



# Full wwPDB EM Validation Report ⓘ

Jul 6, 2024 – 04:01 PM EDT

PDB ID : 8UEZ  
EMDB ID : EMD-42176  
Title : In-situ complex I, Active-Q10 (State-delta)  
Authors : Zheng, W.; Zhu, J.; Zhang, K.  
Deposited on : 2023-10-02  
Resolution : 3.50 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](mailto: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>.

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

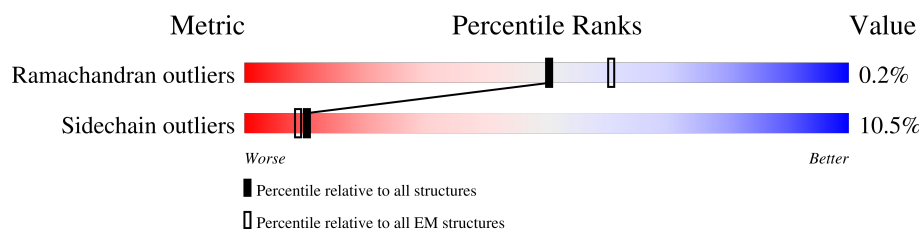
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

# 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 3.50 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  $\geq 3$ , 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	<div> <div>28%</div> <div>90%</div> <div>10%</div> </div>
2	1B	258	<div> <div>56%</div> <div>40%</div> </div>
3	1C	264	<div> <div>74%</div> <div>5%</div> <div>21%</div> </div>
4	1D	476	<div> <div>10%</div> <div>83%</div> <div>7%</div> <div>10%</div> </div>
5	1E	249	<div> <div>81%</div> <div>5%</div> <div>14%</div> </div>
6	1F	464	<div> <div>88%</div> <div>5%</div> <div>7%</div> </div>
7	1G	727	<div> <div>88%</div> <div>8%</div> </div>
8	1H	318	<div> <div>9%</div> <div>91%</div> <div>9%</div> </div>
9	1I	239	<div> <div>68%</div> <div>6%</div> <div>26%</div> </div>

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Mol	Chain	Length	Quality of chain
10	1J	175	
11	1K	98	
12	1L	606	
13	1M	459	
14	1N	347	
15	1O	357	
16	1P	377	
17	1Q	175	
18	1R	123	
19	1S	99	
20	1T	156	
20	1U	156	
21	1V	116	
22	1W	128	
23	1X	172	
24	1Y	141	
25	1Z	144	
26	1a	70	
27	1b	84	
28	1c	76	
29	1d	123	
30	1e	106	
31	1f	135	
32	1g	154	
33	1h	189	

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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 67334 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	115	Total	C	N	O	S	0	0
			916	616	134	159	7		

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

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

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

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

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
4	1D	429	Total	C	N	O	S	0	0
			3452	2207	593	628	24		

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
5	1E	214	Total	C	N	O	S	0	0
			1658	1058	278	312	10		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
24	1Y	139	Total	C	N	O	S	0	0
			1016	648	173	189	6		

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

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

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

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

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

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

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

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

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

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

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
30	1e	99	Total	C	N	O	S	0	0
			816	519	151	140	6		

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

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

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
32	1g	100	Total	C	N	O	S	0	0
			835	535	138	158	4		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1l	156	Total	C	N	O	S	0	0
			1310	847	213	242	8		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	1m	128	Total	C	N	O	0	0
			1062	691	182	189		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1n	172	Total	C	N	O	S	0	0
			1495	956	273	258	8		

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

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

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

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

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

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

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

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

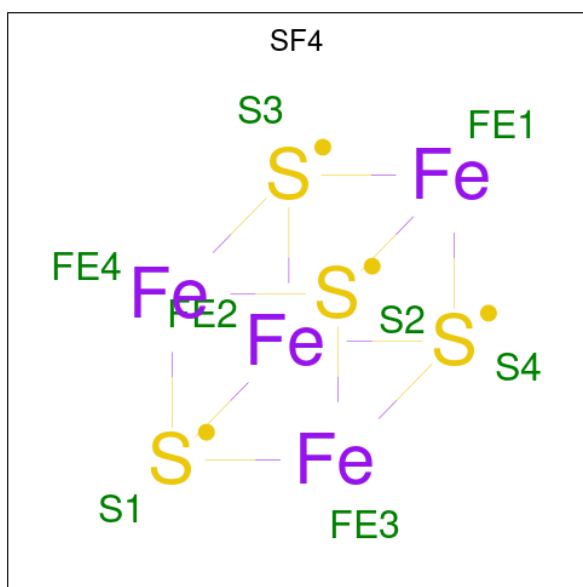
There is a discrepancy between the modelled and reference sequences:

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

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

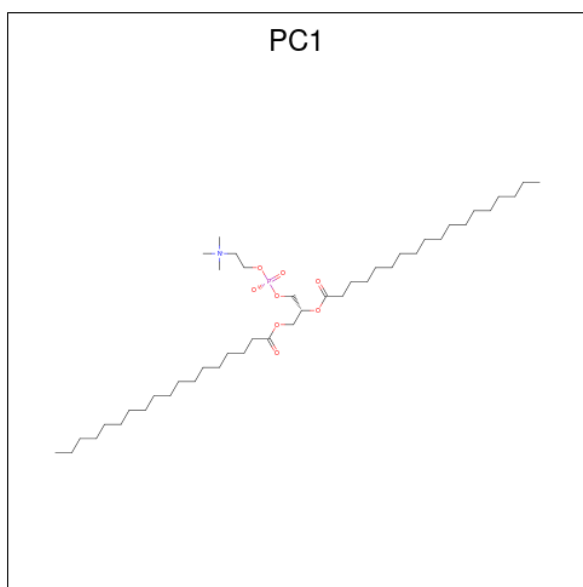
Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



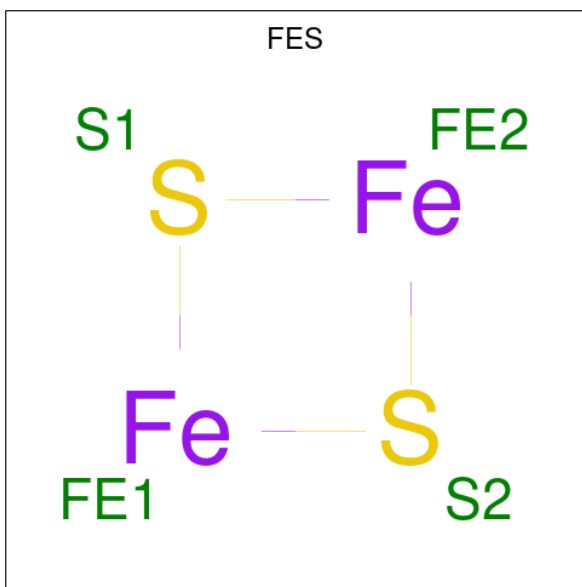
Mol	Chain	Residues	Atoms			AltConf
45	1B	1	Total	Fe	S	0
			8	4	4	
45	1F	1	Total	Fe	S	0
			8	4	4	
45	1G	1	Total	Fe	S	0
			8	4	4	
45	1G	1	Total	Fe	S	0
			8	4	4	
45	1I	1	Total	Fe	S	0
			8	4	4	
45	1I	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C<sub>44</sub>H<sub>88</sub>NO<sub>8</sub>P).



