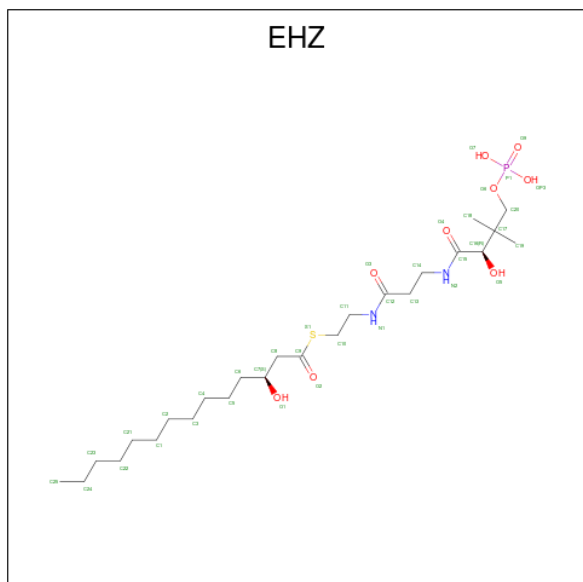


Mol	Chain	Residues	Atoms					AltConf
55	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

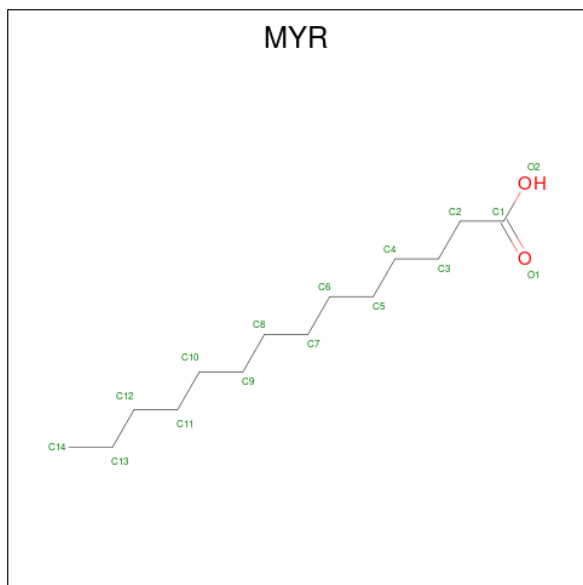
Mol	Chain	Residues	Atoms		AltConf
56	1R	1	Total	Zn	0
			1	1	

- 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: $C_{14}H_{28}O_2$).

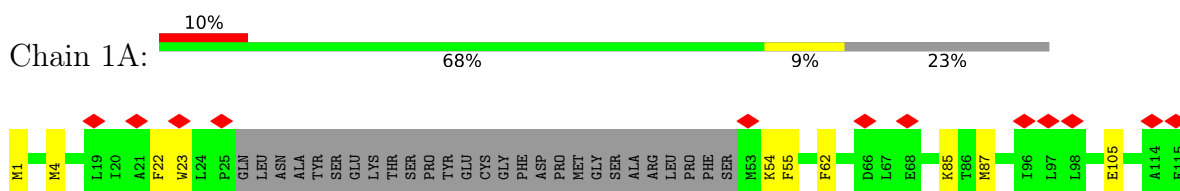


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
58	1l	1	15	14	1	0

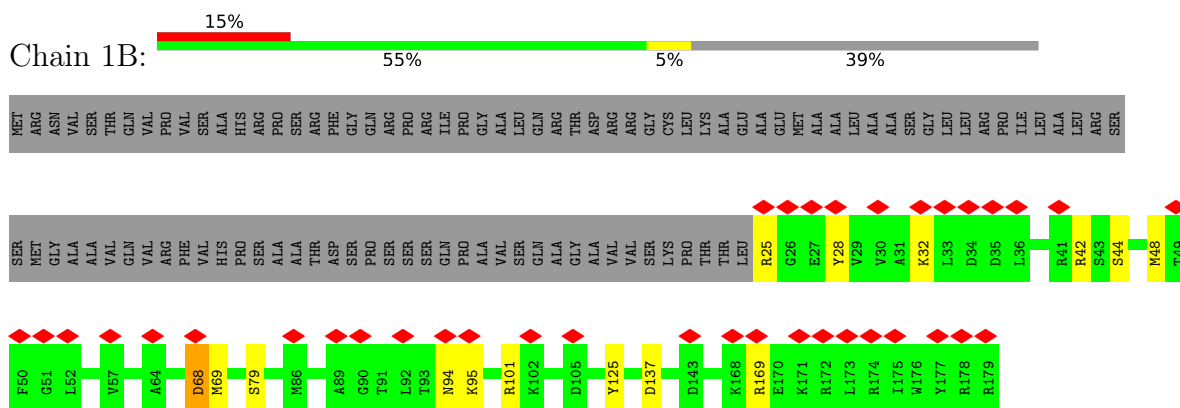
3 Residue-property plots

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 model, but not in the map, are shown in grey.

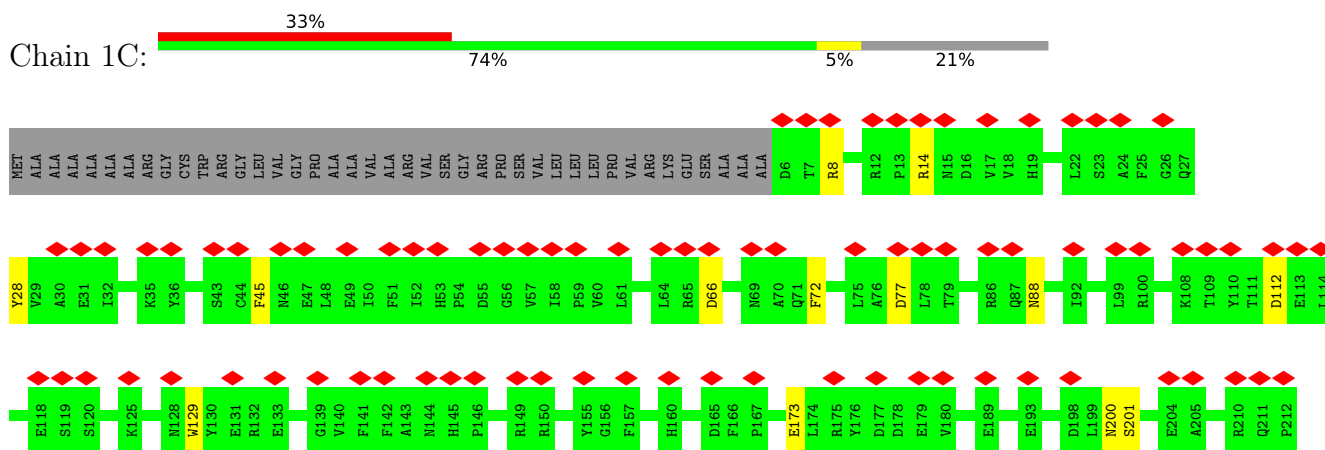
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

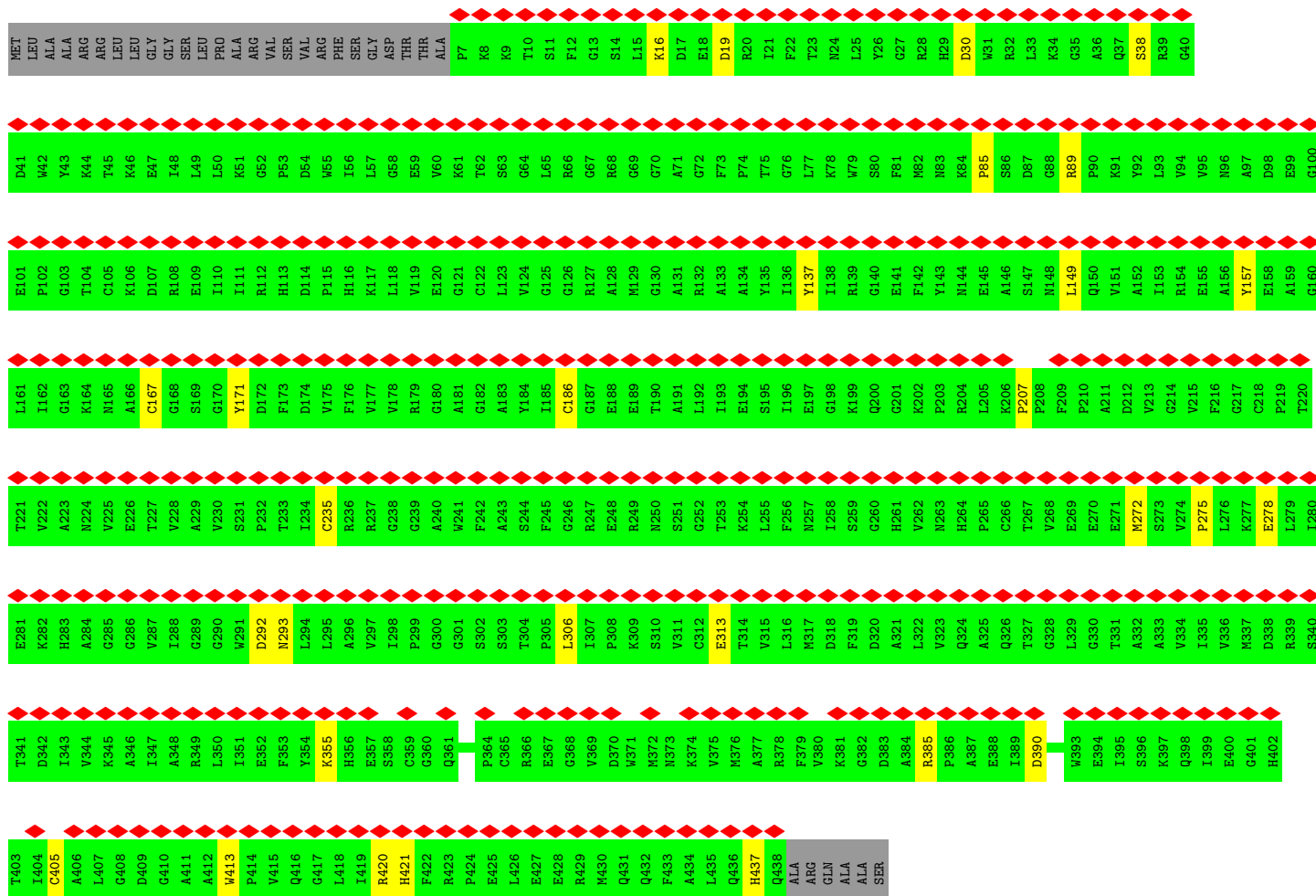


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

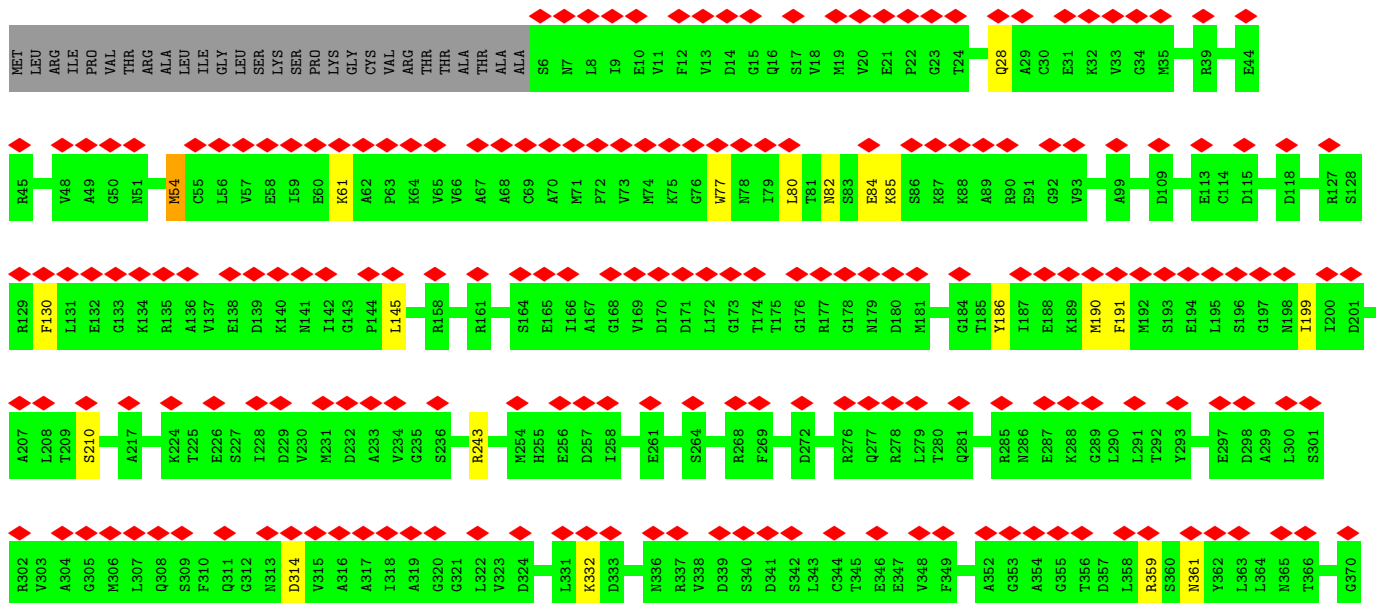
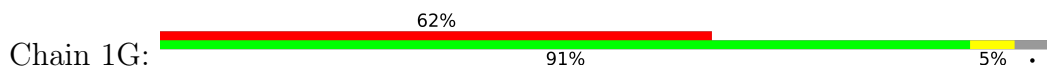


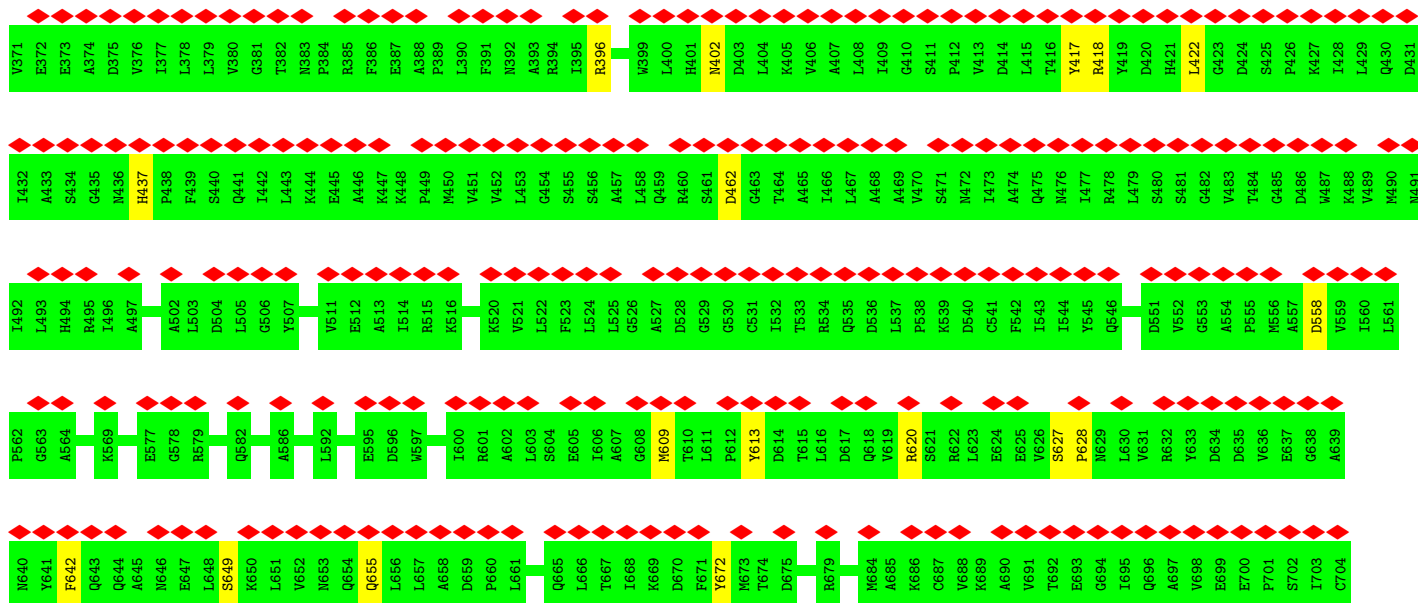
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



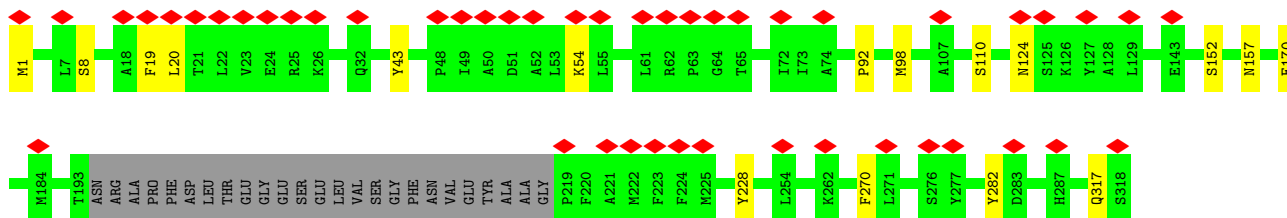
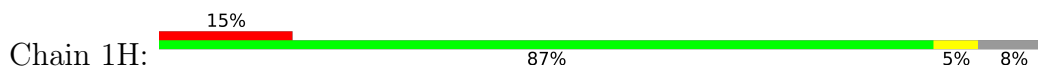


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

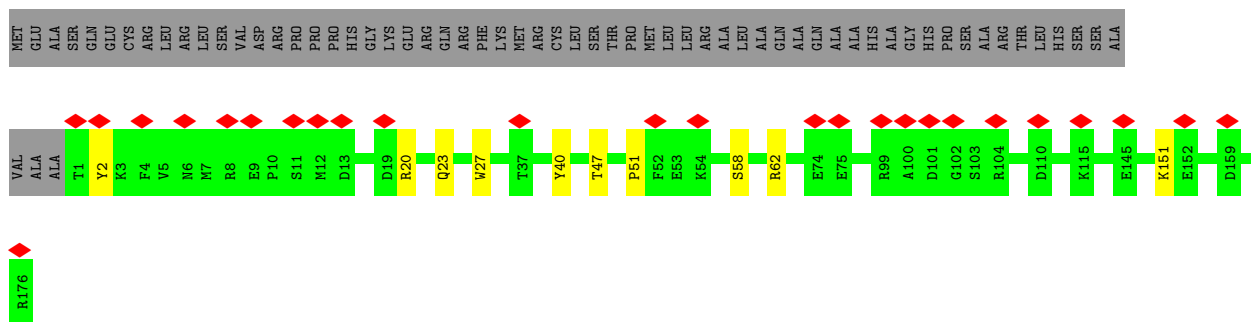




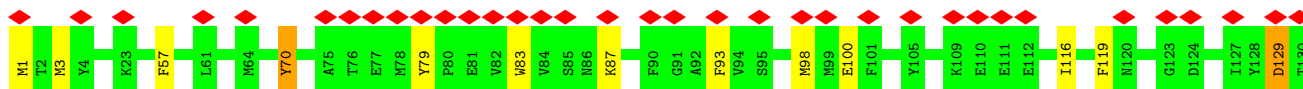
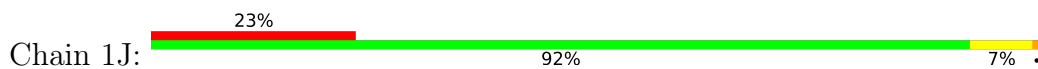
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

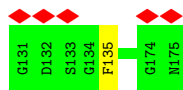


• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



• Molecule 10: NADH-ubiquinone oxidoreductase chain 6





- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5



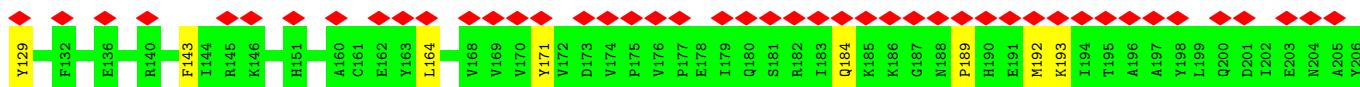
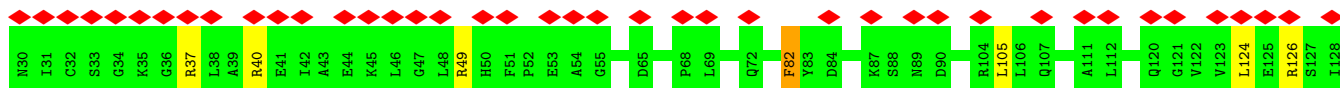
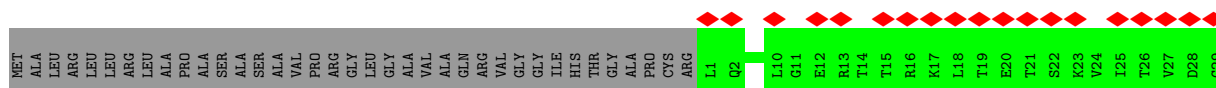
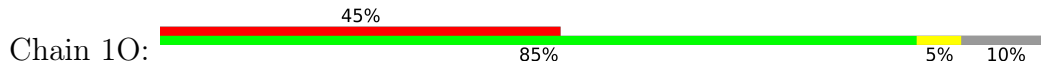
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

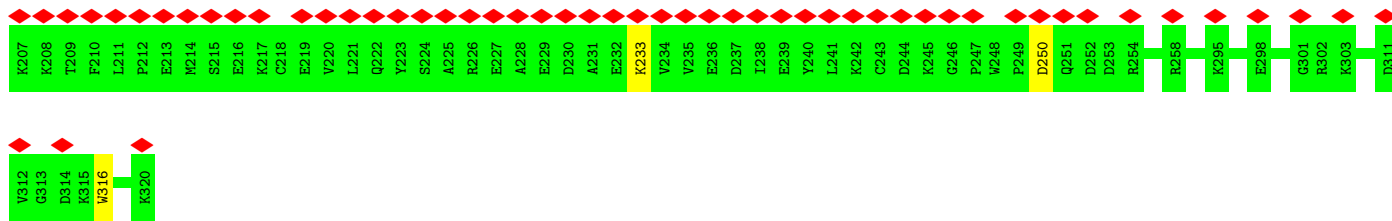


- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

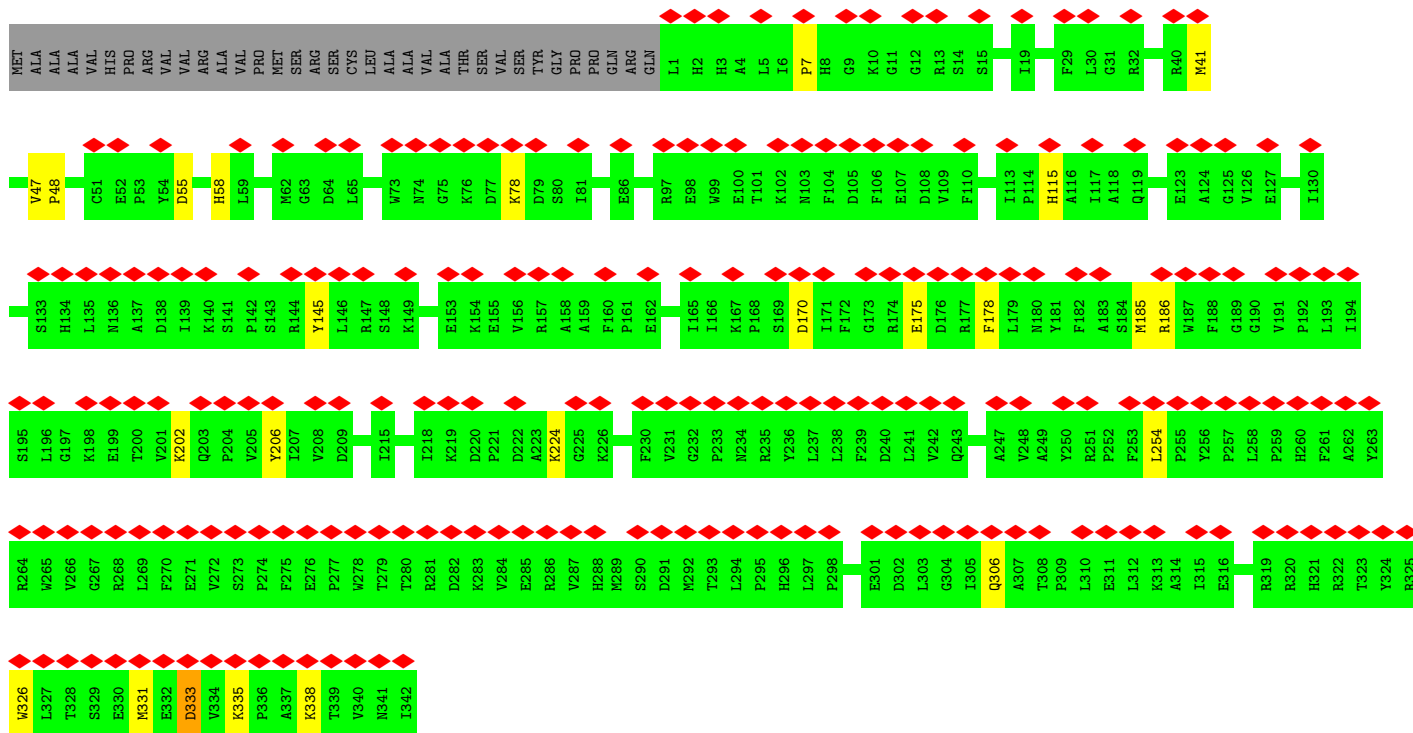
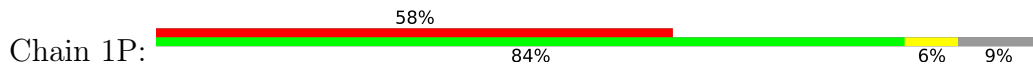


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

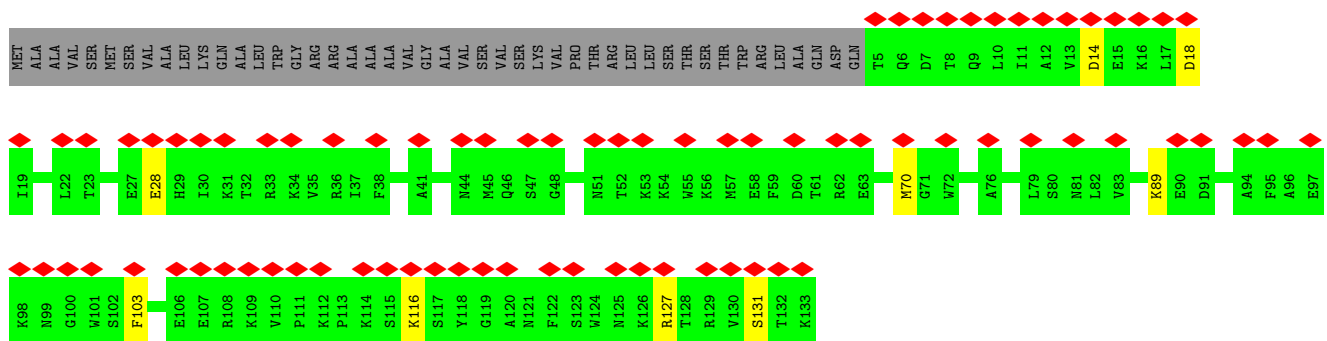




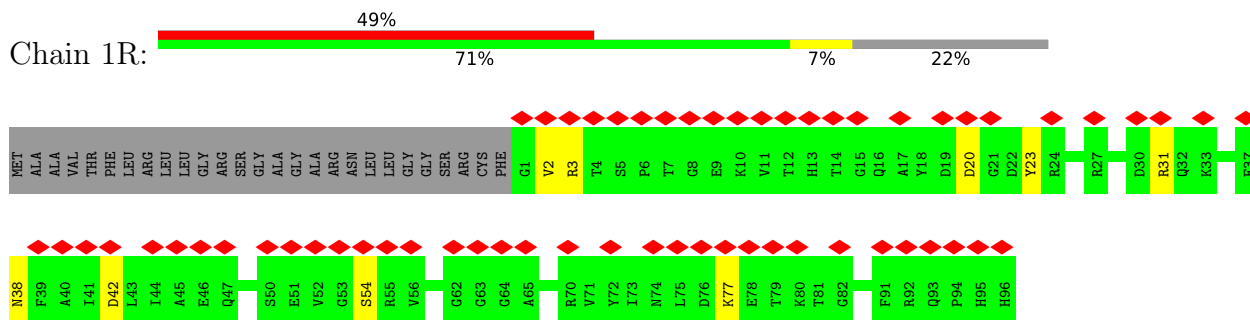
• Molecule 16: NADH:ubiquinone oxidoreductase subunit A9



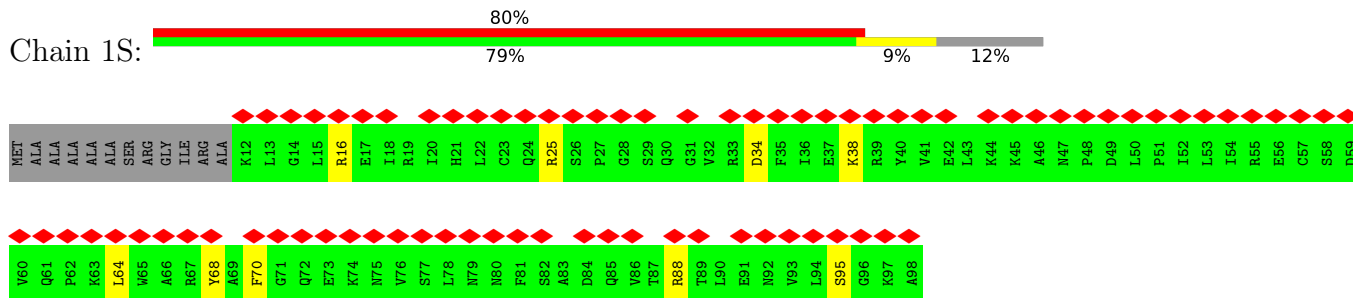
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



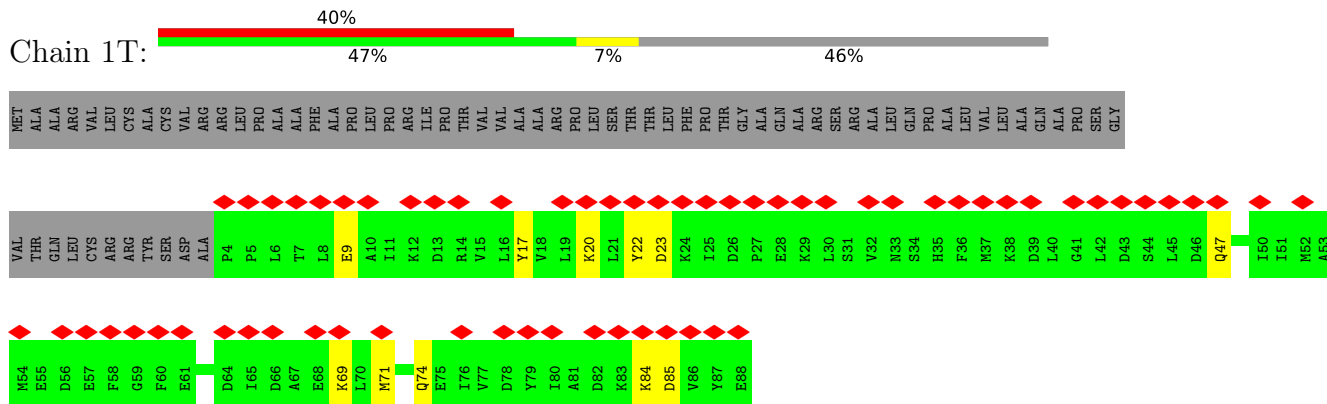
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



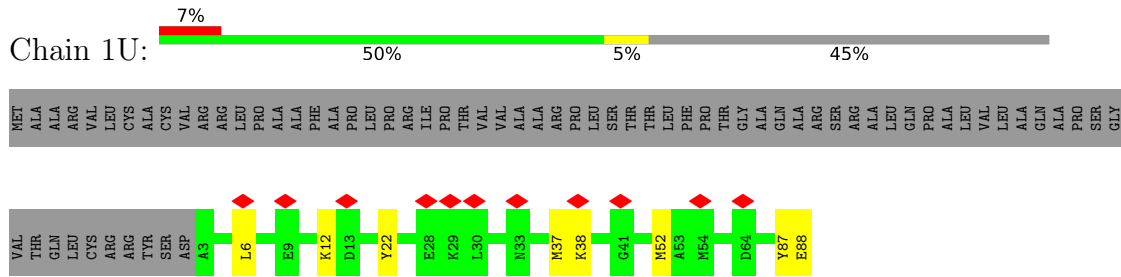
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



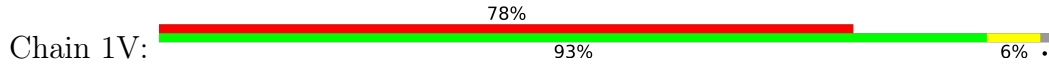
• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

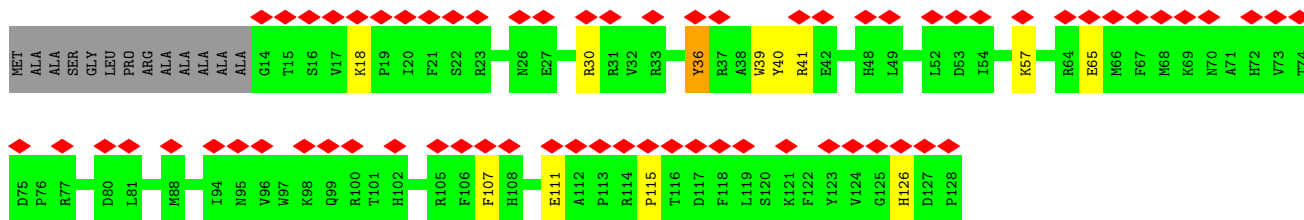
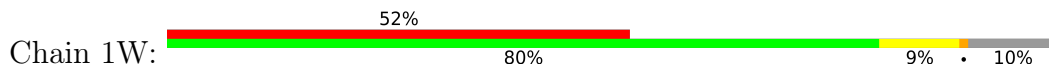


• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

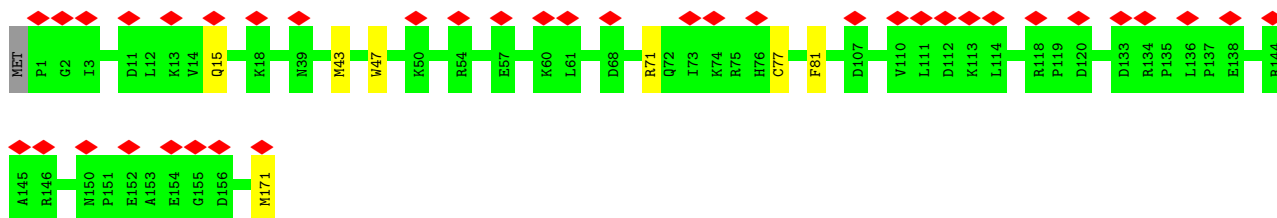




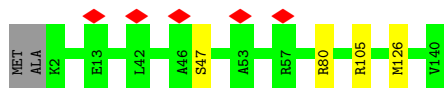
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



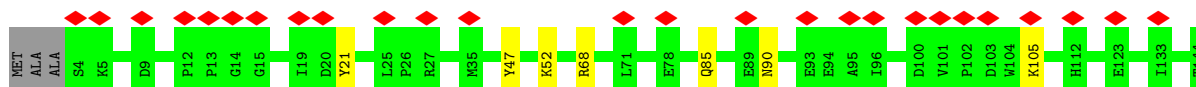
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



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

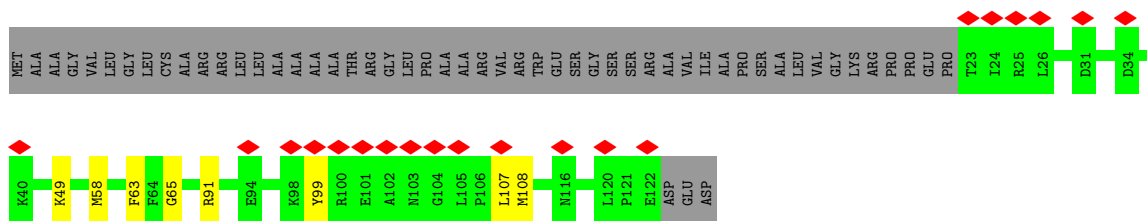


• Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

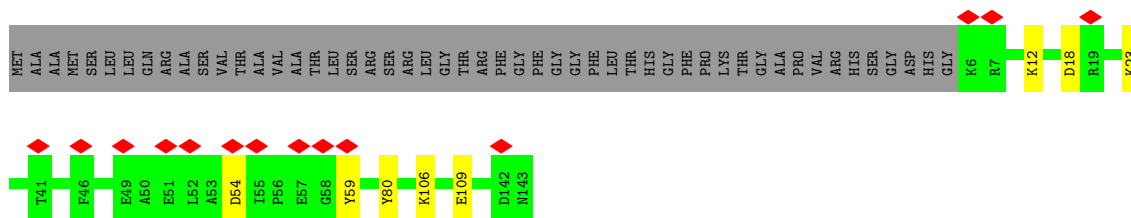


• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

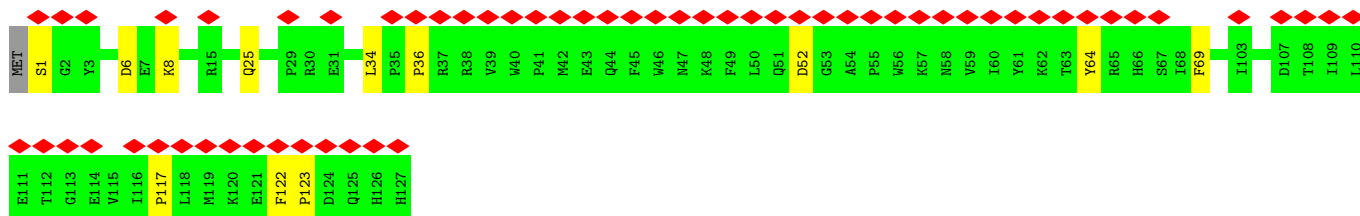
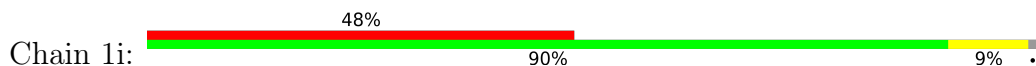




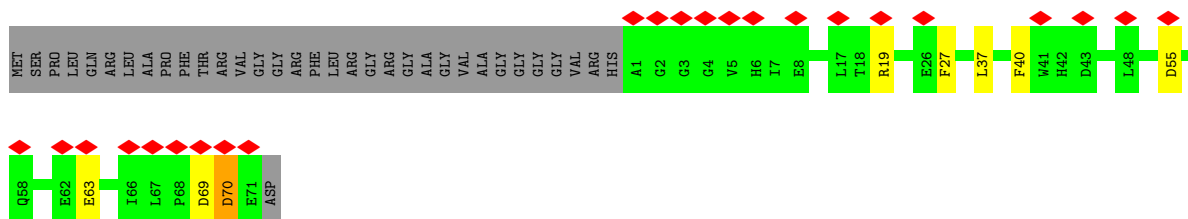
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



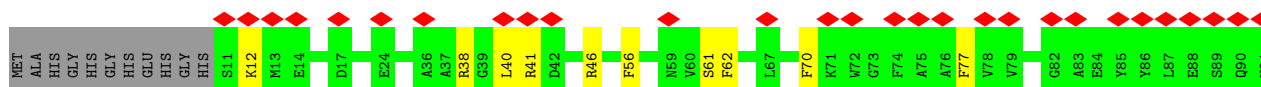
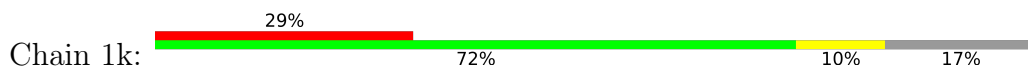
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

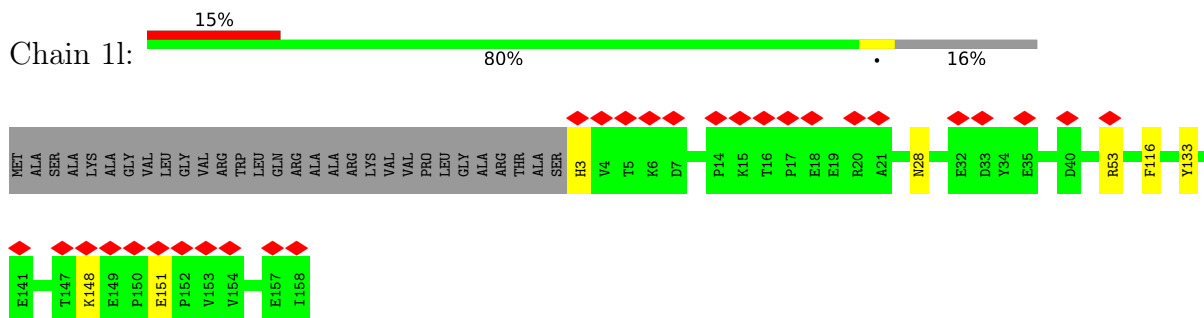


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

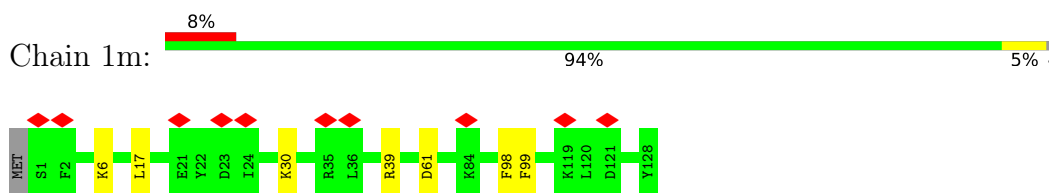


LYS
ASP
LYS
LYS
HIS
HIS

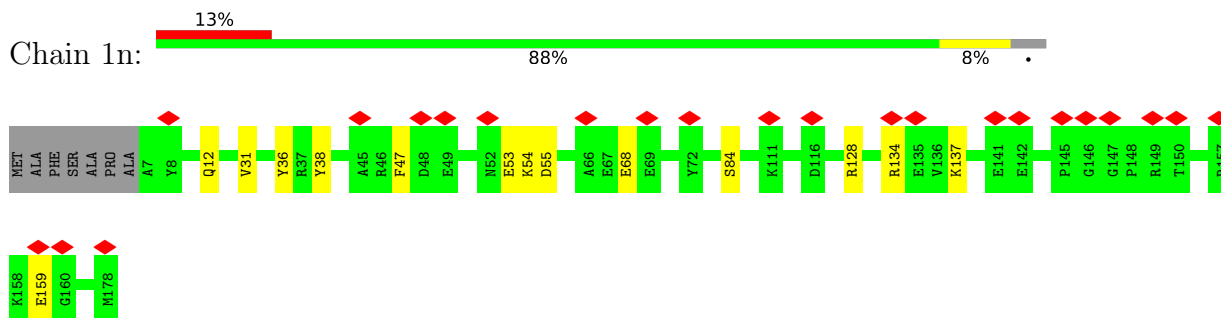
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