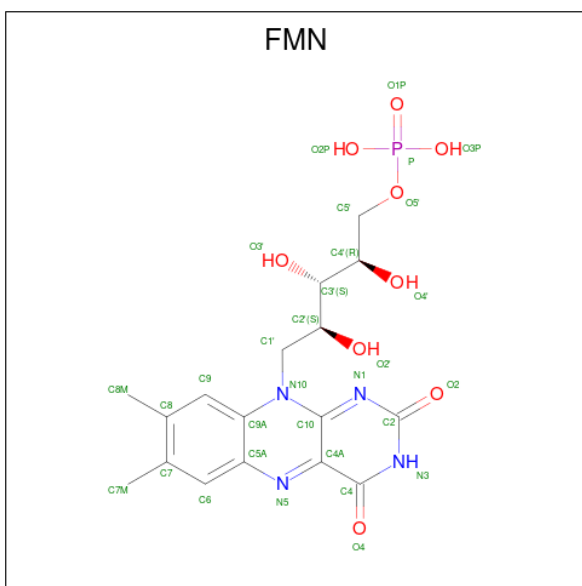
Mol	Chain	Residues	Atoms					AltConf
46	1B	1	Total	C	N	O	P	0
			34	24	1	8	1	
46	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	1M	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	1d	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	1f	1	Total	C	N	O	P	0
			25	15	1	8	1	
46	1q	1	Total	C	N	O	P	0
			48	38	1	8	1	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



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

- Molecule 48 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).

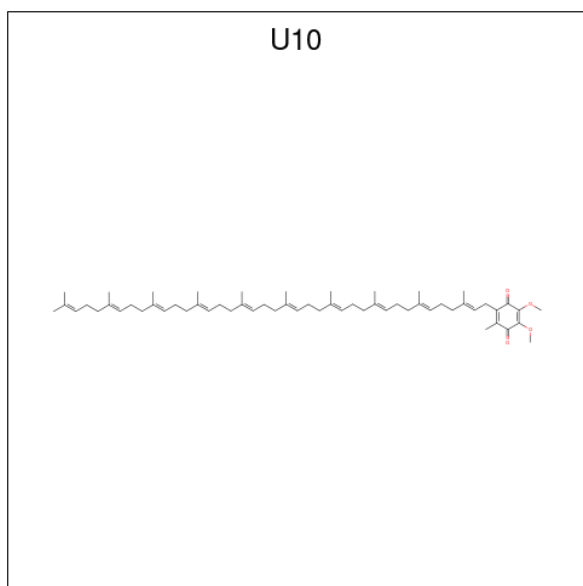


Mol	Chain	Residues	Atoms					AltConf
48	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

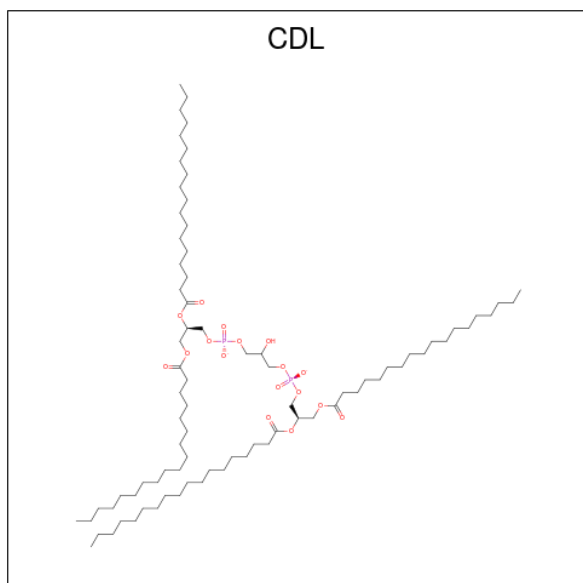
Mol	Chain	Residues	Atoms		AltConf
49	1G	1	Total	K	0
			1	1	

- Molecule 50 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
50	1H	1	Total	C	O	0
			63	59	4	

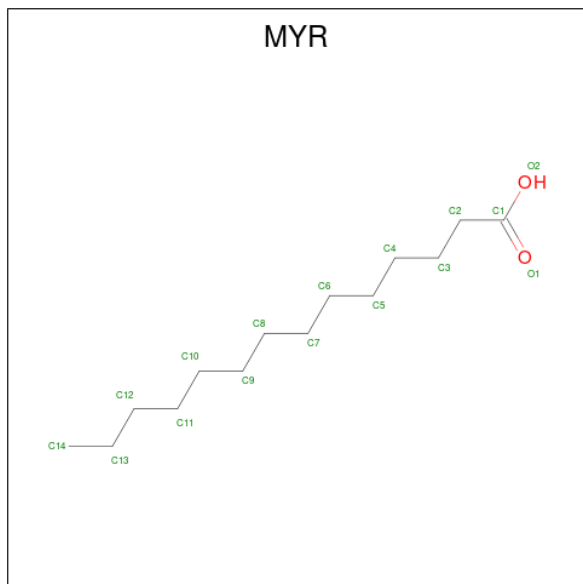
- Molecule 51 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).





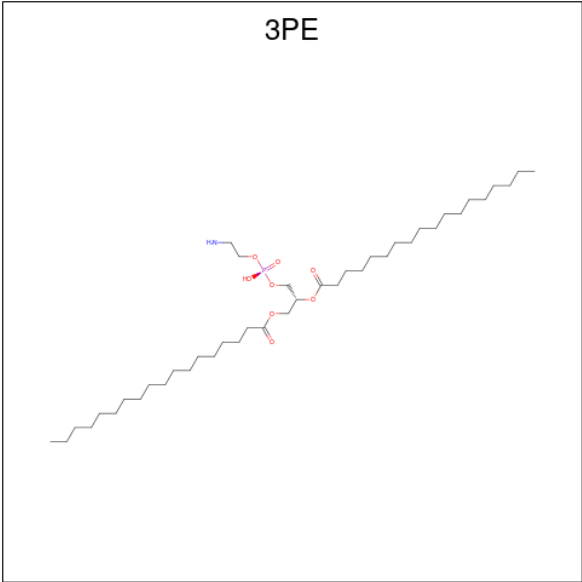
Mol	Chain	Residues	Atoms				AltConf
51	1H	1	Total	C	O	P	0
			51	32	17	2	
51	1O	1	Total	C	O	P	0
			67	48	17	2	
51	1a	1	Total	C	O	P	0
			61	42	17	2	

- Molecule 52 is MYRISTIC ACID (three-letter code: MYR) (formula:  $C_{14}H_{28}O_2$ ).