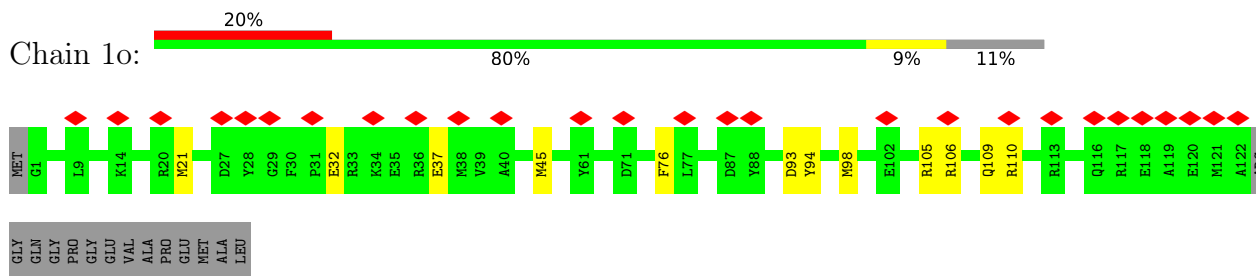
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



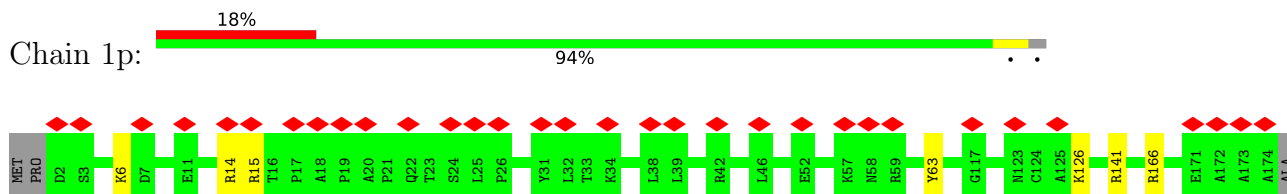
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	0.973	Depositor
Minimum map value	-0.458	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 i

5.1 Standard geometry i

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

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	0.50	0/975
2	1B	0.32	0/1273	0.64	2/1722 (0.1%)
3	1C	0.28	0/1791	0.56	0/2439
4	1D	0.30	1/3274 (0.0%)	0.54	0/4434
5	1E	0.32	0/1698	0.55	0/2311
6	1F	0.32	1/3401 (0.0%)	0.61	2/4595 (0.0%)
7	1G	0.51	4/5451 (0.1%)	0.72	9/7387 (0.1%)
8	1H	0.46	5/2373 (0.2%)	0.54	1/3244 (0.0%)
9	1I	0.31	0/1443	0.64	2/1952 (0.1%)
10	1J	0.39	1/1364 (0.1%)	0.52	1/1850 (0.1%)
11	1K	0.31	0/751	0.61	1/1018 (0.1%)
12	1L	0.27	0/4939	0.51	1/6718 (0.0%)
13	1M	0.31	2/3713 (0.1%)	0.51	1/5063 (0.0%)
14	1N	0.40	2/2765 (0.1%)	0.83	3/3758 (0.1%)
15	1O	0.32	1/2650 (0.0%)	0.51	1/3588 (0.0%)
16	1P	0.65	4/2828 (0.1%)	0.80	8/3834 (0.2%)
17	1Q	0.30	0/1070	0.57	0/1446
18	1R	0.33	0/755	0.61	1/1018 (0.1%)
19	1S	0.39	0/711	0.76	0/956
20	1T	0.31	0/701	0.58	0/946
20	1U	0.40	0/706	0.62	1/954 (0.1%)
21	1V	0.35	0/946	0.66	2/1281 (0.2%)
22	1W	0.54	4/995 (0.4%)	0.76	2/1340 (0.1%)
23	1X	0.27	0/1436	0.54	0/1938
24	1Y	0.25	0/1037	0.47	0/1404
25	1Z	0.27	0/1199	0.56	0/1617
26	1a	0.26	0/577	0.50	0/777
27	1b	0.28	0/664	0.53	0/912
28	1c	0.24	0/430	0.48	0/581
29	1d	0.28	0/1024	0.50	0/1383
30	1e	0.25	0/836	0.53	0/1118
31	1f	0.27	0/499	0.57	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	1g	0.30	0/858	0.54	0/1165
33	1h	0.29	0/1184	0.51	0/1603
34	1i	0.30	0/1131	0.65	2/1541 (0.1%)
35	1j	0.28	0/627	0.58	2/858 (0.2%)
36	1k	0.27	0/668	0.54	0/903
37	1l	0.35	0/1365	0.53	1/1867 (0.1%)
38	1m	0.27	0/1092	0.52	0/1481
39	1n	0.35	0/1549	0.54	0/2098
40	1o	0.28	0/1069	0.59	2/1430 (0.1%)
41	1p	0.26	0/1481	0.52	0/1997
42	1q	0.30	0/1253	0.60	1/1704 (0.1%)
43	1r	0.43	1/782 (0.1%)	0.78	2/1057 (0.2%)
44	1s	0.30	0/394	0.78	1/533 (0.2%)
All	All	0.36	26/67466 (0.0%)	0.60	49/91469 (0.1%)

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
6	1F	0	1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1G	628	PRO	CG-CD	-24.52	0.69	1.50
16	1P	48	PRO	CG-CD	-23.66	0.72	1.50
7	1G	628	PRO	CB-CG	16.14	2.30	1.50
16	1P	48	PRO	CB-CG	15.67	2.28	1.50
14	1N	11	MET	CG-SD	-12.99	1.47	1.81
8	1H	228	TYR	CD2-CE2	-8.84	1.26	1.39
8	1H	228	TYR	CE2-CZ	-8.79	1.27	1.38
13	1M	123	GLU	CD-OE1	-7.58	1.17	1.25
16	1P	47	VAL	C-N	7.40	1.48	1.34
8	1H	228	TYR	CZ-OH	-6.79	1.26	1.37
8	1H	228	TYR	CE1-CZ	-6.57	1.30	1.38
22	1W	36	TYR	CE1-CZ	-6.50	1.30	1.38
7	1G	628	PRO	CA-CB	-6.41	1.40	1.53
7	1G	627	SER	C-N	6.29	1.46	1.34
4	1D	253	TYR	CD2-CE2	-6.25	1.29	1.39
43	1r	47	LYS	CE-NZ	-6.18	1.33	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	1J	70	TYR	CD1-CE1	-6.07	1.30	1.39
8	1H	228	TYR	CD1-CE1	-6.01	1.30	1.39
22	1W	36	TYR	CG-CD1	-5.97	1.31	1.39
16	1P	48	PRO	N-CD	5.76	1.55	1.47
14	1N	11	MET	SD-CE	5.67	2.09	1.77
13	1M	123	GLU	CB-CG	-5.56	1.41	1.52
6	1F	167	CYS	CB-SG	-5.43	1.73	1.81
22	1W	40	TYR	CG-CD1	-5.26	1.32	1.39
22	1W	40	TYR	CD1-CE1	-5.22	1.31	1.39
15	1O	82	PHE	CE2-CZ	-5.02	1.27	1.37

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1N	11	MET	CG-SD-CE	-37.45	40.27	100.20
7	1G	628	PRO	CB-CG-CD	-27.29	0.07	106.50
16	1P	48	PRO	CB-CG-CD	-19.57	30.18	106.50
16	1P	48	PRO	N-CD-CG	-16.41	78.59	103.20
7	1G	628	PRO	CA-N-CD	-15.39	89.95	111.50
16	1P	48	PRO	CA-N-CD	-14.17	91.66	111.50
34	1i	117	PRO	CA-N-CD	-13.13	93.12	111.50
7	1G	627	SER	C-N-CD	11.50	152.54	128.40
16	1P	48	PRO	N-CA-CB	-10.66	90.51	103.30
44	1s	64	PRO	CA-N-CD	-10.60	96.67	111.50
16	1P	48	PRO	CA-CB-CG	-10.26	84.51	104.00
6	1F	275	PRO	CA-N-CD	-10.03	97.45	111.50
7	1G	628	PRO	CA-CB-CG	-10.00	85.00	104.00
9	1I	51	PRO	CA-N-CD	-9.74	97.86	111.50
7	1G	54	MET	CG-SD-CE	-8.99	85.81	100.20
21	1V	106	PRO	CA-N-CD	-8.99	98.92	111.50
14	1N	211	MET	CG-SD-CE	-8.98	85.83	100.20
6	1F	85	PRO	CA-N-CD	-8.63	99.42	111.50
9	1I	47	THR	CA-CB-CG2	-8.11	101.05	112.40
43	1r	110	PRO	CA-N-CD	-8.07	100.21	111.50
15	1O	189	PRO	CA-N-CD	-7.67	100.75	111.50
12	1L	350	LEU	CA-CB-CG	7.65	132.90	115.30
20	1U	88	GLU	OE1-CD-OE2	-7.39	114.43	123.30
7	1G	628	PRO	N-CA-CB	-7.34	94.50	103.30
16	1P	47	VAL	C-N-CD	6.70	142.46	128.40
22	1W	115	PRO	CA-N-CD	-6.67	102.16	111.50
2	1B	68	ASP	CB-CG-OD2	6.50	124.15	118.30
34	1i	117	PRO	N-CD-CG	-6.49	93.47	103.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1V	19	PRO	CA-N-CD	-6.35	102.61	111.50
2	1B	68	ASP	CB-CG-OD1	-6.33	112.60	118.30
40	1o	93	ASP	CB-CG-OD2	-6.29	112.64	118.30
22	1W	36	TYR	CD1-CE1-CZ	6.26	125.43	119.80
16	1P	7	PRO	CA-N-CD	-6.19	102.83	111.50
18	1R	2	VAL	CA-CB-CG1	-6.14	101.68	110.90
43	1r	99	PRO	CA-N-CD	-6.08	102.99	111.50
8	1H	20	LEU	CA-CB-CG	5.90	128.88	115.30
13	1M	437	MET	CG-SD-CE	-5.87	90.81	100.20
7	1G	199	ILE	CG1-CB-CG2	-5.84	98.55	111.40
14	1N	323	MET	CA-CB-CG	5.83	123.20	113.30
7	1G	627	SER	CA-C-N	5.56	132.66	117.10
40	1o	93	ASP	CB-CG-OD1	5.49	123.24	118.30
37	1l	133	TYR	CD1-CE1-CZ	5.44	124.69	119.80
16	1P	254	LEU	CA-CB-CG	5.38	127.67	115.30
42	1q	76	ASP	CB-CG-OD1	5.38	123.14	118.30
35	1j	70	ASP	CB-CG-OD2	5.23	123.01	118.30
7	1G	627	SER	N-CA-CB	-5.09	102.86	110.50
11	1K	96	LEU	CA-CB-CG	5.06	126.94	115.30
35	1j	55	ASP	CB-CG-OD1	5.06	122.85	118.30
10	1J	129	ASP	CB-CG-OD2	5.05	122.84	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1F	207	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%)	78 (93%)	6 (7%)	0	100	100
2	1B	153/255 (60%)	138 (90%)	14 (9%)	1 (1%)	22	61
3	1C	207/264 (78%)	191 (92%)	16 (8%)	0	100	100
4	1D	390/476 (82%)	364 (93%)	26 (7%)	0	100	100
5	1E	212/249 (85%)	195 (92%)	16 (8%)	1 (0%)	29	68
6	1F	430/464 (93%)	401 (93%)	28 (6%)	1 (0%)	47	79
7	1G	697/727 (96%)	648 (93%)	48 (7%)	1 (0%)	51	83
8	1H	289/318 (91%)	270 (93%)	17 (6%)	2 (1%)	22	61
9	1I	174/239 (73%)	166 (95%)	8 (5%)	0	100	100
10	1J	173/175 (99%)	158 (91%)	14 (8%)	1 (1%)	25	64
11	1K	96/98 (98%)	90 (94%)	5 (5%)	1 (1%)	15	55
12	1L	604/606 (100%)	541 (90%)	61 (10%)	2 (0%)	41	75
13	1M	457/459 (100%)	441 (96%)	16 (4%)	0	100	100
14	1N	345/347 (99%)	323 (94%)	22 (6%)	0	100	100
15	1O	318/357 (89%)	302 (95%)	16 (5%)	0	100	100
16	1P	340/377 (90%)	314 (92%)	25 (7%)	1 (0%)	41	75
17	1Q	127/175 (73%)	113 (89%)	13 (10%)	1 (1%)	19	59
18	1R	94/123 (76%)	87 (93%)	7 (7%)	0	100	100
19	1S	85/99 (86%)	73 (86%)	12 (14%)	0	100	100
20	1T	83/156 (53%)	79 (95%)	3 (4%)	1 (1%)	13	51
20	1U	84/156 (54%)	79 (94%)	5 (6%)	0	100	100
21	1V	113/116 (97%)	106 (94%)	7 (6%)	0	100	100
22	1W	113/128 (88%)	108 (96%)	5 (4%)	0	100	100
23	1X	169/172 (98%)	158 (94%)	11 (6%)	0	100	100
24	1Y	137/141 (97%)	131 (96%)	6 (4%)	0	100	100
25	1Z	139/144 (96%)	122 (88%)	17 (12%)	0	100	100
26	1a	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
27	1b	81/84 (96%)	71 (88%)	10 (12%)	0	100	100
28	1c	47/76 (62%)	44 (94%)	3 (6%)	0	100	100
29	1d	117/123 (95%)	106 (91%)	11 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	1e	97/106 (92%)	92 (95%)	5 (5%)	0	100	100
31	1f	55/135 (41%)	47 (86%)	8 (14%)	0	100	100
32	1g	98/154 (64%)	90 (92%)	7 (7%)	1 (1%)	15	55
33	1h	136/189 (72%)	124 (91%)	12 (9%)	0	100	100
34	1i	124/128 (97%)	117 (94%)	7 (6%)	0	100	100
35	1j	69/105 (66%)	65 (94%)	4 (6%)	0	100	100
36	1k	79/98 (81%)	71 (90%)	8 (10%)	0	100	100
37	1l	154/186 (83%)	143 (93%)	11 (7%)	0	100	100
38	1m	126/129 (98%)	119 (94%)	7 (6%)	0	100	100
39	1n	170/179 (95%)	163 (96%)	5 (3%)	2 (1%)	13	51
40	1o	120/137 (88%)	111 (92%)	8 (7%)	1 (1%)	19	59
41	1p	171/176 (97%)	167 (98%)	4 (2%)	0	100	100
42	1q	143/145 (99%)	130 (91%)	11 (8%)	2 (1%)	11	48
43	1r	90/114 (79%)	77 (86%)	13 (14%)	0	100	100
44	1s	43/471 (9%)	37 (86%)	6 (14%)	0	100	100
All	All	8101/9741 (83%)	7516 (93%)	566 (7%)	19 (0%)	50	79

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1F	313	GLU
8	1H	92	PRO
8	1H	170	GLU
20	1T	23	ASP
42	1q	142	THR
10	1J	116	ILE
12	1L	601	LEU
16	1P	333	ASP
39	1n	54	LYS
12	1L	549	ALA
17	1Q	70	MET
32	1g	65	GLY
39	1n	31	VAL
40	1o	32	GLU
7	1G	186	TYR
5	1E	157	ASN
42	1q	143	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1B	79	SER
11	1K	2	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1A	76/99 (77%)	67 (88%)	9 (12%)	5 28
2	1B	131/209 (63%)	117 (89%)	14 (11%)	6 32
3	1C	190/227 (84%)	177 (93%)	13 (7%)	16 50
4	1D	341/405 (84%)	324 (95%)	17 (5%)	24 59
5	1E	183/207 (88%)	171 (93%)	12 (7%)	16 51
6	1F	346/368 (94%)	322 (93%)	24 (7%)	15 49
7	1G	588/610 (96%)	555 (94%)	33 (6%)	21 56
8	1H	255/274 (93%)	243 (95%)	12 (5%)	26 61
9	1I	151/201 (75%)	143 (95%)	8 (5%)	22 58
10	1J	140/140 (100%)	128 (91%)	12 (9%)	10 41
11	1K	84/84 (100%)	79 (94%)	5 (6%)	19 54
12	1L	539/539 (100%)	521 (97%)	18 (3%)	38 69
13	1M	408/408 (100%)	399 (98%)	9 (2%)	52 77
14	1N	310/310 (100%)	295 (95%)	15 (5%)	25 60
15	1O	283/307 (92%)	266 (94%)	17 (6%)	19 54
16	1P	296/323 (92%)	276 (93%)	20 (7%)	16 50
17	1Q	117/152 (77%)	109 (93%)	8 (7%)	16 50
18	1R	79/97 (81%)	71 (90%)	8 (10%)	7 34
19	1S	77/82 (94%)	68 (88%)	9 (12%)	5 29
20	1T	79/133 (59%)	69 (87%)	10 (13%)	4 24
20	1U	79/133 (59%)	72 (91%)	7 (9%)	9 40
21	1V	100/101 (99%)	95 (95%)	5 (5%)	24 59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	1W	107/112 (96%)	97 (91%)	10 (9%)	9	38
23	1X	153/154 (99%)	146 (95%)	7 (5%)	27	61
24	1Y	101/102 (99%)	97 (96%)	4 (4%)	31	65
25	1Z	123/124 (99%)	116 (94%)	7 (6%)	20	55
26	1a	58/58 (100%)	51 (88%)	7 (12%)	5	26
27	1b	69/70 (99%)	63 (91%)	6 (9%)	10	41
28	1c	45/66 (68%)	42 (93%)	3 (7%)	16	50
29	1d	107/109 (98%)	98 (92%)	9 (8%)	11	42
30	1e	87/94 (93%)	82 (94%)	5 (6%)	20	55
31	1f	54/113 (48%)	51 (94%)	3 (6%)	21	56
32	1g	92/129 (71%)	85 (92%)	7 (8%)	13	45
33	1h	121/158 (77%)	113 (93%)	8 (7%)	16	51
34	1i	119/120 (99%)	109 (92%)	10 (8%)	11	42
35	1j	62/84 (74%)	55 (89%)	7 (11%)	6	30
36	1k	63/76 (83%)	53 (84%)	10 (16%)	2	16
37	1l	141/161 (88%)	135 (96%)	6 (4%)	29	63
38	1m	113/114 (99%)	106 (94%)	7 (6%)	18	53
39	1n	156/160 (98%)	144 (92%)	12 (8%)	13	45
40	1o	110/120 (92%)	100 (91%)	10 (9%)	9	39
41	1p	154/156 (99%)	147 (96%)	7 (4%)	27	62
42	1q	131/131 (100%)	124 (95%)	7 (5%)	22	58
43	1r	85/98 (87%)	76 (89%)	9 (11%)	6	32
44	1s	44/351 (12%)	40 (91%)	4 (9%)	9	39
All	All	7147/8269 (86%)	6697 (94%)	450 (6%)	21	53

All (450) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	4	MET
1	1A	22	PHE
1	1A	23	TRP
1	1A	54	LYS
1	1A	55	PHE
1	1A	62	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	85	LYS
1	1A	87	MET
1	1A	105	GLU
2	1B	25	ARG
2	1B	28	TYR
2	1B	32	LYS
2	1B	42	ARG
2	1B	44	SER
2	1B	48	MET
2	1B	68	ASP
2	1B	69	MET
2	1B	94	ASN
2	1B	95	LYS
2	1B	101	ARG
2	1B	125	TYR
2	1B	137	ASP
2	1B	169	ARG
3	1C	8	ARG
3	1C	14	ARG
3	1C	28	TYR
3	1C	45	PHE
3	1C	66	ASP
3	1C	72	PHE
3	1C	77	ASP
3	1C	88	ASN
3	1C	112	ASP
3	1C	129	TRP
3	1C	173	GLU
3	1C	200	ASN
3	1C	201	SER
4	1D	2	ARG
4	1D	74	ARG
4	1D	75	LYS
4	1D	89	LYS
4	1D	90	LEU
4	1D	152	MET
4	1D	171	PHE
4	1D	220	PHE
4	1D	228	MET
4	1D	229	LEU
4	1D	270	ARG
4	1D	318	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	1D	334	LYS
4	1D	389	CYS
4	1D	390	LYS
4	1D	422	ASP
4	1D	429	ASP
5	1E	9	HIS
5	1E	22	ASP
5	1E	37	ASN
5	1E	38	TYR
5	1E	98	TYR
5	1E	109	MET
5	1E	141	GLU
5	1E	144	CYS
5	1E	150	ASN
5	1E	153	MET
5	1E	160	TYR
5	1E	188	SER
6	1F	16	LYS
6	1F	19	ASP
6	1F	30	ASP
6	1F	38	SER
6	1F	89	ARG
6	1F	137	TYR
6	1F	149	LEU
6	1F	157	TYR
6	1F	171	TYR
6	1F	186	CYS
6	1F	235	CYS
6	1F	272	MET
6	1F	278	GLU
6	1F	292	ASP
6	1F	293	ASN
6	1F	306	LEU
6	1F	355	LYS
6	1F	385	ARG
6	1F	390	ASP
6	1F	405	CYS
6	1F	413	TRP
6	1F	420	ARG
6	1F	421	HIS
6	1F	437	HIS
7	1G	28	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	1G	54	MET
7	1G	61	LYS
7	1G	77	TRP
7	1G	80	LEU
7	1G	82	ASN
7	1G	84	GLU
7	1G	85	LYS
7	1G	130	PHE
7	1G	145	LEU
7	1G	190	MET
7	1G	191	PHE
7	1G	210	SER
7	1G	243	ARG
7	1G	314	ASP
7	1G	332	LYS
7	1G	359	ARG
7	1G	361	ASN
7	1G	396	ARG
7	1G	402	ASN
7	1G	417	TYR
7	1G	418	ARG
7	1G	422	LEU
7	1G	437	HIS
7	1G	462	ASP
7	1G	558	ASP
7	1G	609	MET
7	1G	613	TYR
7	1G	620	ARG
7	1G	642	PHE
7	1G	649	SER
7	1G	655	GLN
7	1G	672	TYR
8	1H	8	SER
8	1H	19	PHE
8	1H	43	TYR
8	1H	54	LYS
8	1H	98	MET
8	1H	110	SER
8	1H	124	ASN
8	1H	152	SER
8	1H	157	ASN
8	1H	270	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	1H	282	TYR
8	1H	317	GLN
9	1I	2	TYR
9	1I	20	ARG
9	1I	23	GLN
9	1I	27	TRP
9	1I	40	TYR
9	1I	58	SER
9	1I	62	ARG
9	1I	151	LYS
10	1J	3	MET
10	1J	57	PHE
10	1J	70	TYR
10	1J	79	TYR
10	1J	83	TRP
10	1J	87	LYS
10	1J	93	PHE
10	1J	98	MET
10	1J	100	GLU
10	1J	119	PHE
10	1J	129	ASP
10	1J	135	PHE
11	1K	21	MET
11	1K	23	ARG
11	1K	53	PHE
11	1K	59	MET
11	1K	66	PHE
12	1L	7	LEU
12	1L	23	ASN
12	1L	52	LEU
12	1L	66	TRP
12	1L	83	ASP
12	1L	179	ASP
12	1L	185	SER
12	1L	186	MET
12	1L	250	SER
12	1L	271	LYS
12	1L	276	MET
12	1L	300	LYS
12	1L	328	HIS
12	1L	401	MET
12	1L	482	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	1L	500	LEU
12	1L	602	PHE
12	1L	605	HIS
13	1M	57	PHE
13	1M	76	MET
13	1M	148	TYR
13	1M	152	TYR
13	1M	228	SER
13	1M	255	ASN
13	1M	336	ARG
13	1M	359	TRP
13	1M	437	MET
14	1N	14	MET
14	1N	21	MET
14	1N	48	PHE
14	1N	98	MET
14	1N	100	MET
14	1N	140	SER
14	1N	175	LEU
14	1N	200	MET
14	1N	204	ASN
14	1N	211	MET
14	1N	213	LEU
14	1N	237	MET
14	1N	278	MET
14	1N	298	TYR
14	1N	323	MET
15	1O	37	ARG
15	1O	40	ARG
15	1O	49	ARG
15	1O	82	PHE
15	1O	105	LEU
15	1O	124	LEU
15	1O	126	ARG
15	1O	129	TYR
15	1O	143	PHE
15	1O	164	LEU
15	1O	171	TYR
15	1O	184	GLN
15	1O	192	MET
15	1O	193	LYS
15	1O	233	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	1O	250	ASP
15	1O	316	TRP
16	1P	41	MET
16	1P	55	ASP
16	1P	58	HIS
16	1P	78	LYS
16	1P	115	HIS
16	1P	145	TYR
16	1P	170	ASP
16	1P	175	GLU
16	1P	178	PHE
16	1P	185	MET
16	1P	186	ARG
16	1P	202	LYS
16	1P	206	TYR
16	1P	224	LYS
16	1P	306	GLN
16	1P	326	TRP
16	1P	331	MET
16	1P	333	ASP
16	1P	335	LYS
16	1P	338	LYS
17	1Q	14	ASP
17	1Q	18	ASP
17	1Q	28	GLU
17	1Q	89	LYS
17	1Q	103	PHE
17	1Q	116	LYS
17	1Q	127	ARG
17	1Q	131	SER
18	1R	3	ARG
18	1R	20	ASP
18	1R	23	TYR
18	1R	31	ARG
18	1R	38	ASN
18	1R	42	ASP
18	1R	54	SER
18	1R	77	LYS
19	1S	16	ARG
19	1S	25	ARG
19	1S	34	ASP
19	1S	38	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	1S	64	LEU
19	1S	68	TYR
19	1S	70	PHE
19	1S	88	ARG
19	1S	95	SER
20	1T	9	GLU
20	1T	17	TYR
20	1T	20	LYS
20	1T	22	TYR
20	1T	47	GLN
20	1T	69	LYS
20	1T	71	MET
20	1T	74	GLN
20	1T	84	LYS
20	1T	85	ASP
20	1U	6	LEU
20	1U	12	LYS
20	1U	22	TYR
20	1U	37	MET
20	1U	38	LYS
20	1U	52	MET
20	1U	87	TYR
21	1V	4	LEU
21	1V	5	LYS
21	1V	6	LYS
21	1V	48	GLU
21	1V	93	MET
22	1W	18	LYS
22	1W	30	ARG
22	1W	36	TYR
22	1W	39	TRP
22	1W	41	ARG
22	1W	57	LYS
22	1W	65	GLU
22	1W	107	PHE
22	1W	111	GLU
22	1W	126	HIS
23	1X	15	GLN
23	1X	43	MET
23	1X	47	TRP
23	1X	71	ARG
23	1X	77	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	1X	81	PHE
23	1X	171	MET
24	1Y	47	SER
24	1Y	80	ARG
24	1Y	105	ARG
24	1Y	126	MET
25	1Z	21	TYR
25	1Z	47	TYR
25	1Z	52	LYS
25	1Z	68	ARG
25	1Z	85	GLN
25	1Z	90	ASN
25	1Z	105	LYS
26	1a	48	MET
26	1a	50	ARG
26	1a	59	ARG
26	1a	60	TYR
26	1a	61	HIS
26	1a	67	GLU
26	1a	68	ASN
27	1b	15	GLU
27	1b	33	SER
27	1b	59	ASP
27	1b	62	MET
27	1b	76	SER
27	1b	79	TRP
28	1c	5	ARG
28	1c	30	TYR
28	1c	48	LEU
29	1d	8	ARG
29	1d	26	LEU
29	1d	39	TYR
29	1d	51	ARG
29	1d	88	HIS
29	1d	95	LYS
29	1d	100	ASP
29	1d	104	LYS
29	1d	105	ASP
30	1e	20	GLN
30	1e	21	SER
30	1e	52	GLU
30	1e	74	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	1e	91	TYR
31	1f	1	MET
31	1f	22	PHE
31	1f	45	LYS
32	1g	49	LYS
32	1g	58	MET
32	1g	63	PHE
32	1g	91	ARG
32	1g	99	TYR
32	1g	107	LEU
32	1g	108	MET
33	1h	12	LYS
33	1h	18	ASP
33	1h	23	LYS
33	1h	54	ASP
33	1h	59	TYR
33	1h	80	TYR
33	1h	106	LYS
33	1h	109	GLU
34	1i	6	ASP
34	1i	8	LYS
34	1i	25	GLN
34	1i	34	LEU
34	1i	36	PRO
34	1i	52	ASP
34	1i	64	TYR
34	1i	69	PHE
34	1i	122	PHE
34	1i	123	PRO
35	1j	19	ARG
35	1j	27	PHE
35	1j	37	LEU
35	1j	40	PHE
35	1j	63	GLU
35	1j	69	ASP
35	1j	70	ASP
36	1k	12	LYS
36	1k	38	ARG
36	1k	40	LEU
36	1k	41	ARG
36	1k	46	ARG
36	1k	56	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1k	61	SER
36	1k	62	PHE
36	1k	70	PHE
36	1k	77	PHE
37	1l	3	HIS
37	1l	28	ASN
37	1l	53	ARG
37	1l	116	PHE
37	1l	148	LYS
37	1l	151	GLU
38	1m	6	LYS
38	1m	17	LEU
38	1m	30	LYS
38	1m	39	ARG
38	1m	61	ASP
38	1m	98	PHE
38	1m	99	PHE
39	1n	12	GLN
39	1n	36	TYR
39	1n	38	TYR
39	1n	47	PHE
39	1n	53	GLU
39	1n	55	ASP
39	1n	68	GLU
39	1n	84	SER
39	1n	128	ARG
39	1n	134	ARG
39	1n	137	LYS
39	1n	159	GLU
40	1o	21	MET
40	1o	37	GLU
40	1o	45	MET
40	1o	76	PHE
40	1o	94	TYR
40	1o	98	MET
40	1o	105	ARG
40	1o	106	ARG
40	1o	109	GLN
40	1o	110	ARG
41	1p	6	LYS
41	1p	14	ARG
41	1p	15	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1p	63	TYR
41	1p	126	LYS
41	1p	141	ARG
41	1p	166	ARG
42	1q	1	MET
42	1q	9	ARG
42	1q	58	ARG
42	1q	78	ASP
42	1q	81	MET
42	1q	106	ARG
42	1q	135	GLN
43	1r	11	ARG
43	1r	19	LEU
43	1r	22	LYS
43	1r	25	LEU
43	1r	51	ASN
43	1r	60	ARG
43	1r	91	LYS
43	1r	104	GLU
43	1r	109	GLN
44	1s	51	PHE
44	1s	60	LYS
44	1s	61	PHE
44	1s	63	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
3	1C	41	GLN
4	1D	237	ASN
5	1E	55	GLN
5	1E	159	ASN
6	1F	83	ASN
6	1F	200	GLN
7	1G	100	ASN
7	1G	491	ASN
7	1G	549	HIS
7	1G	581	GLN
8	1H	124	ASN
8	1H	287	HIS
9	1I	157	ASN
11	1K	7	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	1L	194	ASN
12	1L	506	ASN
13	1M	168	GLN
13	1M	415	GLN
13	1M	425	ASN
13	1M	450	ASN
16	1P	36	ASN
17	1Q	6	GLN
18	1R	93	GLN
19	1S	80	ASN
20	1T	35	HIS
21	1V	49	GLN
21	1V	85	ASN
22	1W	126	HIS
34	1i	13	GLN
38	1m	74	ASN
40	1o	54	GLN
40	1o	116	GLN
41	1p	27	ASN
42	1q	91	HIS
43	1r	24	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	$\# Z > 2$
12	FME	1L	1	12	8,9,10	0.52	0	7,9,11	1.10	1 (14%)
11	FME	1K	1	11	8,9,10	0.51	0	7,9,11	1.83	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	FME	1M	1	13	8,9,10	0.52	0	7,9,11	1.03	1 (14%)
14	FME	1N	1	14	8,9,10	0.48	0	7,9,11	1.08	1 (14%)
1	FME	1A	1	1	8,9,10	0.50	0	7,9,11	1.03	1 (14%)
10	FME	1J	1	10	8,9,10	0.53	0	7,9,11	0.99	1 (14%)
8	FME	1H	1	8	8,9,10	0.51	0	7,9,11	1.14	1 (14%)
34	SAC	1i	1	-	7,8,9	0.52	0	8,9,11	1.93	2 (25%)

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
12	FME	1L	1	12	-	0/7/9/11	-
11	FME	1K	1	11	-	0/7/9/11	-
13	FME	1M	1	13	-	1/7/9/11	-
14	FME	1N	1	14	-	0/7/9/11	-
1	FME	1A	1	1	-	2/7/9/11	-
10	FME	1J	1	10	-	0/7/9/11	-
8	FME	1H	1	8	-	0/7/9/11	-
34	SAC	1i	1	-	-	6/7/8/10	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1K	1	FME	CA-N-CN	3.72	128.54	122.82
34	1i	1	SAC	CA-N-C1A	3.69	129.95	123.15
34	1i	1	SAC	O-C-CA	-2.93	117.10	124.78
8	1H	1	FME	O-C-CA	-2.75	117.57	124.78
12	1L	1	FME	O-C-CA	-2.66	117.81	124.78
14	1N	1	FME	O-C-CA	-2.61	117.94	124.78
11	1K	1	FME	O-C-CA	-2.52	118.19	124.78
13	1M	1	FME	O-C-CA	-2.50	118.23	124.78
1	1A	1	FME	O-C-CA	-2.47	118.30	124.78
10	1J	1	FME	O-C-CA	-2.44	118.39	124.78

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1	FME	N-CA-CB-CG
13	1M	1	FME	C-CA-CB-CG
34	1i	1	SAC	C-CA-CB-OG
34	1i	1	SAC	C2A-C1A-N-CA
34	1i	1	SAC	OAC-C1A-N-CA
34	1i	1	SAC	N-CA-CB-OG
1	1A	1	FME	C-CA-CB-CG
34	1i	1	SAC	C-CA-N-C1A
34	1i	1	SAC	CB-CA-N-C1A

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	$\# Z > 2$
45	3PE	1L	701	-	45,45,50	0.28	0	48,50,55	0.31	0
47	SF4	1G	802	7	0,12,12	-	-	-		
47	SF4	1F	502	6	0,12,12	-	-	-		
46	PC1	1I	203	-	53,53,53	0.27	0	59,61,61	0.30	0
46	PC1	1I	204	-	43,43,53	0.29	0	49,51,61	0.35	0
49	FMN	1F	501	-	33,33,33	0.59	0	48,50,50	0.66	1 (2%)
46	PC1	1L	702	-	43,43,53	0.29	0	49,51,61	0.38	0
45	3PE	1Y	201	-	30,30,50	0.34	0	33,35,55	0.59	1 (3%)
57	EHZ	1W	201	-	29,36,37	0.18	0	35,44,47	1.06	1 (2%)
57	EHZ	1n	201	-	29,36,37	0.16	0	35,44,47	1.22	1 (2%)
47	SF4	1I	202	9	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	MYR	1l	201	-	14,14,15	0.34	0	13,13,15	0.38	0
47	SF4	1I	201	9	0,12,12	-	-	-	-	-
53	GTP	1O	401	54	26,34,34	0.95	2 (7%)	32,54,54	0.89	1 (3%)
48	FES	1E	301	5	0,4,4	-	-	-	-	-
47	SF4	1G	801	7	0,12,12	-	-	-	-	-
52	CDL	1q	201	-	60,60,99	0.34	0	66,72,111	0.43	0
45	3PE	1L	703	-	41,41,50	0.30	0	44,46,55	1.26	5 (11%)
45	3PE	1N	401	-	50,50,50	0.27	0	53,55,55	0.41	0
46	PC1	1f	101	-	45,45,53	0.27	0	51,53,61	0.34	0
46	PC1	1A	202	-	34,34,53	0.32	0	40,42,61	0.35	0
45	3PE	1Y	202	-	50,50,50	0.26	0	53,55,55	0.41	0
51	PGT	1M	501	-	50,50,50	0.49	0	53,56,56	0.49	0
47	SF4	1B	201	2	0,12,12	-	-	-	-	-
45	3PE	1A	201	-	46,46,50	0.28	0	49,51,55	0.38	0
52	CDL	1N	402	-	76,76,99	0.77	2 (2%)	82,88,111	0.60	2 (2%)
55	NDP	1P	501	-	45,52,52	0.61	0	53,80,80	0.72	1 (1%)
48	FES	1G	803	7	0,4,4	-	-	-	-	-

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
45	3PE	1L	701	-	-	3/49/49/54	-
47	SF4	1G	802	7	-	-	0/6/5/5
47	SF4	1F	502	6	-	-	0/6/5/5
46	PC1	1I	203	-	-	3/57/57/57	-
46	PC1	1I	204	-	-	6/47/47/57	-
49	FMN	1F	501	-	-	1/18/18/18	0/3/3/3
46	PC1	1L	702	-	-	5/47/47/57	-
45	3PE	1Y	201	-	-	8/34/34/54	-
57	EHZ	1W	201	-	-	14/42/44/45	-
57	EHZ	1n	201	-	-	4/42/44/45	-
47	SF4	1I	202	9	-	-	0/6/5/5
58	MYR	1l	201	-	-	1/11/12/13	-
47	SF4	1I	201	9	-	-	0/6/5/5
53	GTP	1O	401	54	-	0/18/38/38	0/3/3/3
48	FES	1E	301	5	-	-	0/1/1/1
47	SF4	1G	801	7	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	CDL	1q	201	-	-	19/71/71/110	-
45	3PE	1L	703	-	-	6/45/45/54	-
45	3PE	1N	401	-	-	6/54/54/54	-
46	PC1	1f	101	-	-	6/49/49/57	-
46	PC1	1A	202	-	-	4/38/38/57	-
45	3PE	1Y	202	-	-	9/54/54/54	-
51	PGT	1M	501	-	-	23/55/55/55	-
47	SF4	1B	201	2	-	-	0/6/5/5
45	3PE	1A	201	-	-	2/50/50/54	-
52	CDL	1N	402	-	-	10/87/87/110	-
55	NDP	1P	501	-	-	8/30/77/77	0/5/5/5
48	FES	1G	803	7	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	1N	402	CDL	C15-C14	5.03	1.79	1.51
52	1N	402	CDL	C16-C15	2.72	1.66	1.51
53	1O	401	GTP	C5-C6	-2.58	1.42	1.47
53	1O	401	GTP	C8-N7	-2.00	1.31	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1n	201	EHZ	C10-S1-C9	6.77	122.94	101.87
45	1L	703	3PE	O21-C21-C22	6.11	124.66	111.50
57	1W	201	EHZ	C10-S1-C9	5.86	120.11	101.87
53	1O	401	GTP	O4'-C1'-C2'	-2.79	102.85	106.93
52	1N	402	CDL	C17-C16-C15	2.66	139.96	115.30
45	1L	703	3PE	O21-C21-O22	-2.64	117.31	123.70
45	1L	703	3PE	C2-O21-C21	2.58	124.14	117.79
52	1N	402	CDL	C16-C15-C14	2.50	127.13	114.42
45	1L	703	3PE	O21-C2-C1	2.34	116.87	108.40
45	1Y	201	3PE	O21-C21-C22	2.30	116.45	111.50
55	1P	501	NDP	C5A-C6A-N6A	2.22	123.73	120.35
45	1L	703	3PE	O21-C2-C3	2.05	115.83	108.40
49	1F	501	FMN	C4-N3-C2	-2.04	121.88	125.64

There are no chirality outliers.

All (138) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	1L	703	3PE	O22-C21-O21-C2
45	1L	703	3PE	C22-C21-O21-C2
45	1Y	201	3PE	O32-C31-O31-C3
45	1Y	201	3PE	C32-C31-O31-C3
45	1Y	201	3PE	O22-C21-O21-C2
45	1Y	201	3PE	C22-C21-O21-C2
45	1Y	202	3PE	C1-O11-P-O14
46	1A	202	PC1	C1-O11-P-O14
46	1A	202	PC1	C1-O11-P-O13
46	1I	204	PC1	C11-O13-P-O14
46	1I	204	PC1	C11-O13-P-O11
46	1L	702	PC1	C1-O11-P-O14
46	1f	101	PC1	O32-C31-O31-C3
46	1f	101	PC1	C32-C31-O31-C3
51	1M	501	PGT	C32-C31-O2-C2
51	1M	501	PGT	C1-O3P-P-O1P
51	1M	501	PGT	O11-C11-O3-C3
51	1M	501	PGT	C12-C11-O3-C3
52	1q	201	CDL	CA3-OA5-PA1-OA2
52	1q	201	CDL	CA4-CA3-OA5-PA1
52	1q	201	CDL	CB4-CB3-OB5-PB2
57	1W	201	EHZ	C11-C10-S1-C9
57	1W	201	EHZ	N2-C15-C16-C17
57	1W	201	EHZ	N2-C15-C16-O5
57	1W	201	EHZ	O4-C15-C16-C17
57	1W	201	EHZ	C16-C17-C20-O6
57	1W	201	EHZ	O2-C9-S1-C10
57	1W	201	EHZ	C8-C9-S1-C10
57	1n	201	EHZ	S1-C10-C11-N1
57	1n	201	EHZ	O2-C9-S1-C10
57	1n	201	EHZ	C8-C9-S1-C10
57	1W	201	EHZ	C13-C12-N1-C11
51	1M	501	PGT	O31-C31-O2-C2
45	1Y	202	3PE	C2-C1-O11-P
51	1M	501	PGT	C5-C4-O4P-P
57	1W	201	EHZ	O3-C12-N1-C11
51	1M	501	PGT	C31-C32-C33-C34
51	1M	501	PGT	C15-C16-C17-C18
52	1N	402	CDL	C12-C13-C14-C15
51	1M	501	PGT	C4-O4P-P-O3P
57	1W	201	EHZ	C18-C17-C20-O6
57	1W	201	EHZ	C19-C17-C20-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	1q	201	CDL	O1-C1-CB2-OB2
51	1M	501	PGT	C40-C41-C42-C43
51	1M	501	PGT	C14-C15-C16-C17
46	1I	204	PC1	C36-C37-C38-C39
51	1M	501	PGT	C22-C23-C24-C25
46	1I	203	PC1	C24-C25-C26-C27
52	1N	402	CDL	C15-C16-C17-C18
51	1M	501	PGT	C34-C35-C36-C37
45	1N	401	3PE	C35-C36-C37-C38
46	1I	204	PC1	O21-C2-C3-O31
45	1N	401	3PE	C37-C38-C39-C3A
49	1F	501	FMN	C4'-C5'-O5'-P
45	1Y	202	3PE	C3C-C3D-C3E-C3F
46	1I	204	PC1	C1-C2-C3-O31
52	1q	201	CDL	CA3-CA4-CA6-OA8
57	1W	201	EHZ	C3-C4-C5-C6
58	1l	201	MYR	C2-C3-C4-C5
57	1W	201	EHZ	O4-C15-C16-O5
57	1W	201	EHZ	C2-C3-C4-C5
45	1Y	202	3PE	C35-C36-C37-C38
45	1L	703	3PE	O11-C1-C2-O21
51	1M	501	PGT	O3P-C1-C2-O2
51	1M	501	PGT	C32-C33-C34-C35
52	1N	402	CDL	OA6-CA4-CA6-OA8
45	1N	401	3PE	C2-C3-O31-C31
51	1M	501	PGT	C44-C45-C46-C47
45	1N	401	3PE	O11-C1-C2-O21
57	1n	201	EHZ	C11-C10-S1-C9
45	1A	201	3PE	O21-C2-C3-O31
52	1q	201	CDL	OB6-CB4-CB6-OB8
55	1P	501	NDP	C3B-C2B-O2B-P2B
52	1N	402	CDL	CA3-CA4-CA6-OA8
45	1Y	202	3PE	O11-C1-C2-O21
55	1P	501	NDP	C2D-C1D-N1N-C6N
52	1q	201	CDL	CA2-C1-CB2-OB2
51	1M	501	PGT	C16-C17-C18-C19
52	1N	402	CDL	C32-C33-C34-C35
45	1N	401	3PE	C1-O11-P-O13
45	1Y	202	3PE	C1-O11-P-O13
51	1M	501	PGT	C1-O3P-P-O4P
52	1q	201	CDL	C1-CA2-OA2-PA1
51	1M	501	PGT	C4-O4P-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	1q	201	CDL	CA3-OA5-PA1-OA4
45	1Y	202	3PE	O11-C1-C2-C3
45	1A	201	3PE	C12-C11-O13-P
45	1Y	202	3PE	C12-C11-O13-P
55	1P	501	NDP	C1B-C2B-O2B-P2B
46	1I	203	PC1	C3A-C3B-C3C-C3D
51	1M	501	PGT	C21-C22-C23-C24
46	1A	202	PC1	O13-C11-C12-N
45	1Y	201	3PE	O21-C2-C3-O31
52	1q	201	CDL	C12-C13-C14-C15
55	1P	501	NDP	O4D-C1D-N1N-C6N
46	1L	702	PC1	C31-C32-C33-C34
52	1q	201	CDL	C52-C51-CB5-OB6
52	1q	201	CDL	OA6-CA4-CA6-OA8
51	1M	501	PGT	C41-C42-C43-C44
45	1Y	201	3PE	C1-O11-P-O13
46	1f	101	PC1	C11-O13-P-O11
52	1q	201	CDL	CA2-OA2-PA1-OA5
52	1q	201	CDL	CB2-OB2-PB2-OB5
52	1N	402	CDL	CA7-C31-C32-C33
46	1I	203	PC1	C32-C33-C34-C35
46	1f	101	PC1	C21-C22-C23-C24
52	1N	402	CDL	C55-C56-C57-C58
52	1N	402	CDL	C76-C77-C78-C79
45	1N	401	3PE	C22-C23-C24-C25
45	1L	703	3PE	C1-C2-O21-C21
55	1P	501	NDP	C2D-C1D-N1N-C2N
46	1L	702	PC1	O11-C1-C2-C3
51	1M	501	PGT	O3P-C1-C2-C3
46	1A	202	PC1	O21-C2-C3-O31
52	1N	402	CDL	C53-C54-C55-C56
52	1q	201	CDL	CB3-CB4-CB6-OB8
46	1f	101	PC1	C36-C37-C38-C39
46	1I	204	PC1	C1-O11-P-O13
45	1L	701	3PE	C22-C23-C24-C25
45	1L	703	3PE	C32-C33-C34-C35
45	1L	703	3PE	C1-C2-C3-O31
55	1P	501	NDP	O4D-C1D-N1N-C2N
45	1Y	201	3PE	C1-C2-C3-O31
45	1Y	201	3PE	C1-O11-P-O14
46	1f	101	PC1	C11-O13-P-O14
52	1q	201	CDL	CA2-OA2-PA1-OA3

Continued on next page...