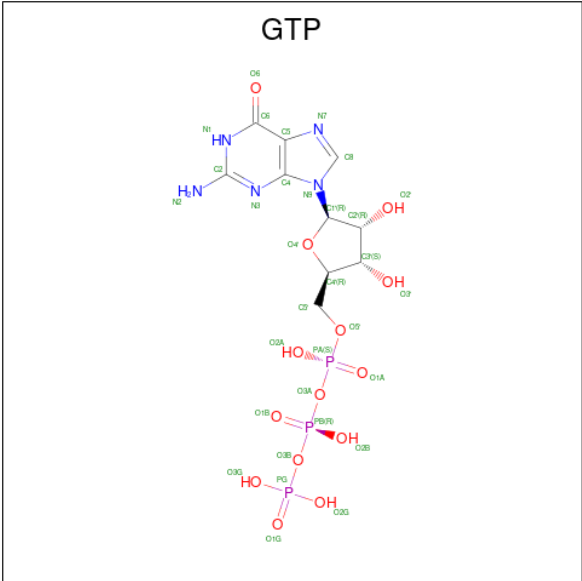
Mol	Chain	Residues	Atoms				AltConf
52	1L	1	Total	C	O		0
			15	14	1		

- Molecule 53 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
53	1M	1	Total	C	N	O	P	0
			38	28	1	8	1	
53	1Y	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).

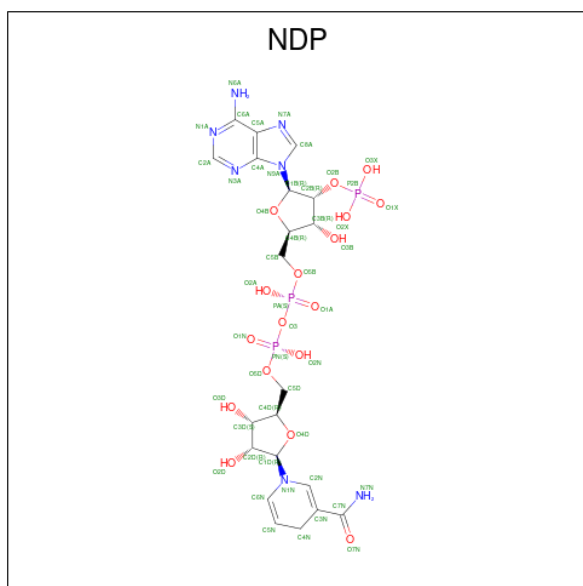


Mol	Chain	Residues	Atoms					AltConf
54	1O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	1O	1	Total	Mg	0
			1	1	

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).

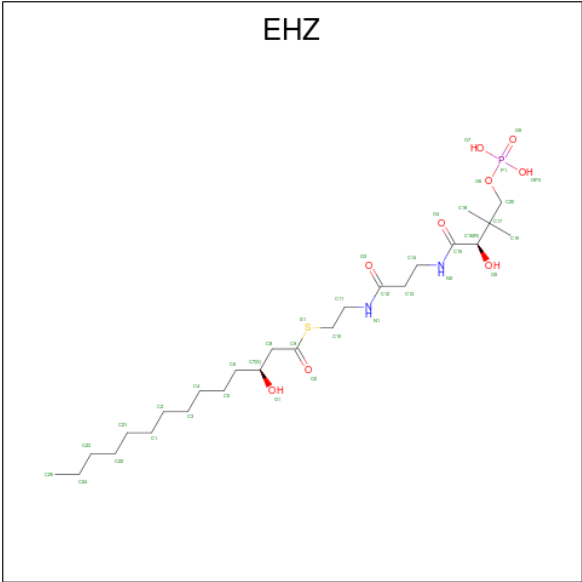


Mol	Chain	Residues	Atoms					AltConf
56	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	1R	1	Total	Zn	0
			1	1	

- Molecule 58 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>9</sub>PS).

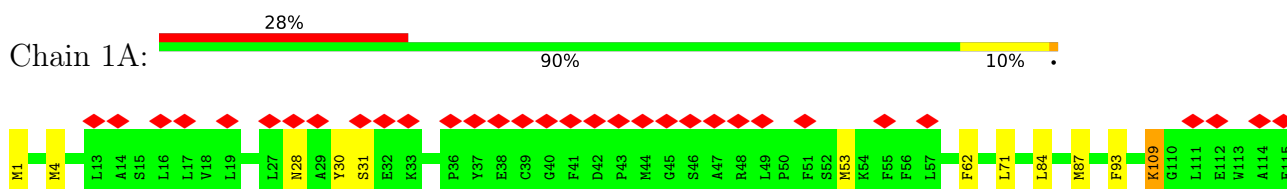


Mol	Chain	Residues	Atoms						AltConf
58	1W	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
58	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

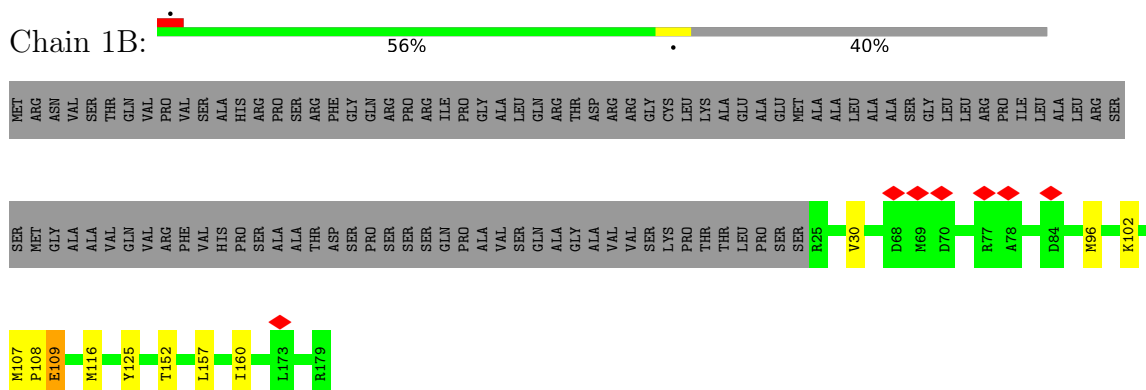
### 3 Residue-property plots

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

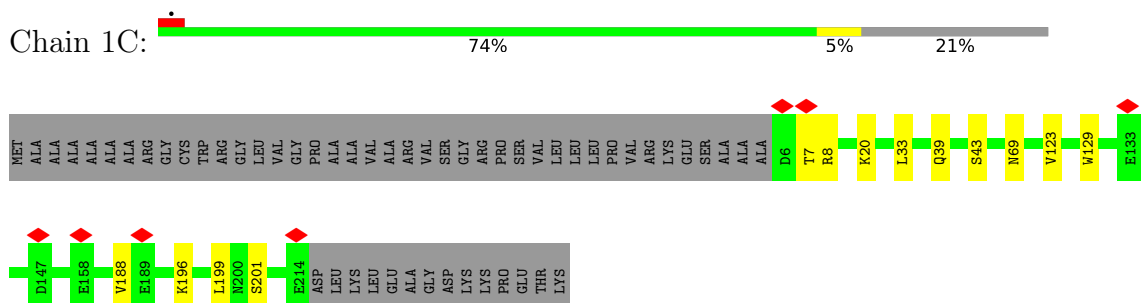
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



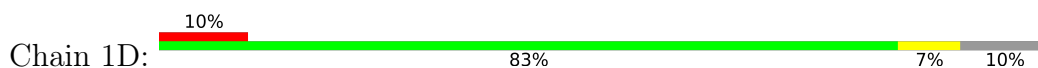
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