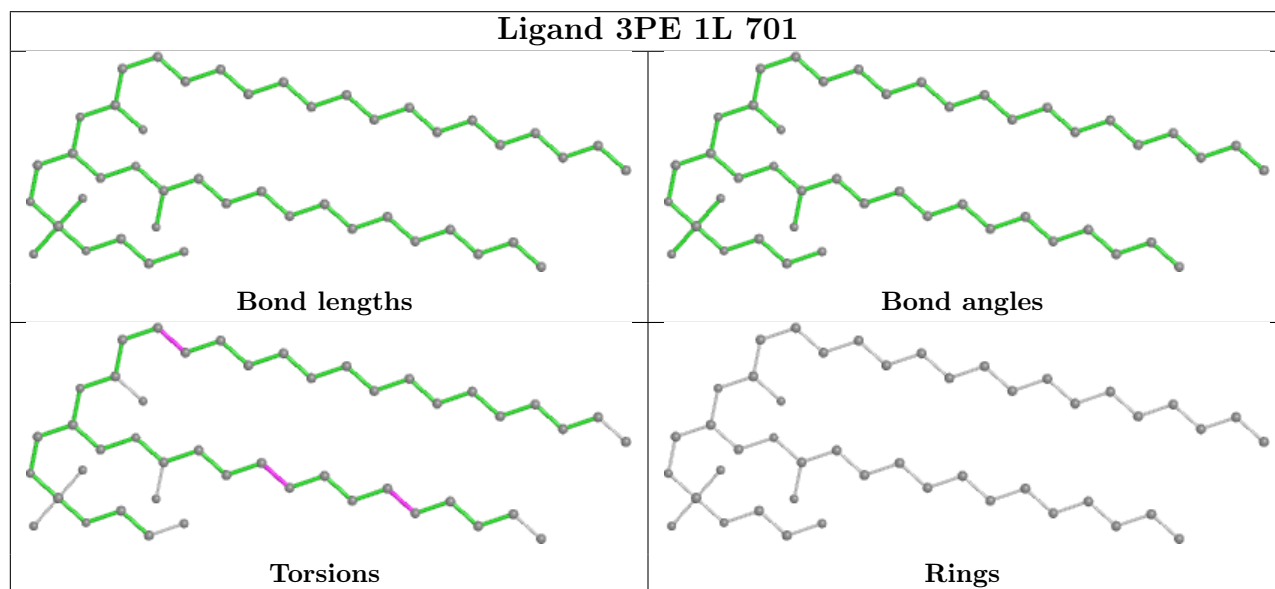
Continued from previous page...

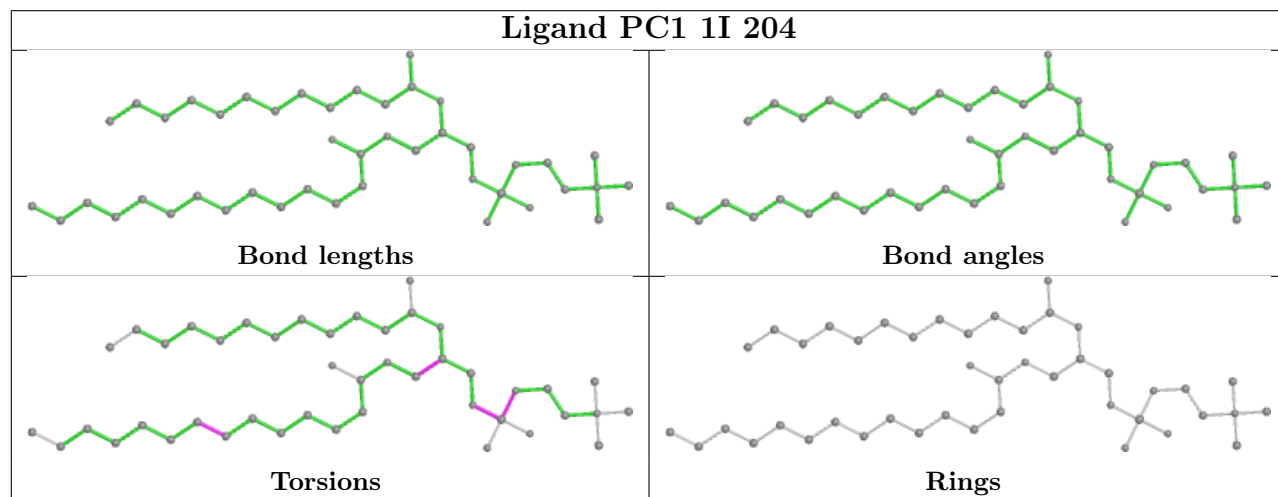
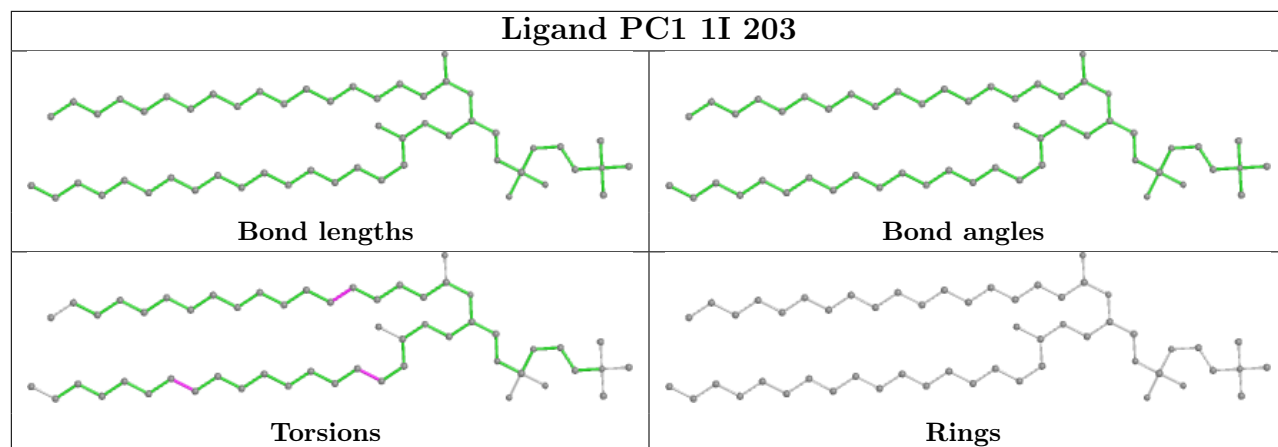
Mol	Chain	Res	Type	Atoms
52	1q	201	CDL	CB3-OB5-PB2-OB3
55	1P	501	NDP	O4B-C4B-C5B-O5B
55	1P	501	NDP	O4D-C4D-C5D-O5D
46	1L	702	PC1	O31-C31-C32-C33
45	1L	701	3PE	C33-C34-C35-C36
51	1M	501	PGT	C39-C40-C41-C42
52	1q	201	CDL	O1-C1-CA2-OA2
52	1q	201	CDL	C32-C31-CA7-OA8
52	1N	402	CDL	C33-C34-C35-C36
45	1L	701	3PE	C37-C38-C39-C3A
45	1Y	202	3PE	C24-C25-C26-C27
46	1L	702	PC1	O32-C31-C32-C33

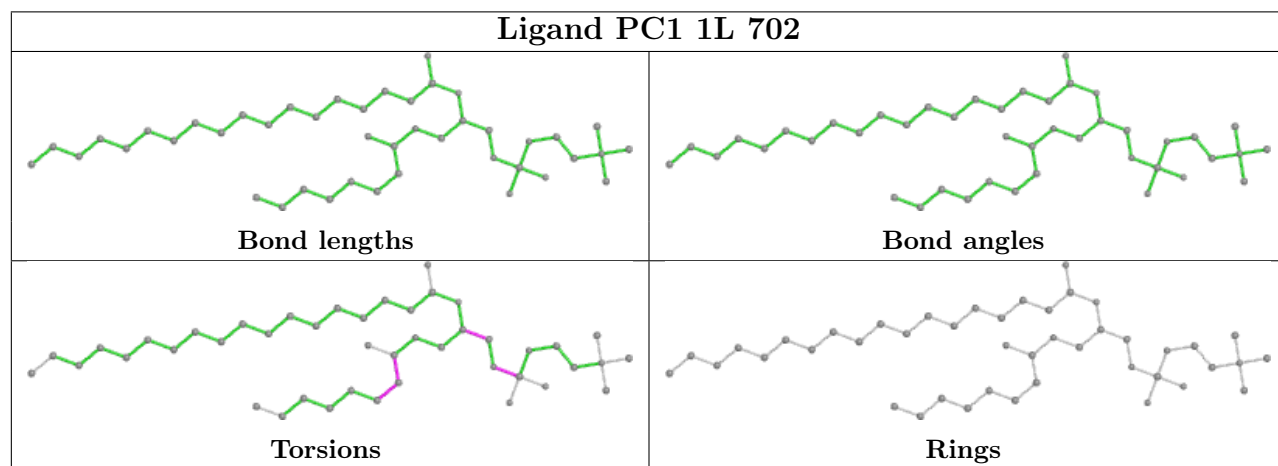
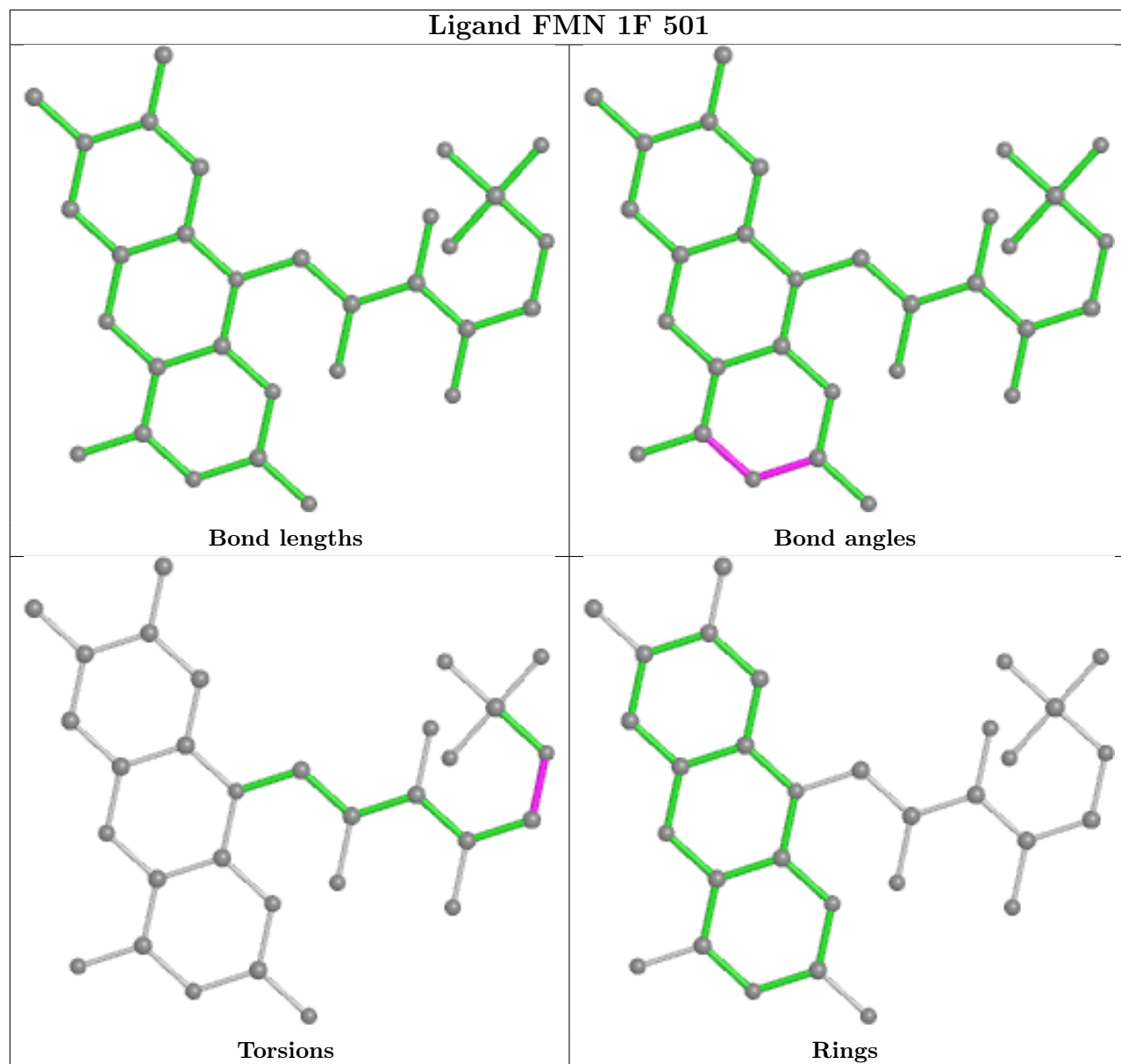
There are no ring outliers.

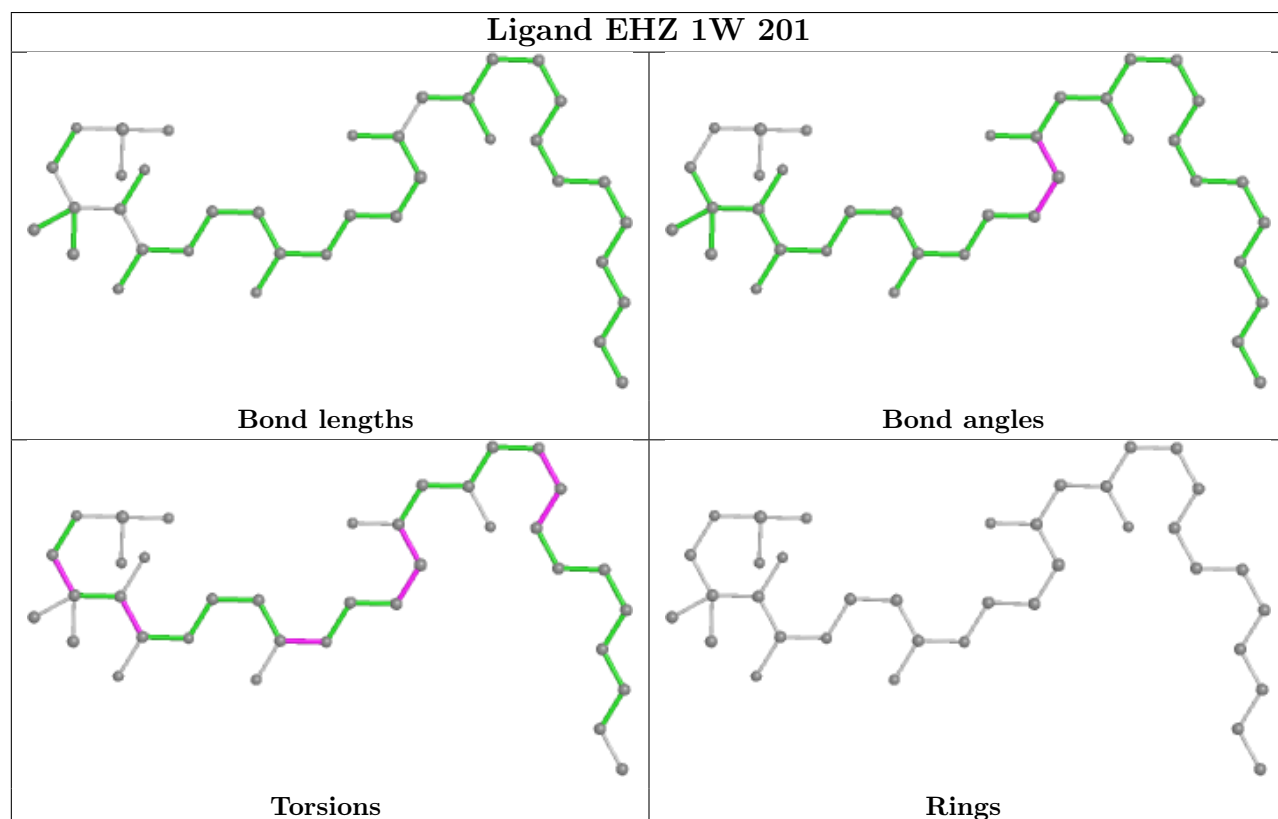
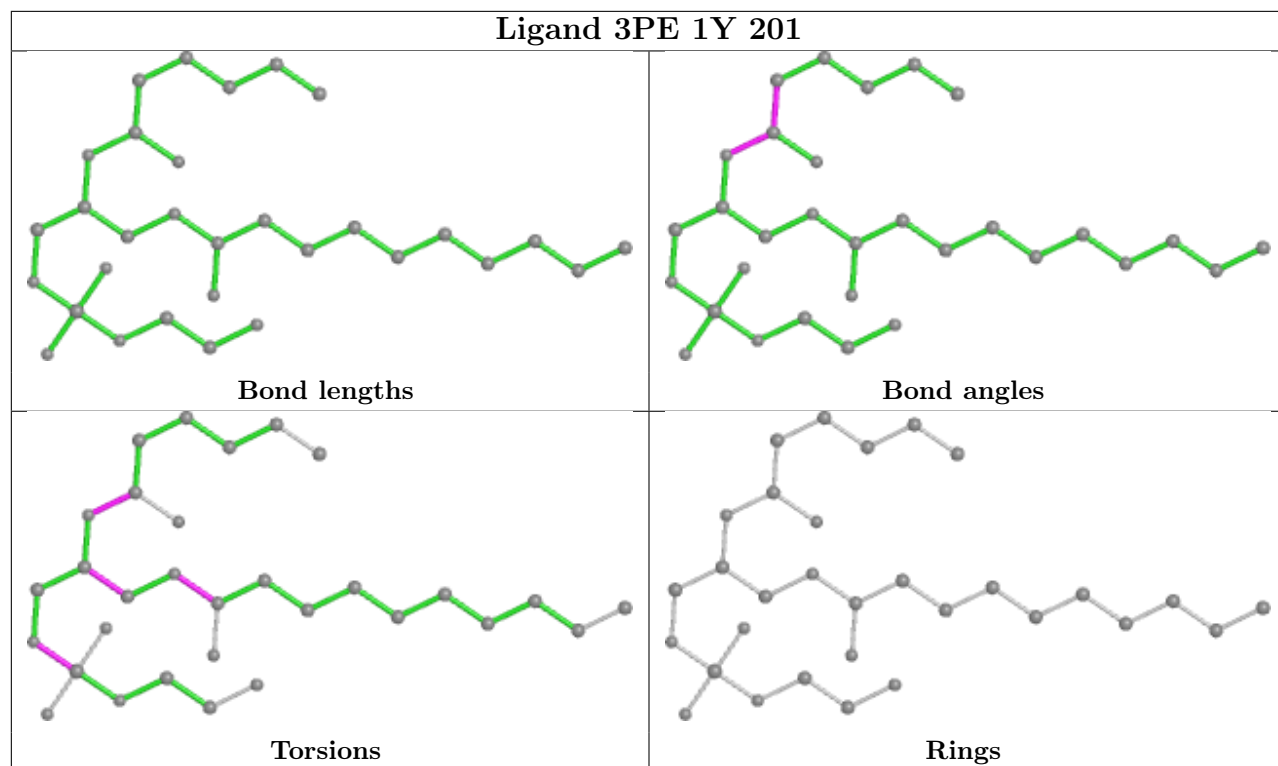
No monomer is involved in short contacts.

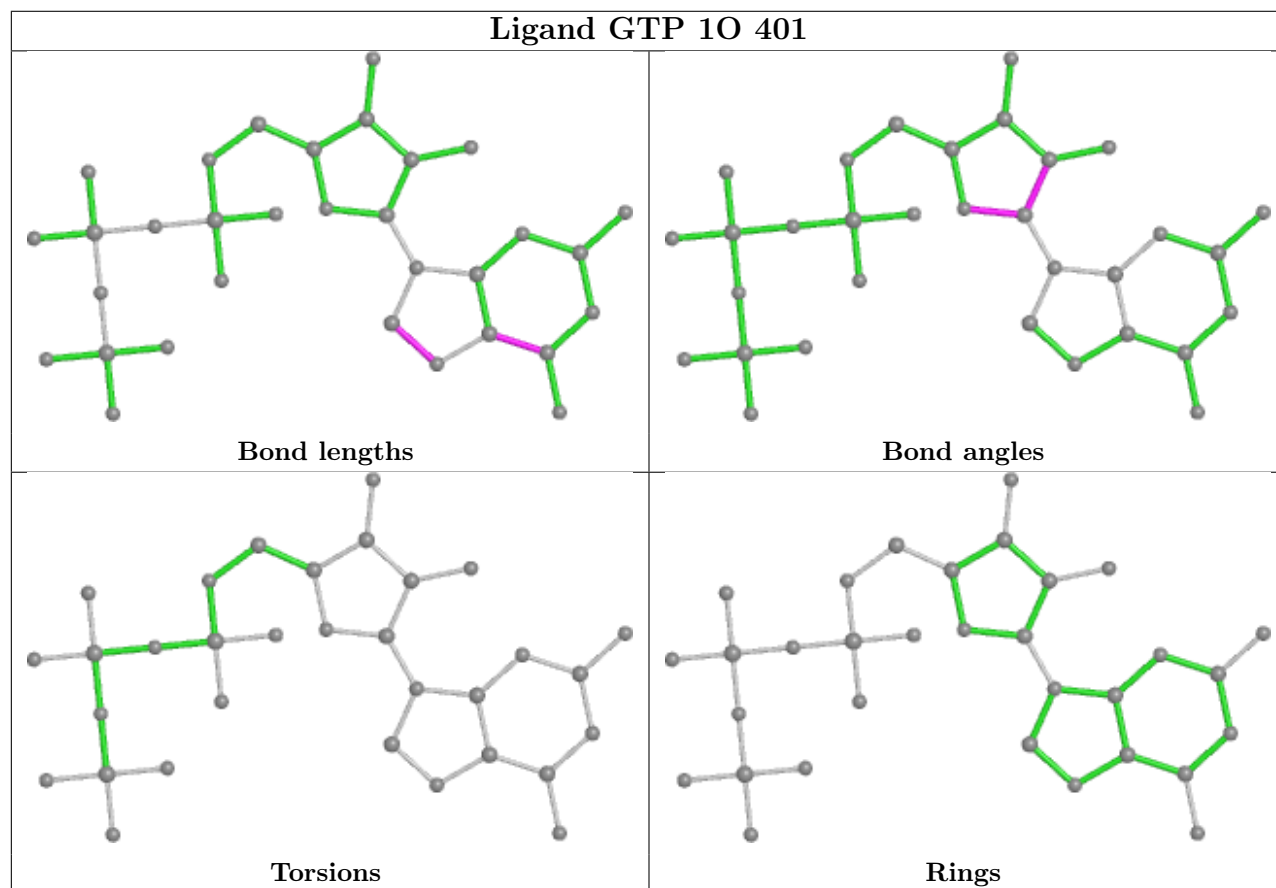
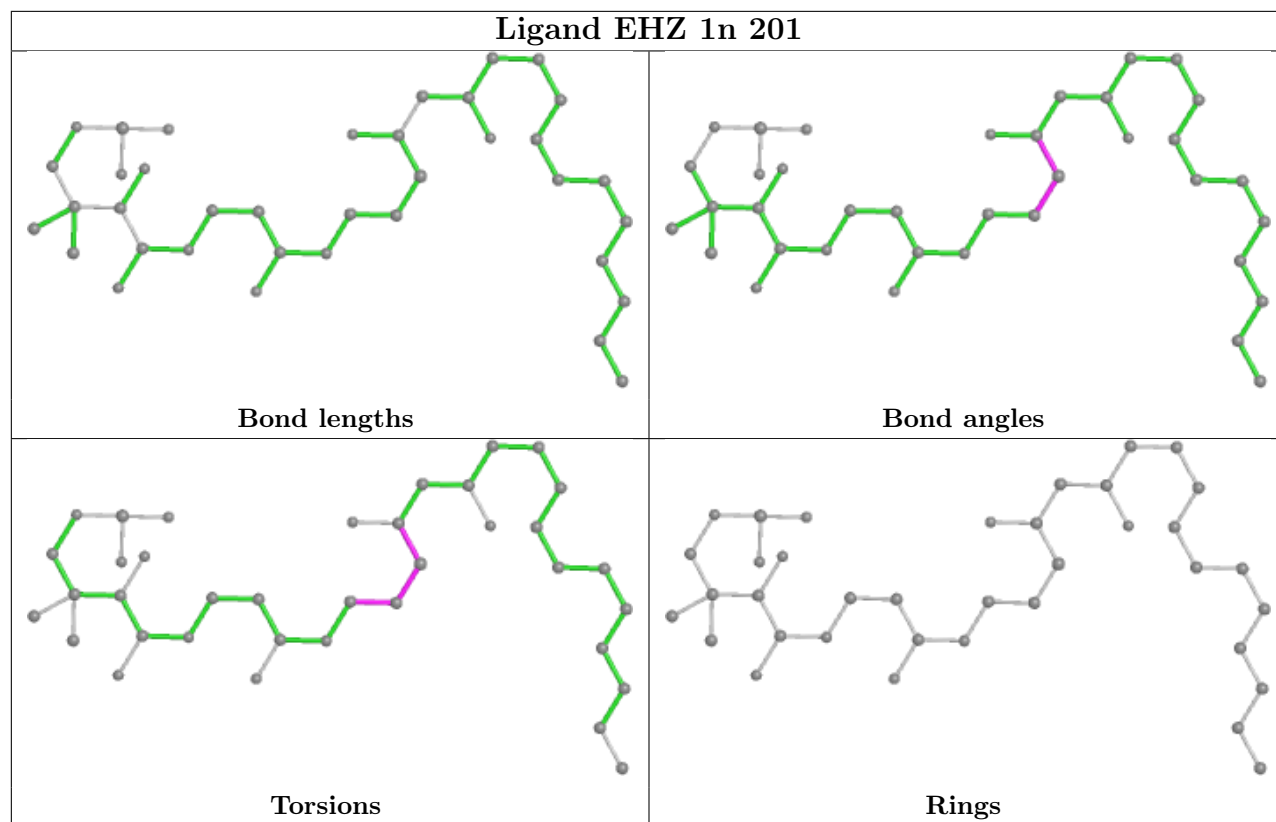
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

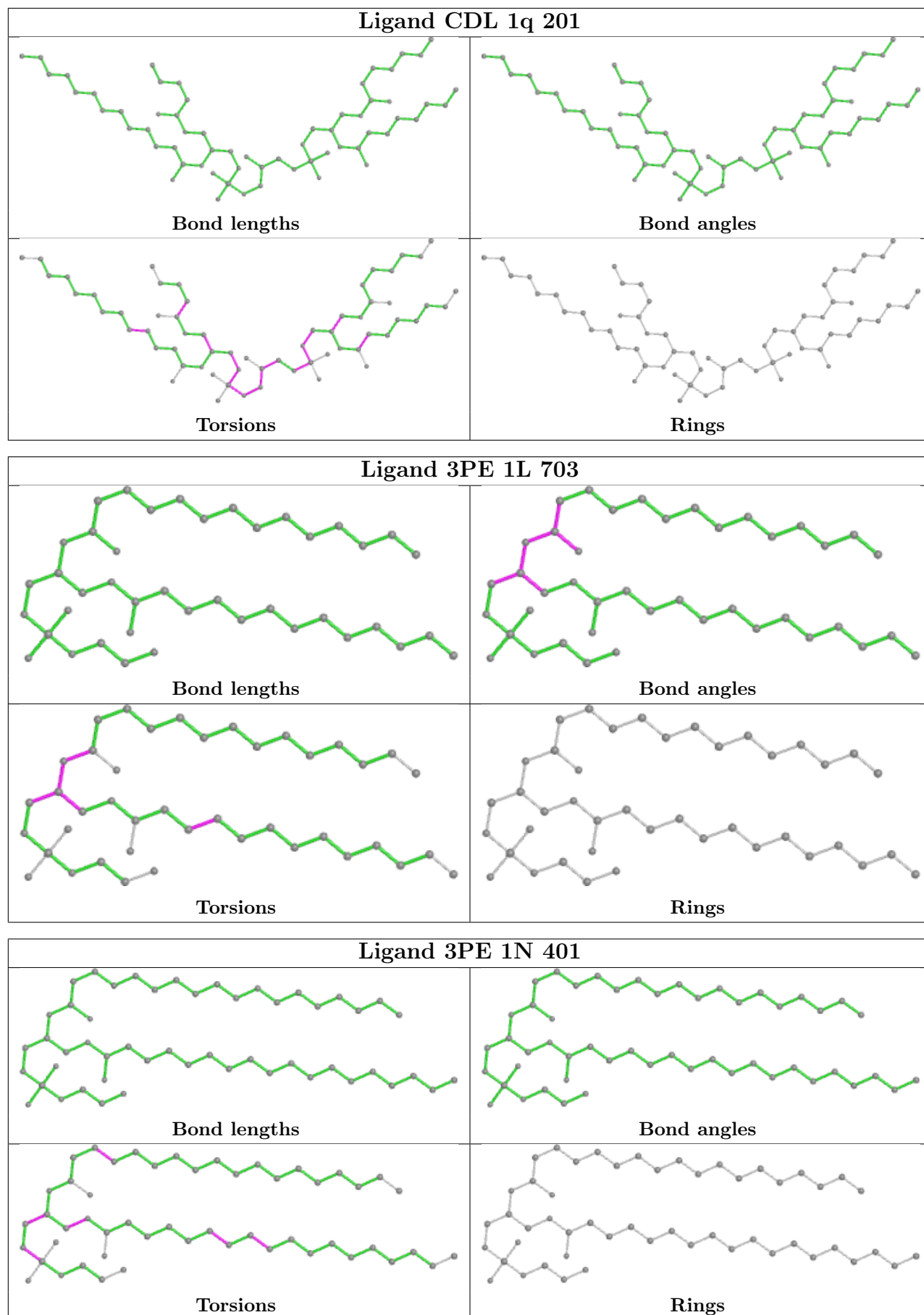


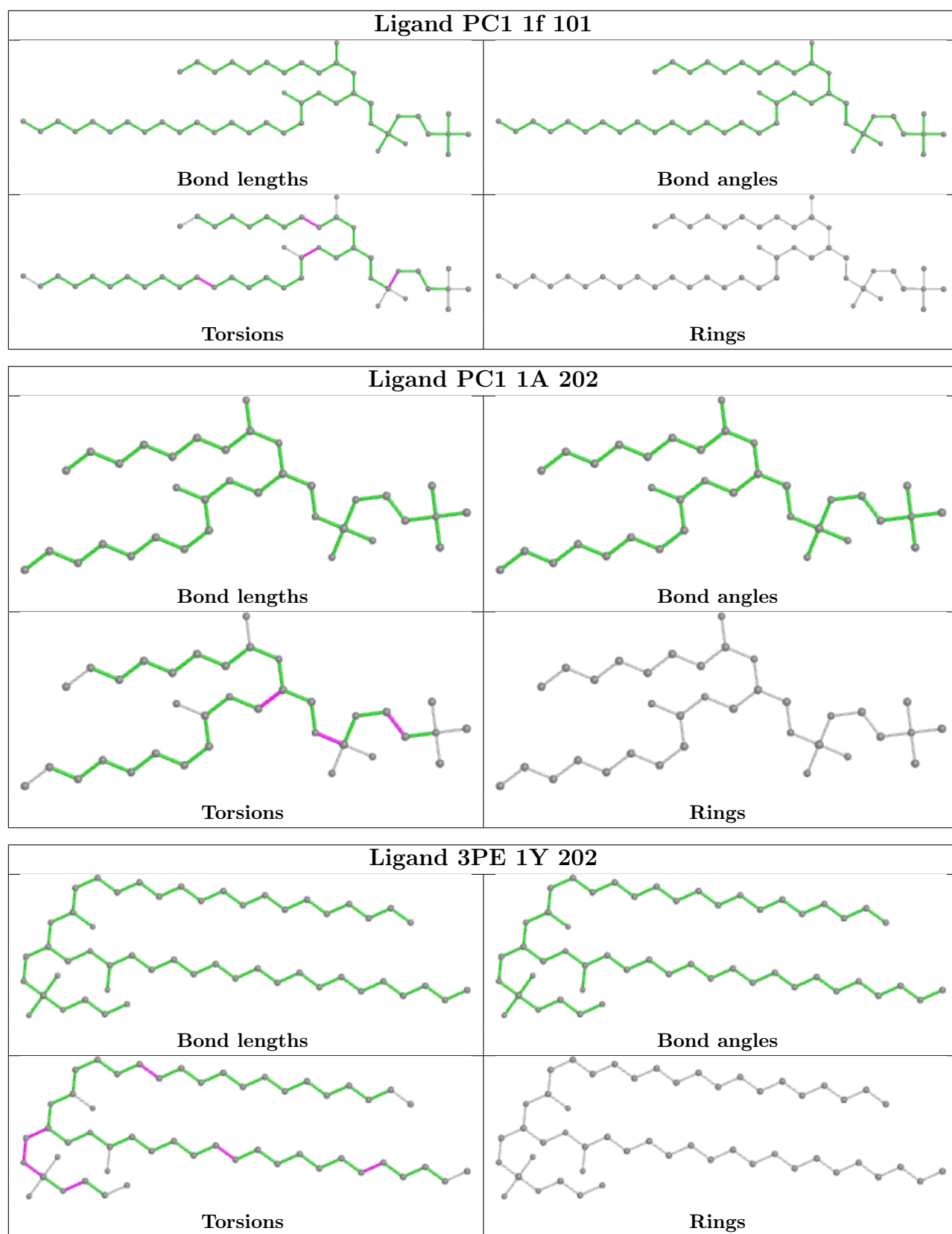


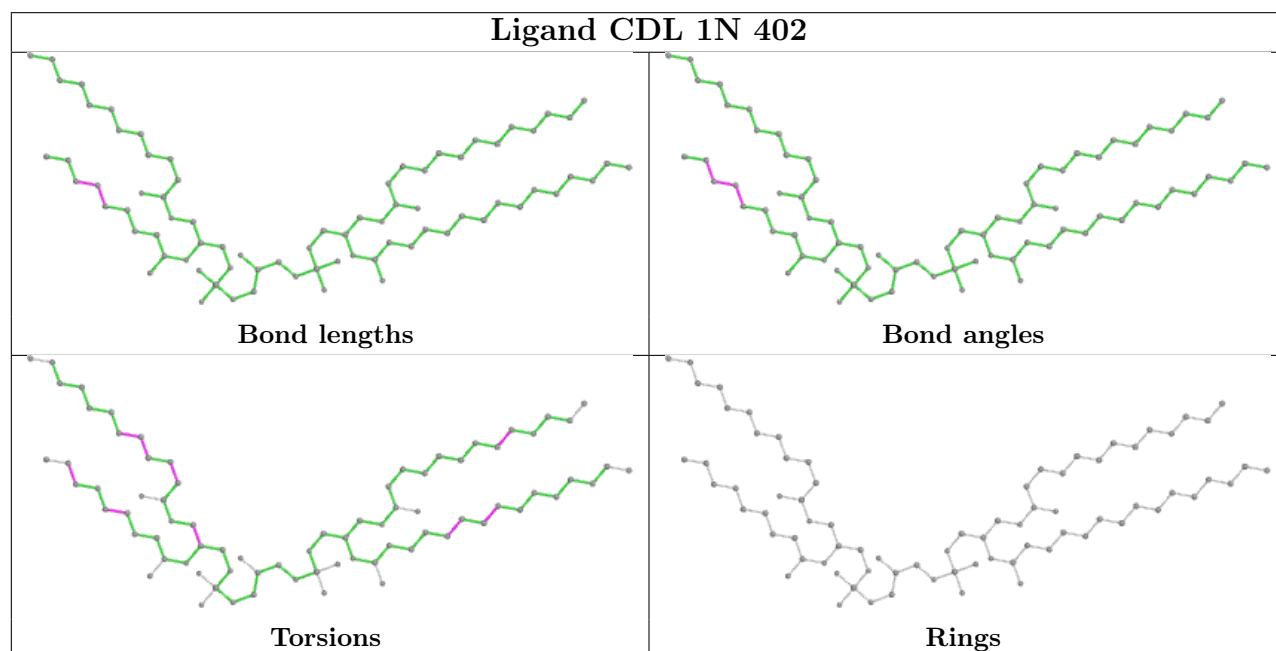
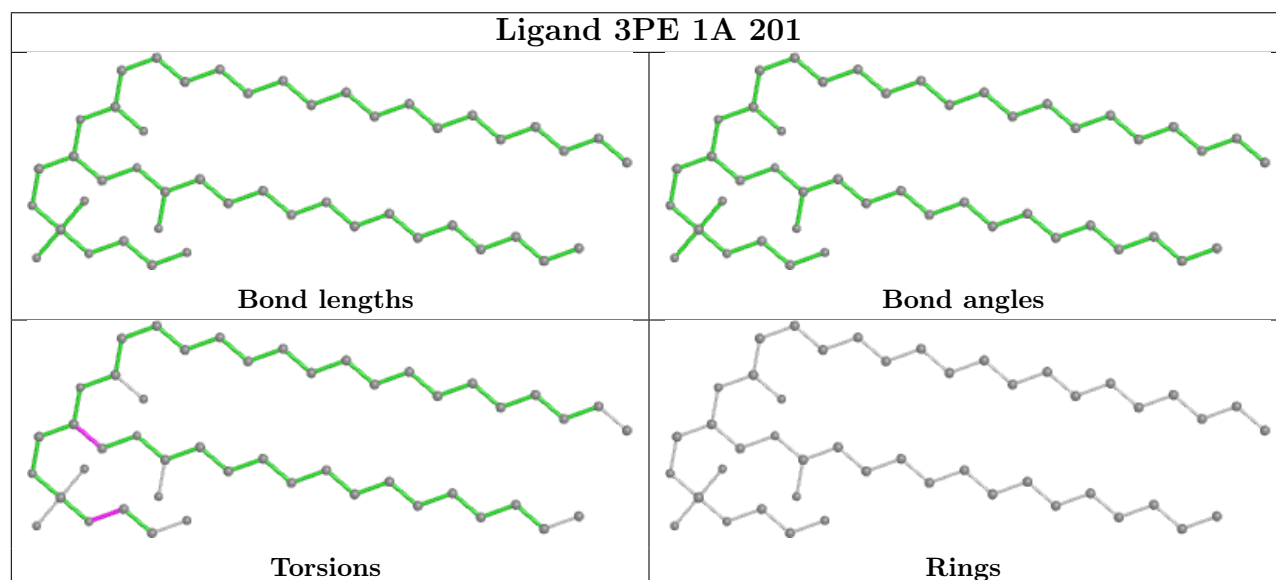
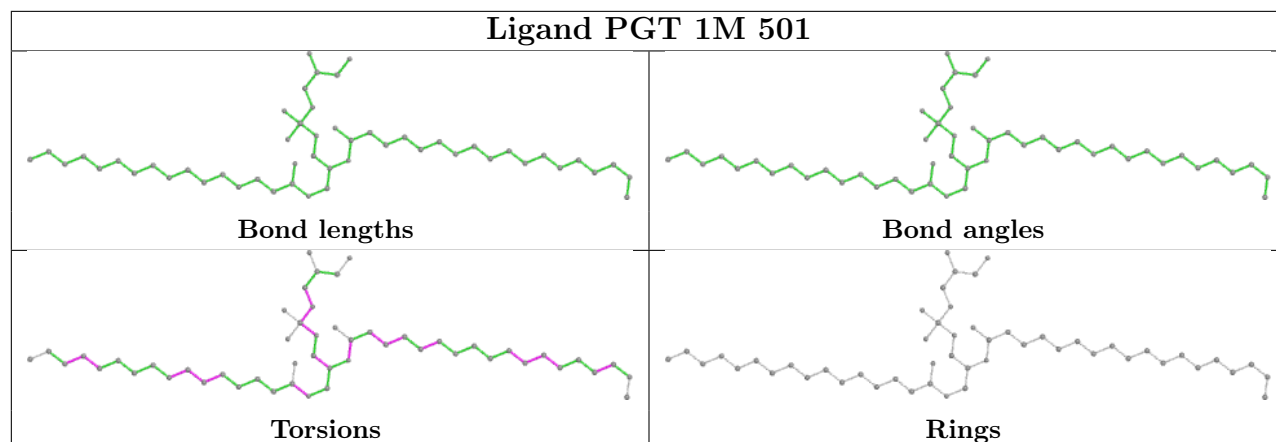


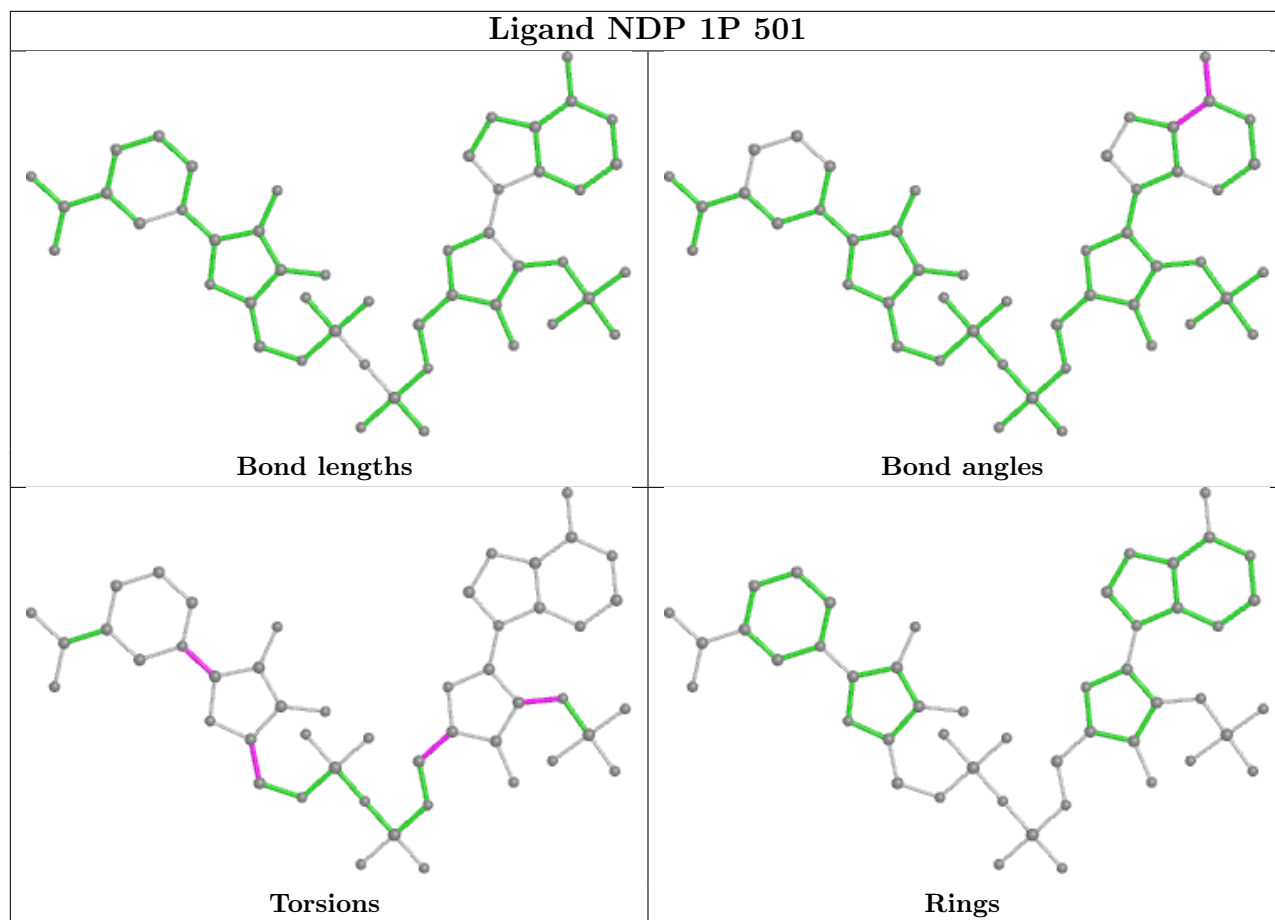












5.7 Other polymers [\(i\)](#)

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	3.75
1	1r	1:ALA	C	2:SER	N	3.09

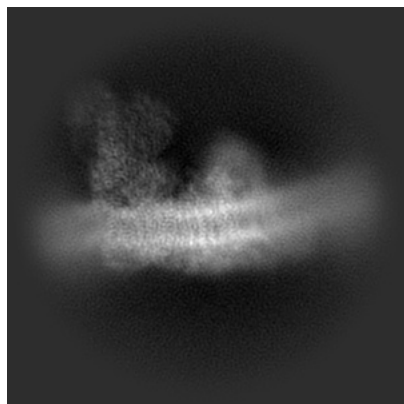
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42175. These allow visual inspection of the internal detail of the map and identification of artifacts.