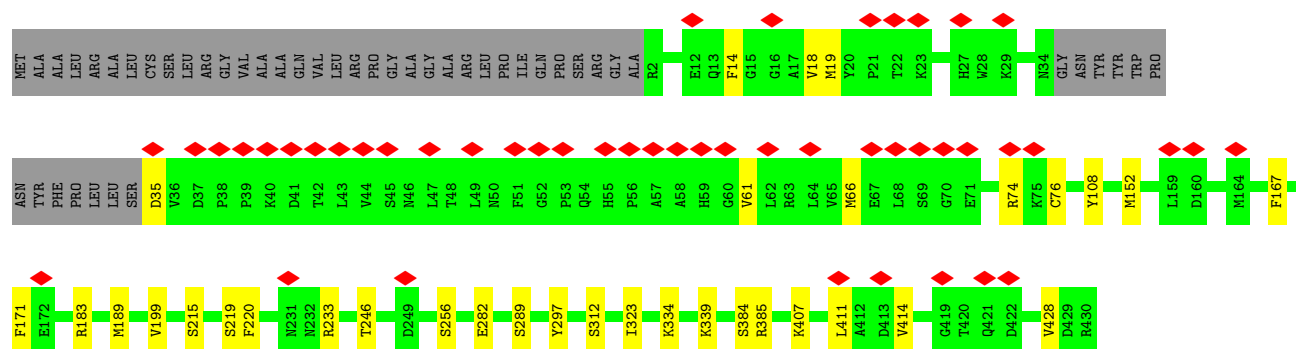


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



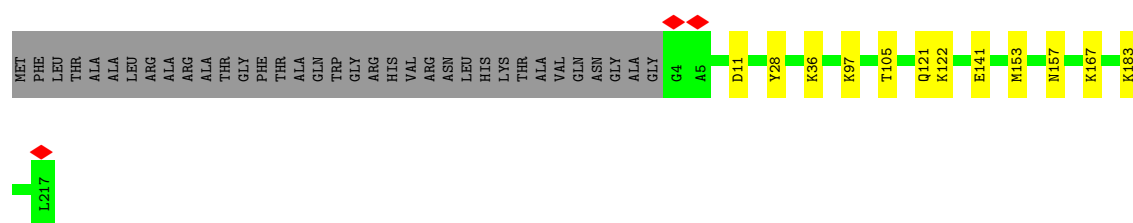
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial





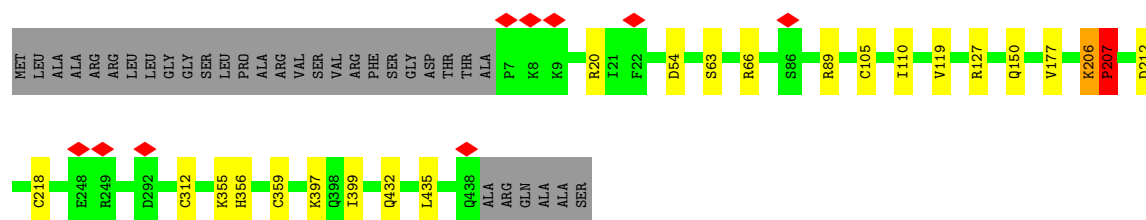
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain 1E:



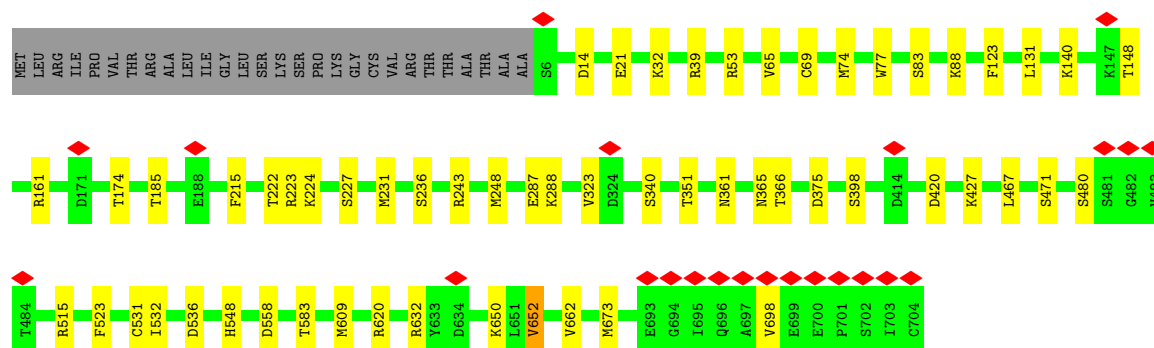
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1F:

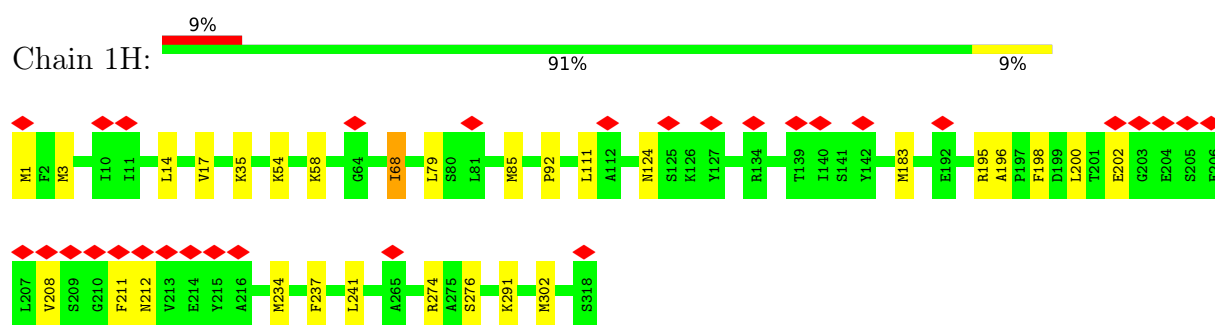


- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

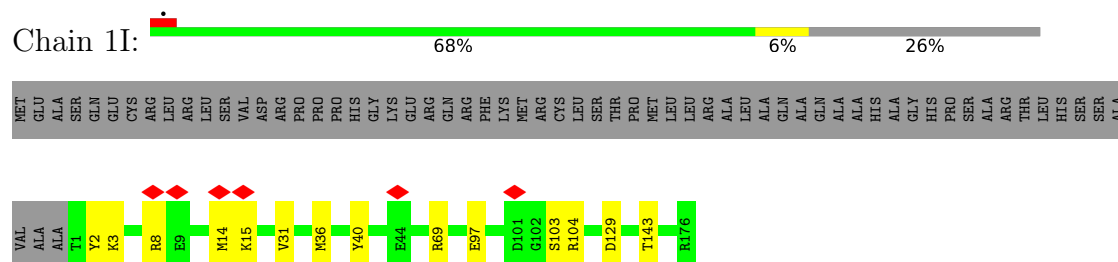
Chain 1G:



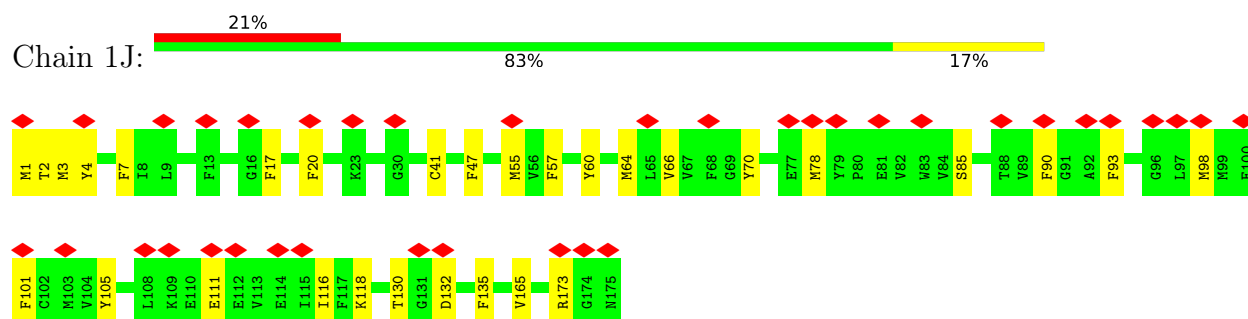
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



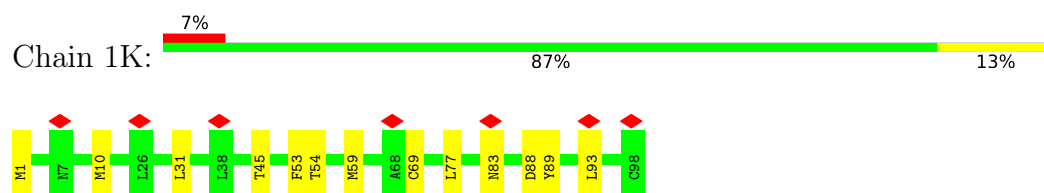
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



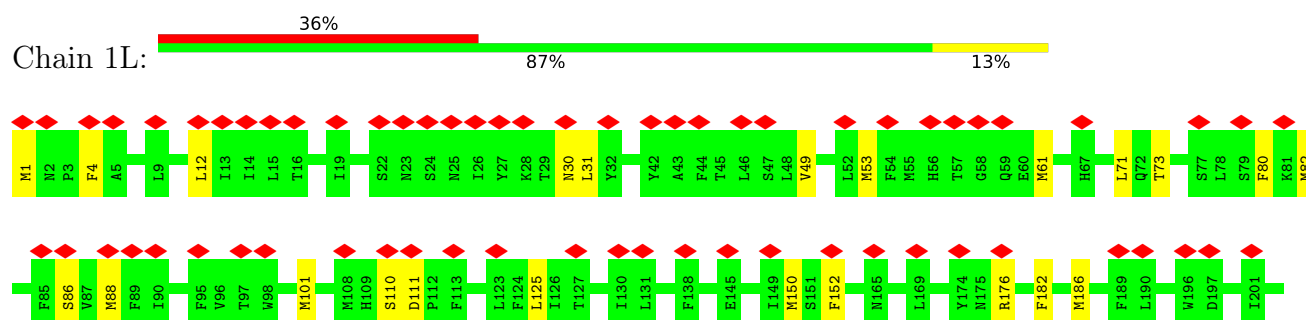
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

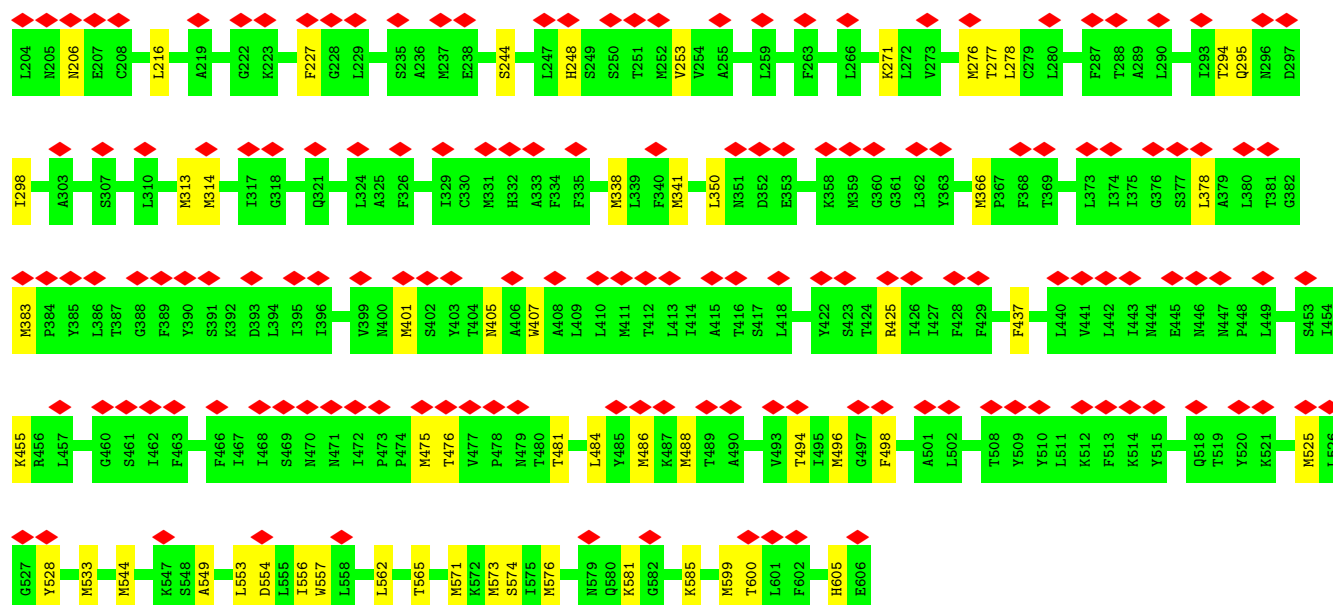


- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

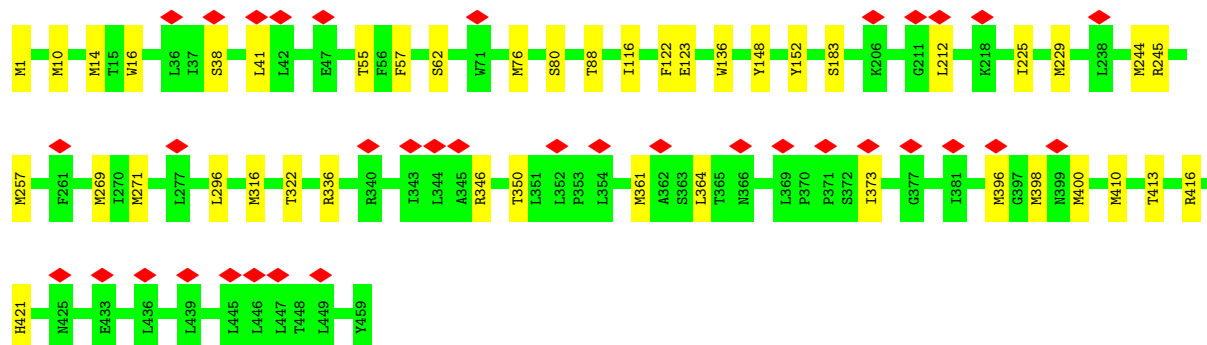


- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

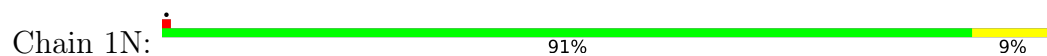




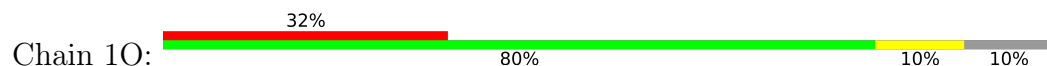
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