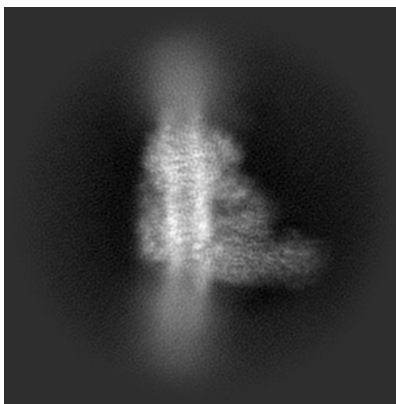
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

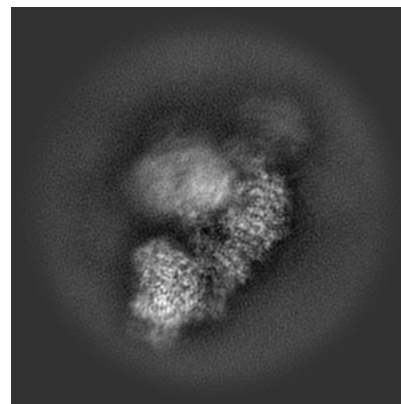
6.1.1 Primary map



X

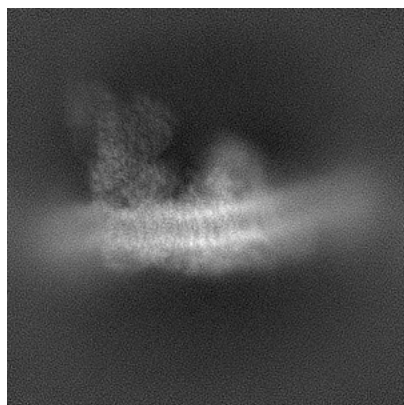


Y

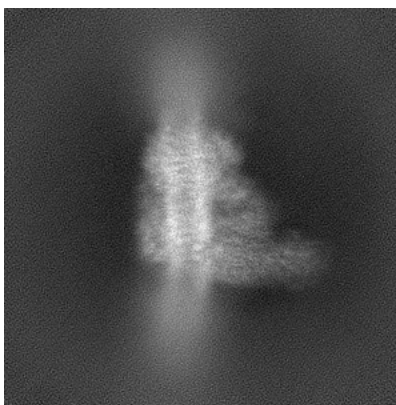


Z

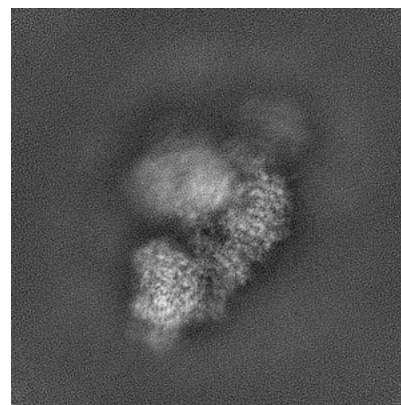
6.1.2 Raw map



X



Y

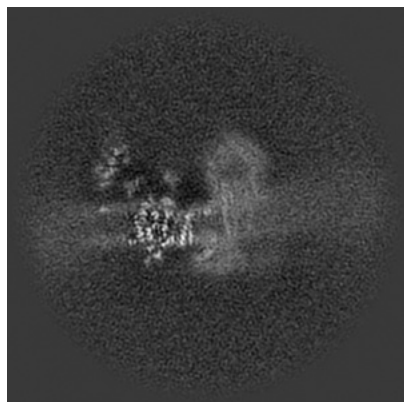


Z

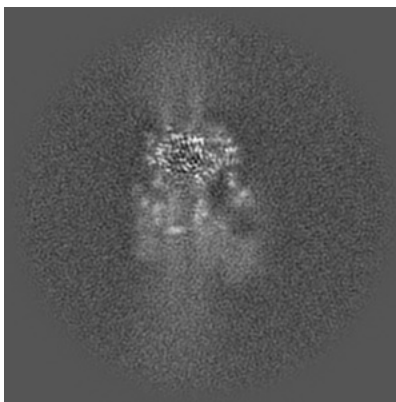
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

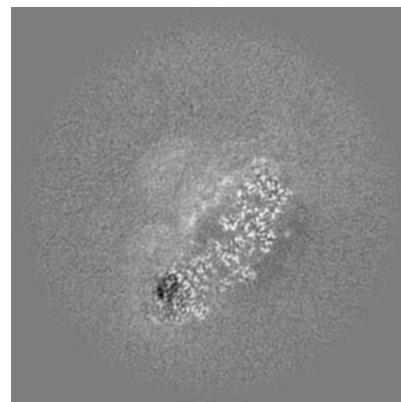
6.2.1 Primary map



X Index: 160



Y Index: 160

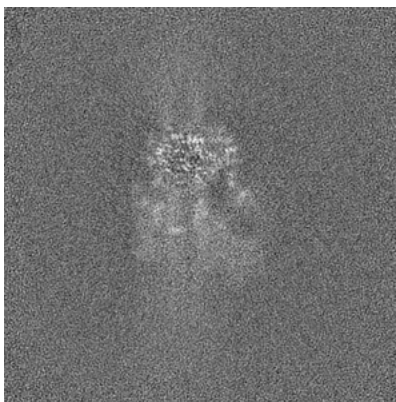


Z Index: 160

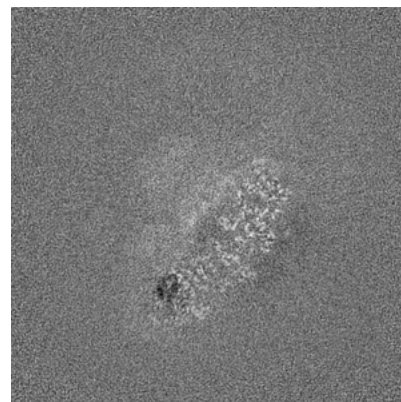
6.2.2 Raw map



X Index: 160



Y Index: 160

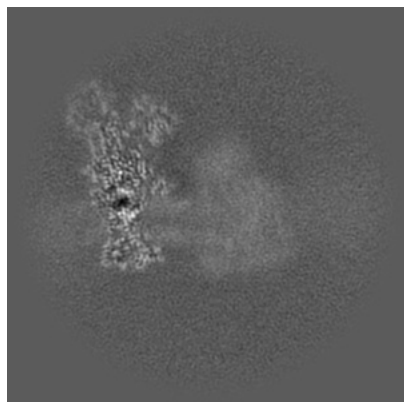


Z Index: 160

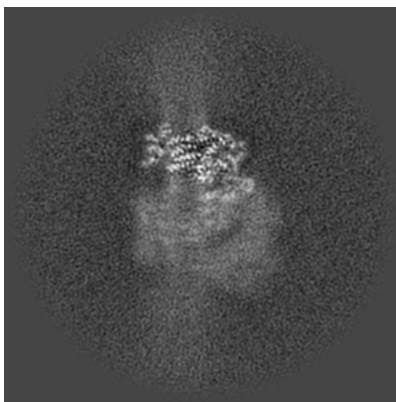
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

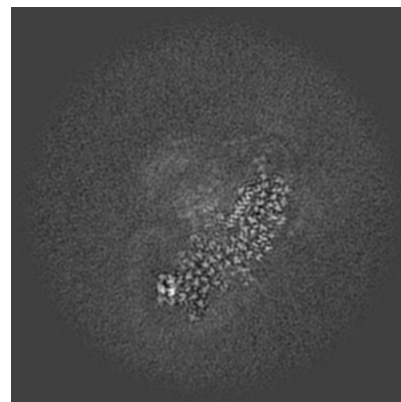
6.3.1 Primary map



X Index: 127

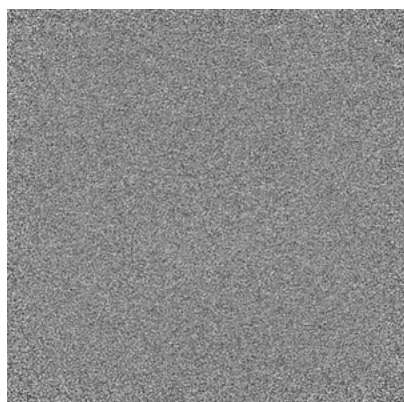


Y Index: 171

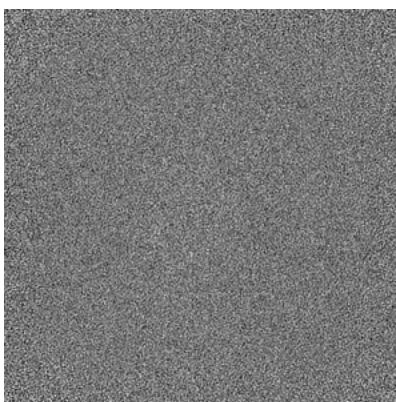


Z Index: 155

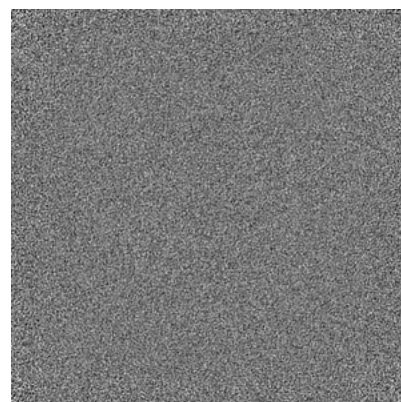
6.3.2 Raw map



X Index: 0



Y Index: 0

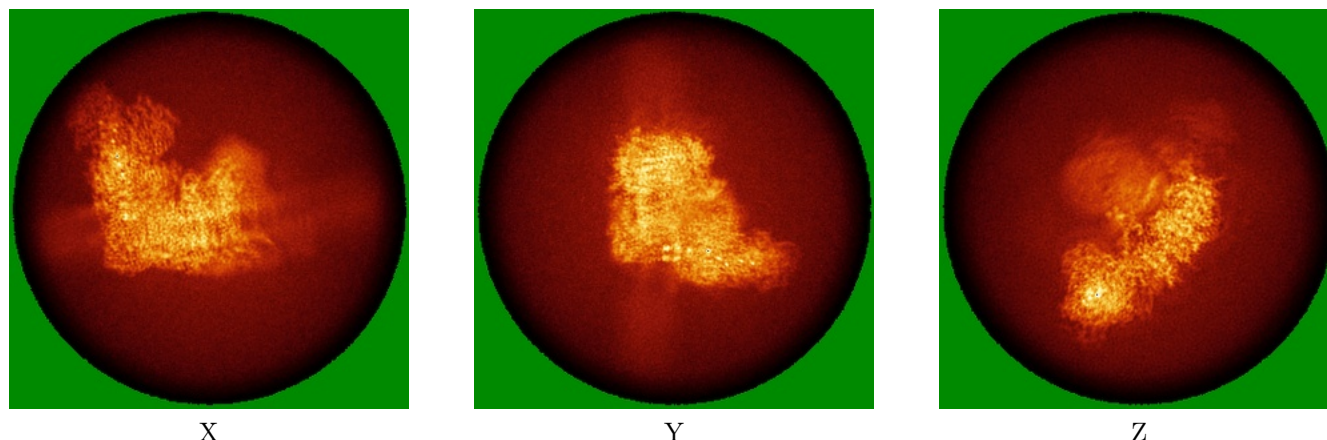


Z Index: 0

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

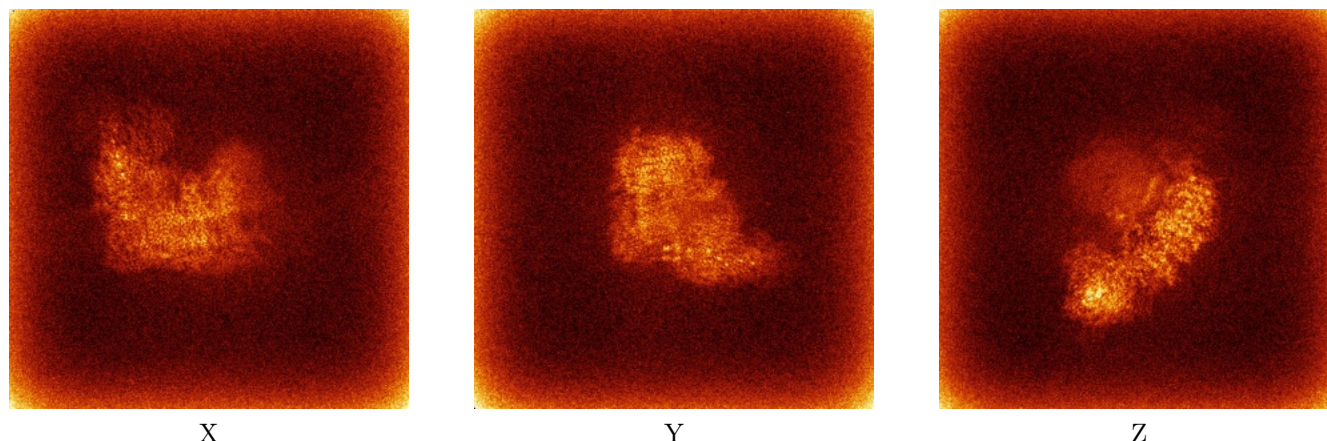


X

Y

Z

6.4.2 Raw map



X

Y

Z

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

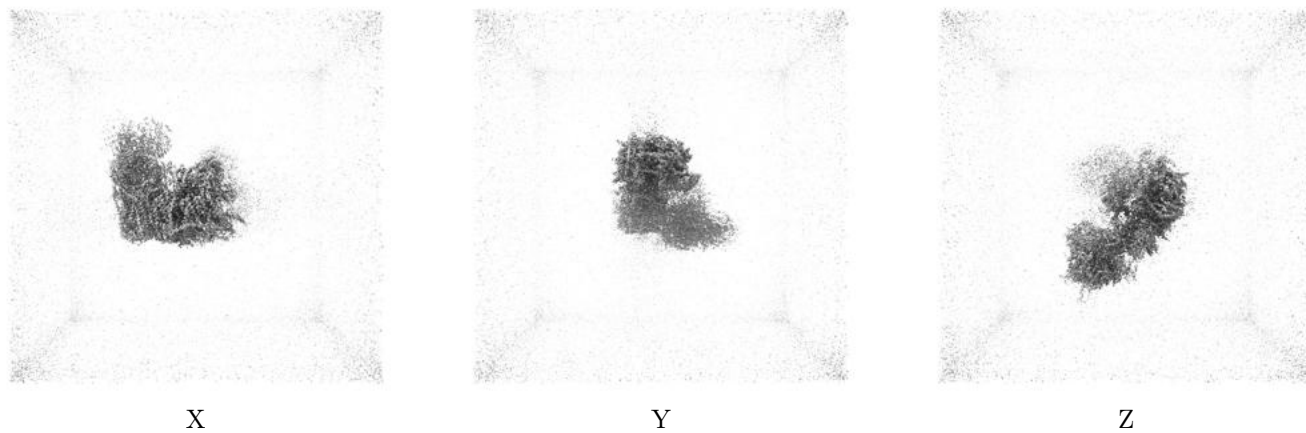
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

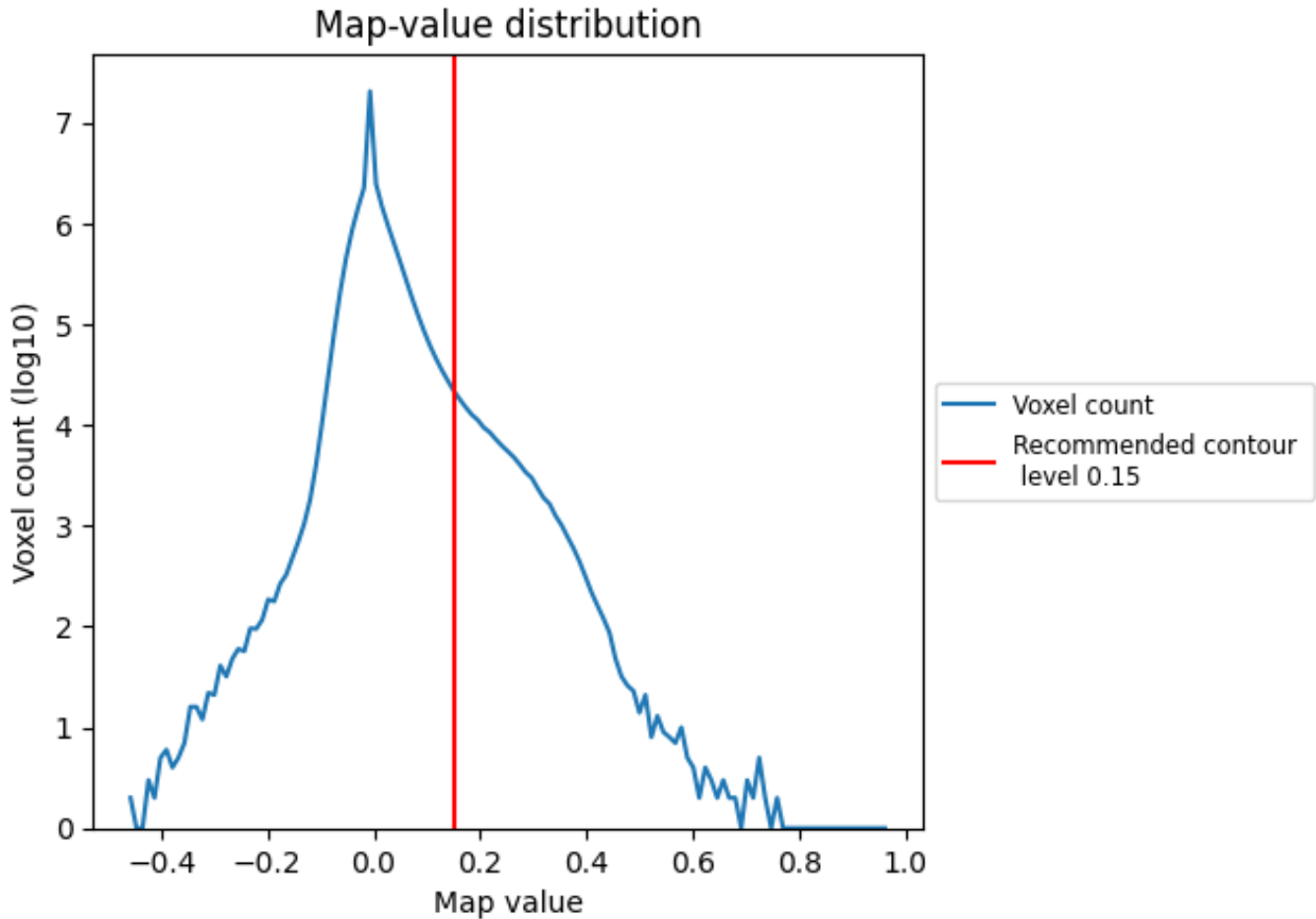
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

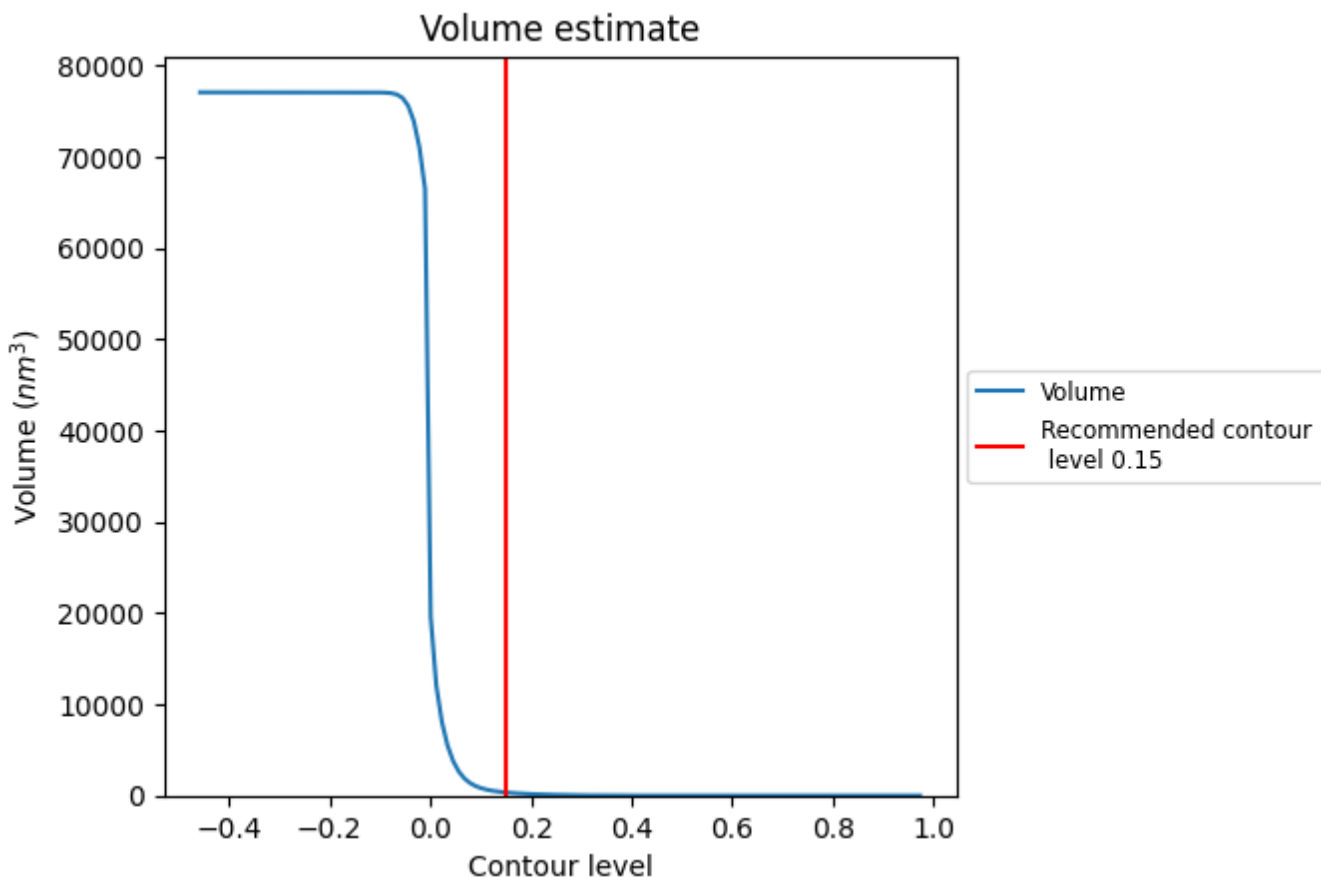
This section contains the results of statistical analysis of the map.

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.

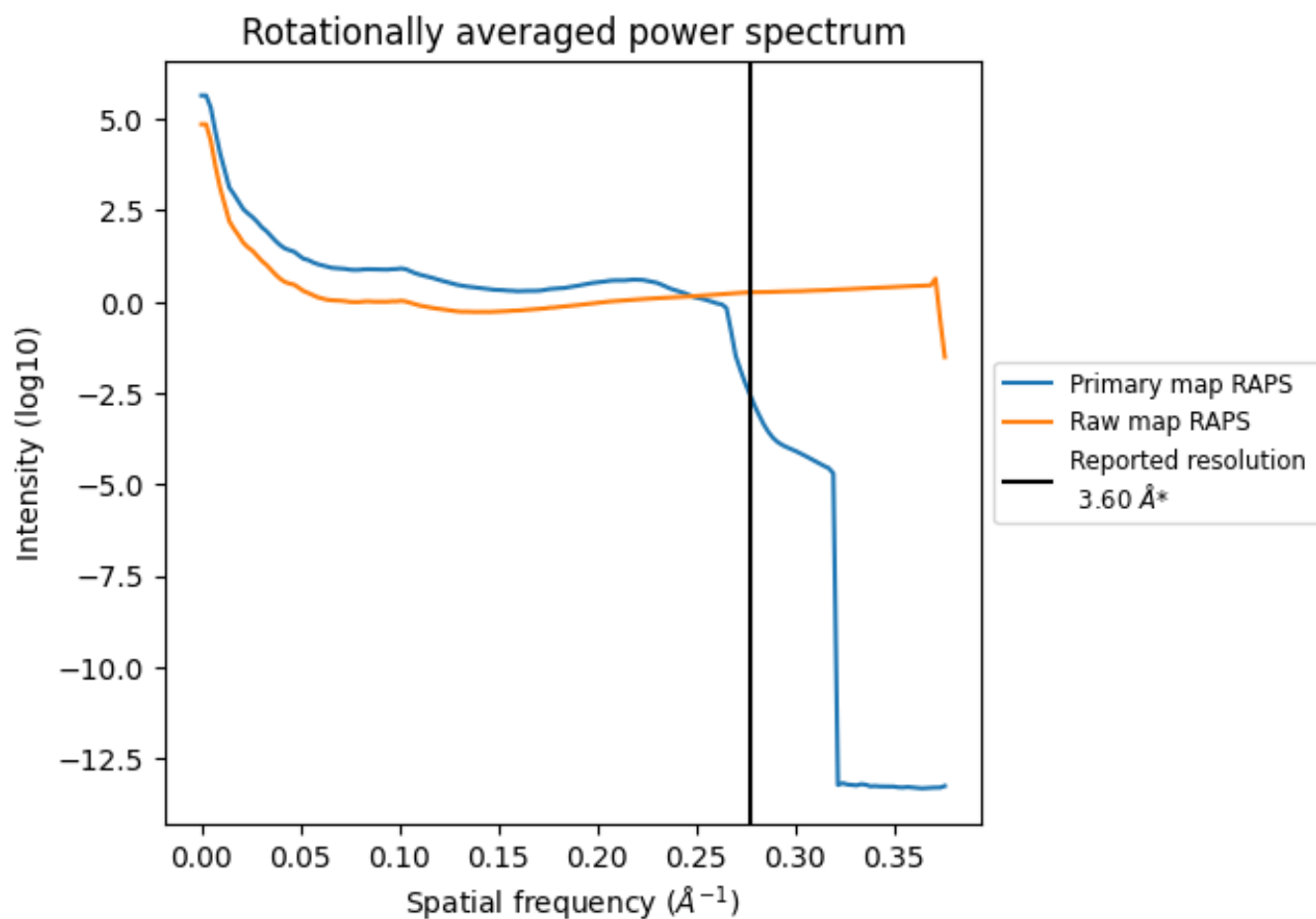
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 338 nm³; this corresponds to an approximate mass of 306 kDa.

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

7.3 Rotationally averaged power spectrum i

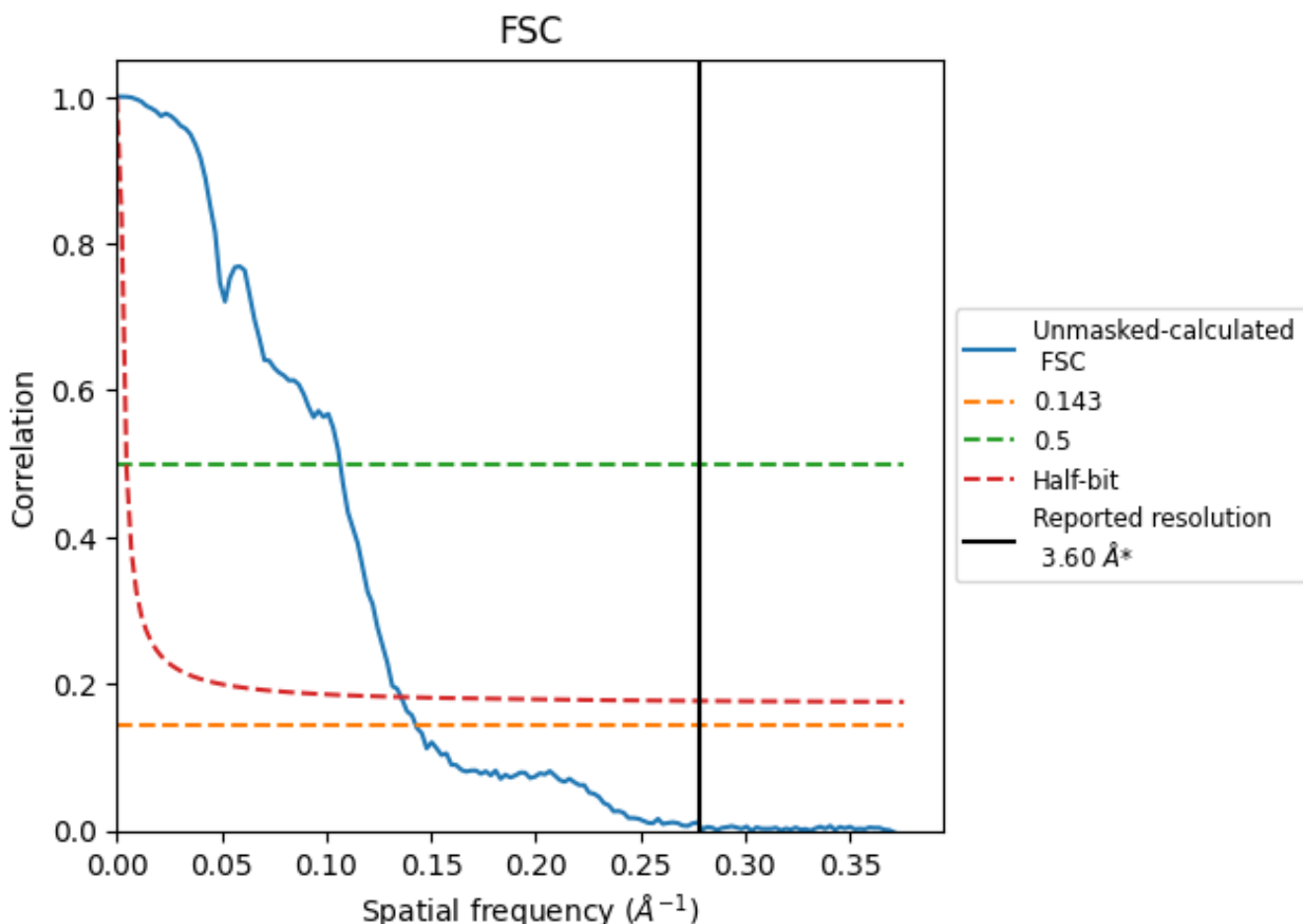


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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](#)

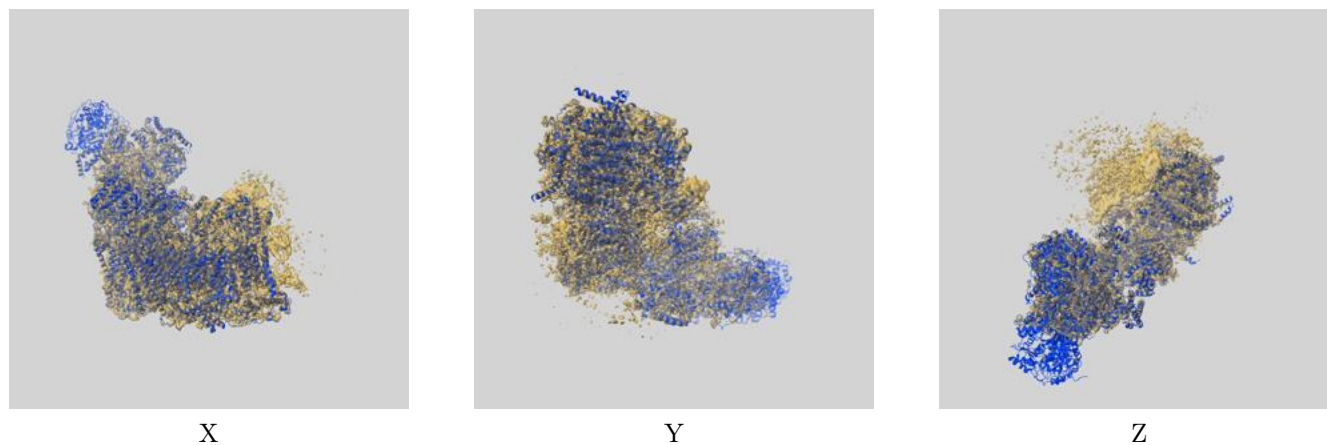
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.00	9.37	7.36

*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 7.00 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

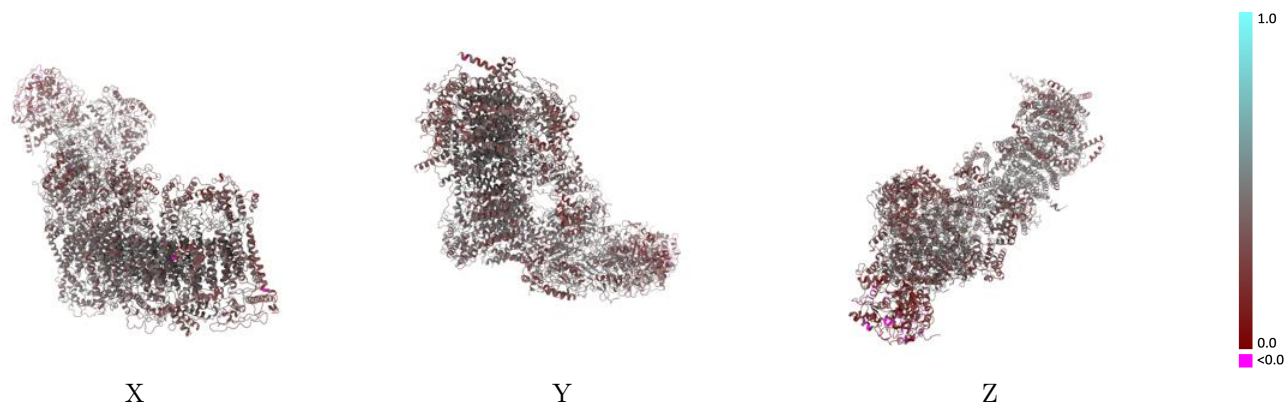
This section contains information regarding the fit between EMDB map EMD-42175 and PDB model 8UEY. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



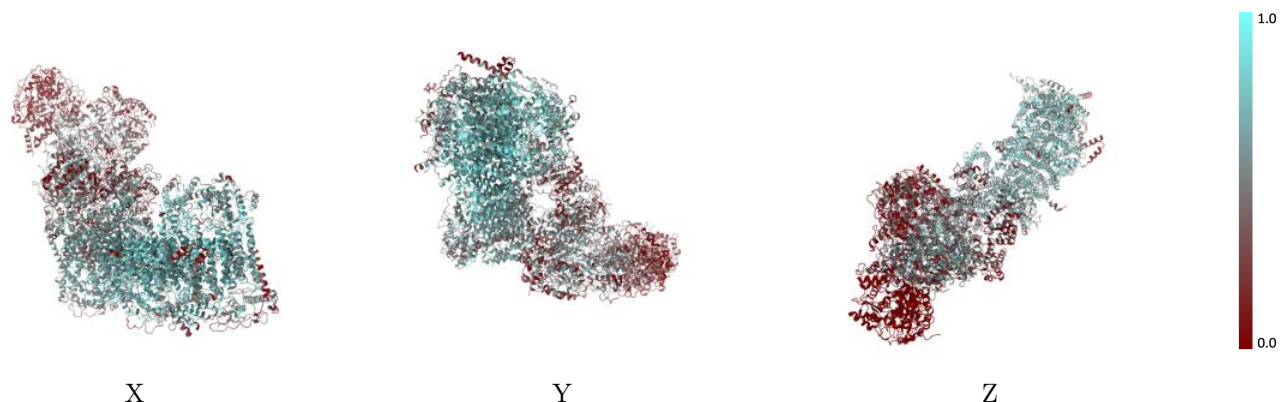
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



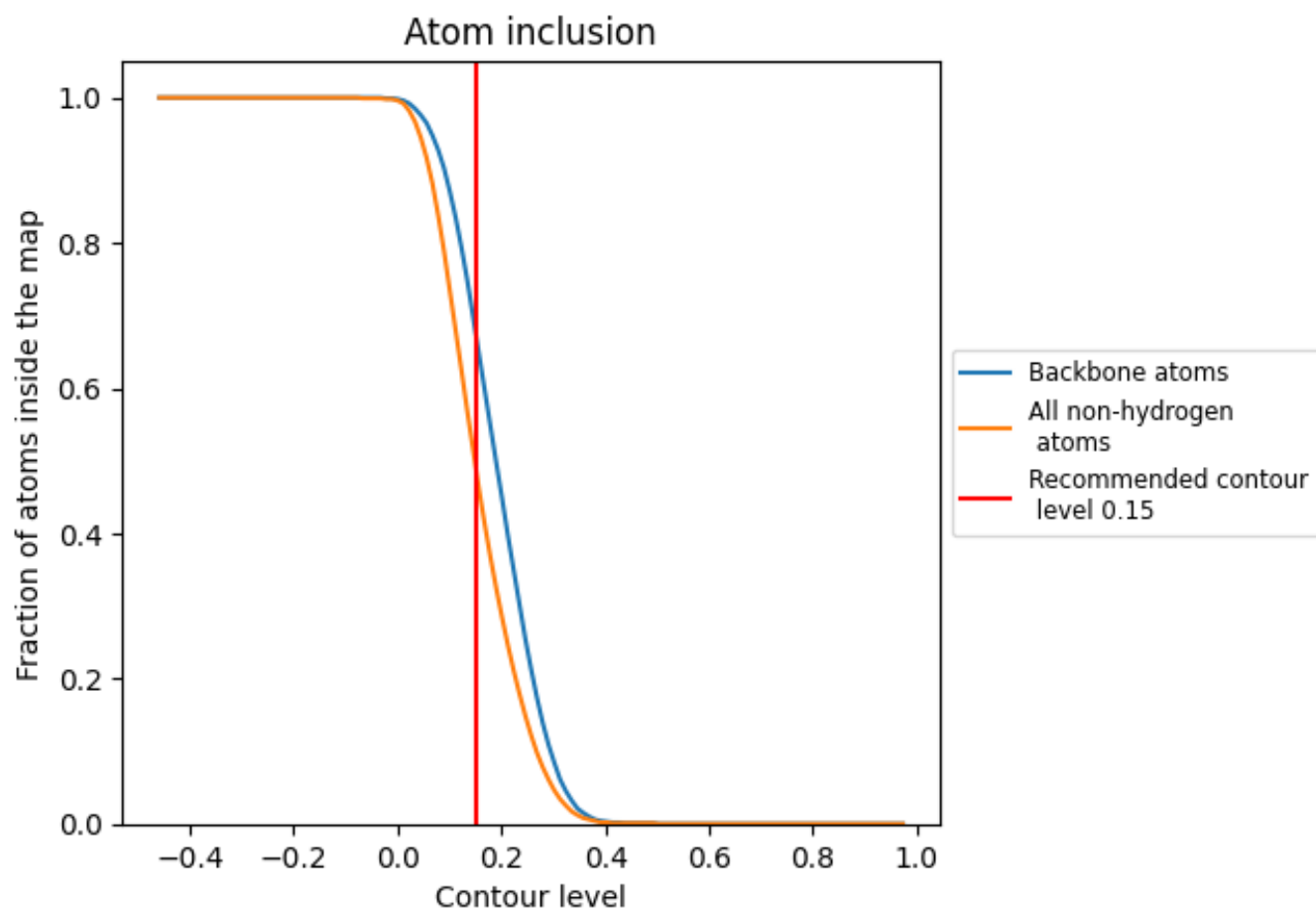
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 68% of all backbone atoms, 50% 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	0.4950	0.3830
1A	0.5300	0.4180
1B	0.5860	0.4290
1C	0.4340	0.4060
1D	0.5590	0.4080
1E	0.0450	0.2950
1F	0.0480	0.2570
1G	0.3120	0.3680
1H	0.5930	0.4130
1I	0.5670	0.4210
1J	0.5290	0.3800
1K	0.6290	0.4090
1L	0.7110	0.4100
1M	0.7630	0.4420
1N	0.6850	0.4310
1O	0.4050	0.3700
1P	0.3270	0.3470
1Q	0.3250	0.3840
1R	0.3320	0.4040
1S	0.1620	0.3070
1T	0.2640	0.2940
1U	0.6120	0.3580
1V	0.2440	0.3400
1W	0.3370	0.3580
1X	0.5630	0.4110
1Y	0.6790	0.3880
1Z	0.5820	0.4200
1a	0.6840	0.4140
1b	0.5690	0.4180
1c	0.4460	0.3740
1d	0.6800	0.4180
1e	0.6120	0.4290
1f	0.4740	0.3860
1g	0.5960	0.4040
1h	0.6890	0.4230



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
1i	 0.4070	 0.3590
1j	 0.5220	 0.3630
1k	 0.5200	 0.3610
1l	 0.6540	 0.3940
1m	 0.6900	 0.3870
1n	 0.6560	 0.3760
1o	 0.5350	 0.3320
1p	 0.6210	 0.3920
1q	 0.4310	 0.4050
1r	 0.4140	 0.3990
1s	 0.0000	 0.2350