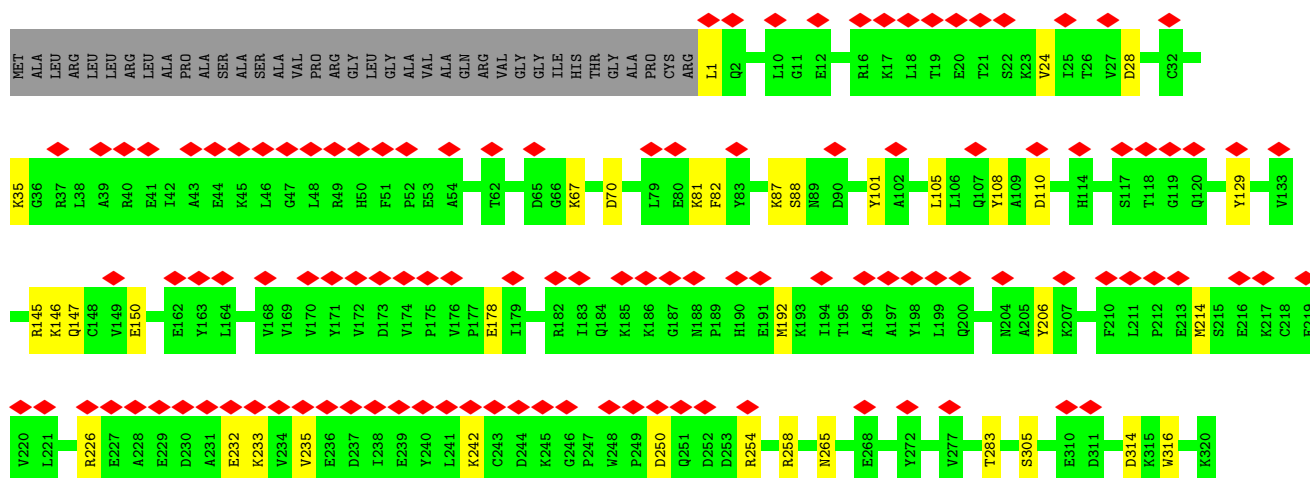
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2



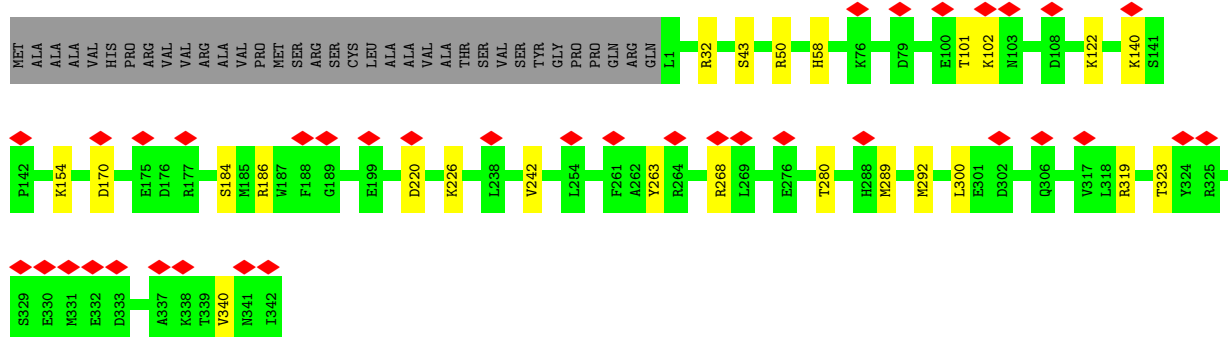
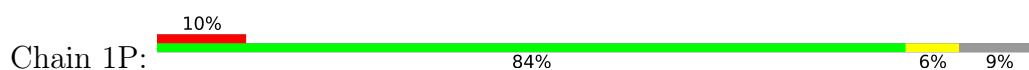
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



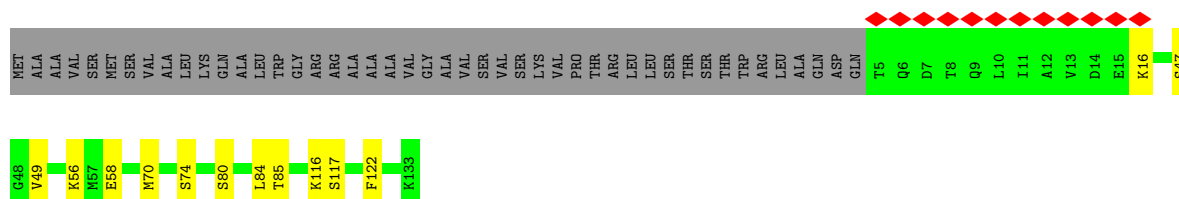




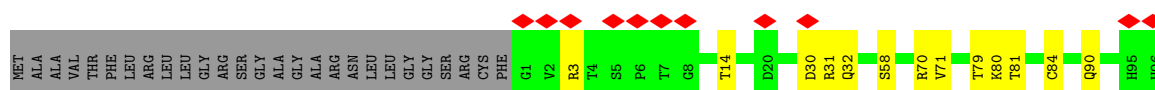
- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9



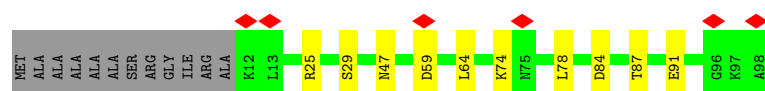
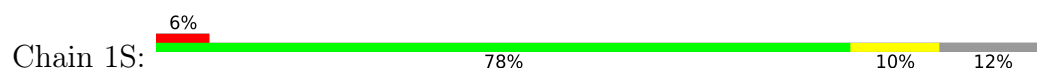
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



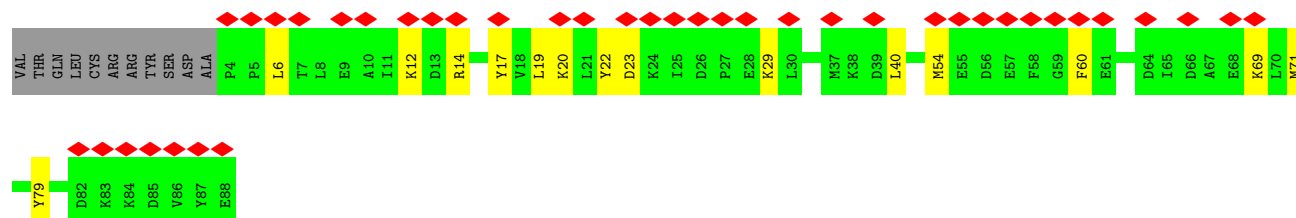
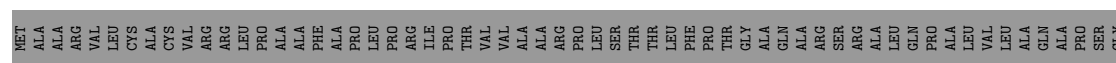
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



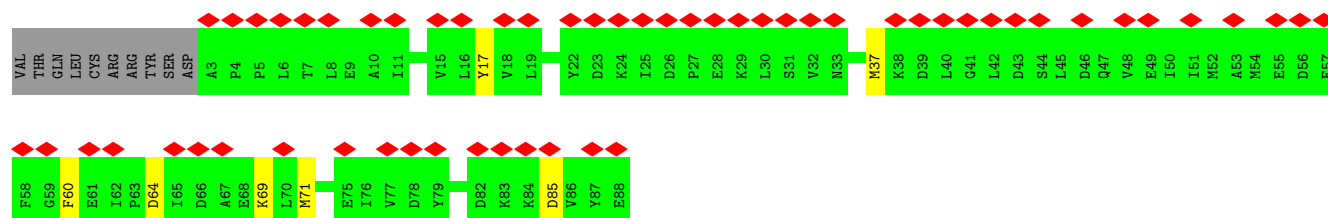
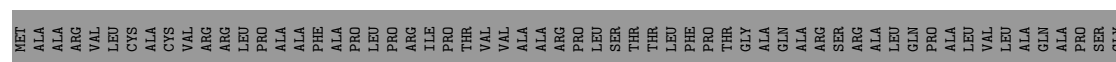
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



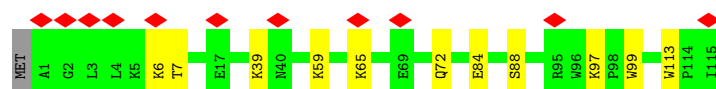
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



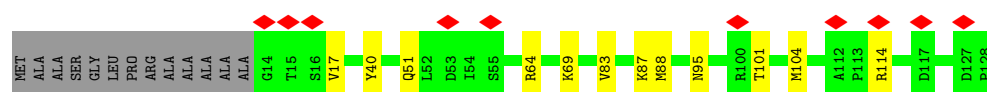
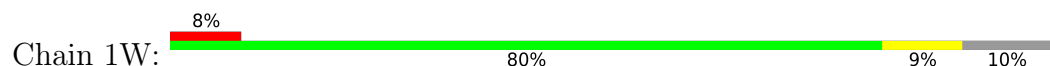
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



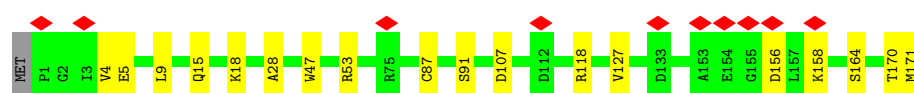
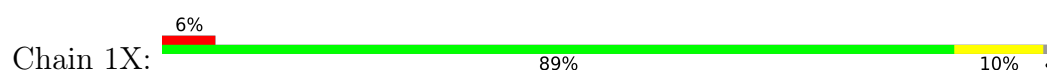
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



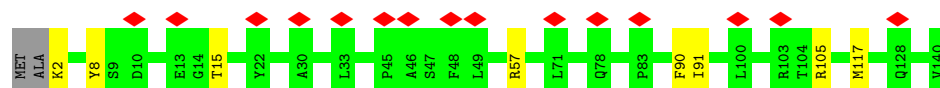
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



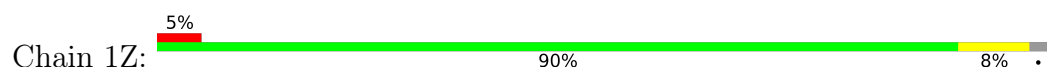
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



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



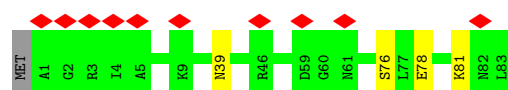
- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



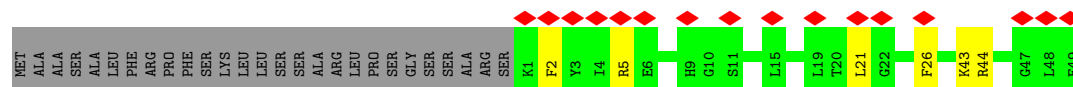
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



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

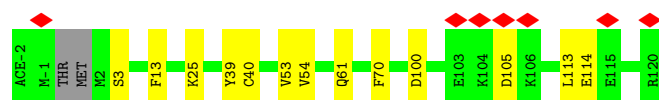


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

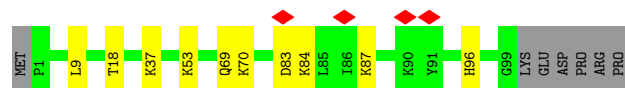
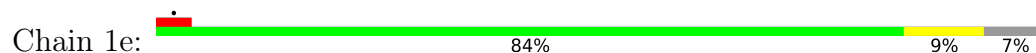


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

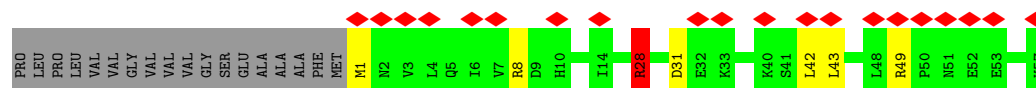
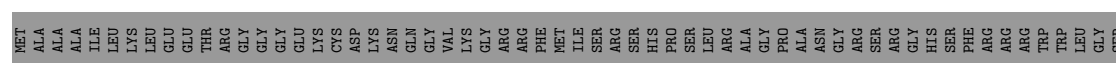




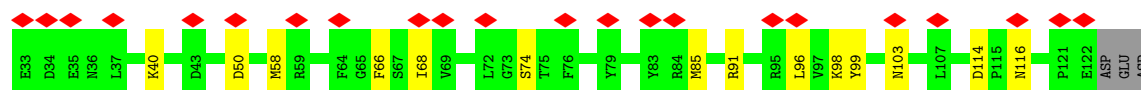
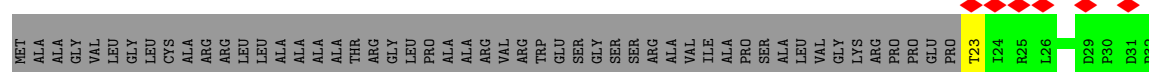
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



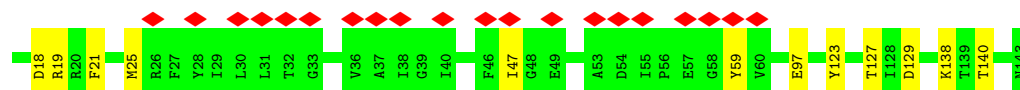
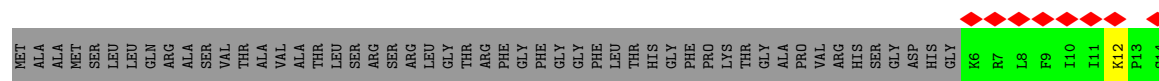
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]



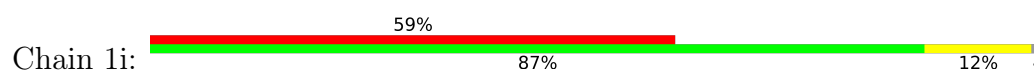
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

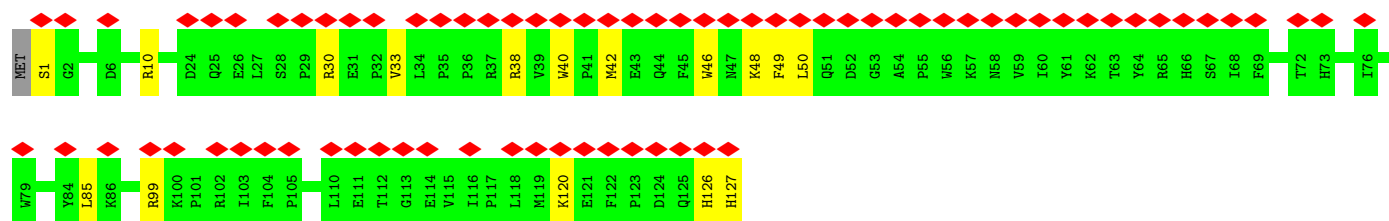


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

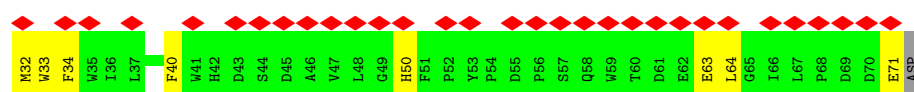
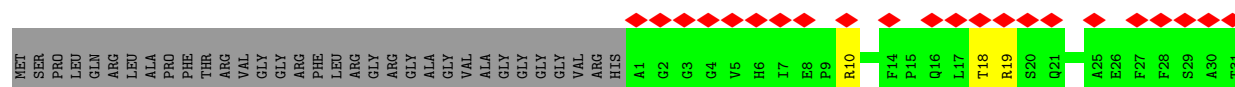


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

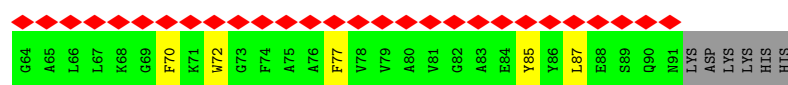
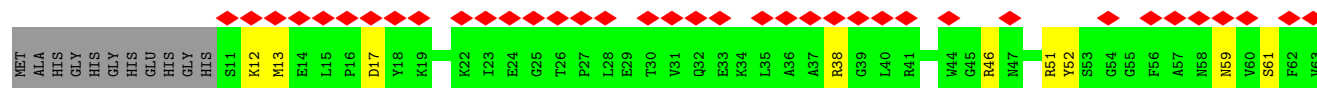




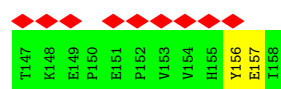
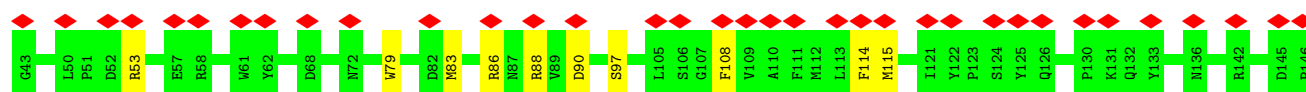
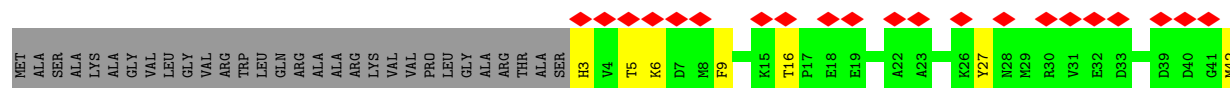
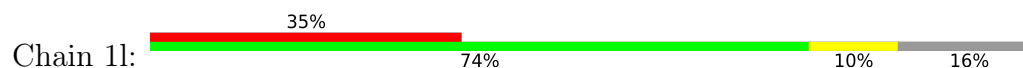
• Molecule 35: NADH:ubiquinone oxidoreductase subunit B2



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

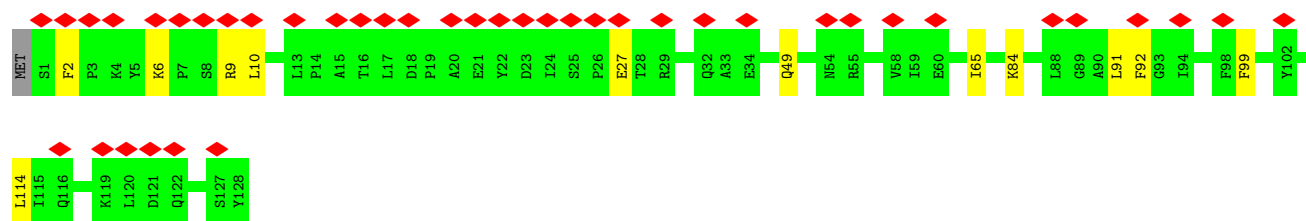


• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

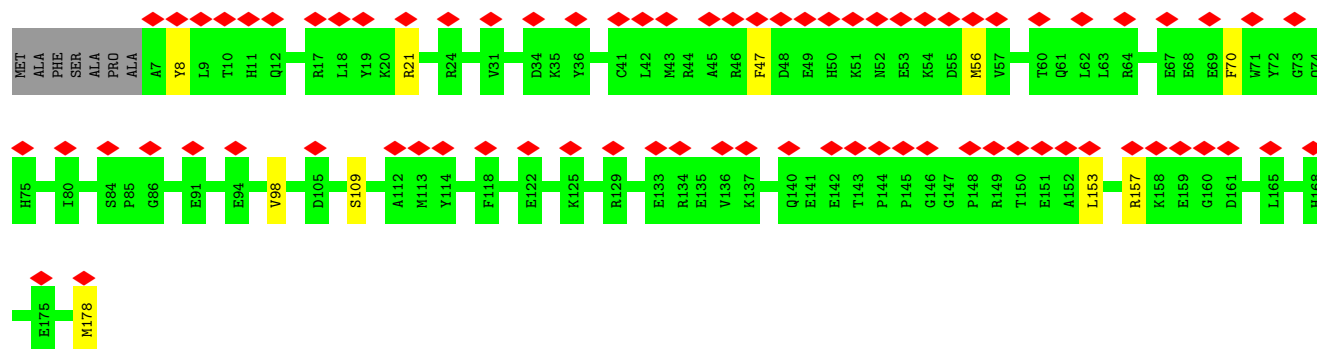
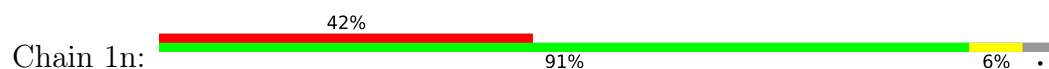


• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

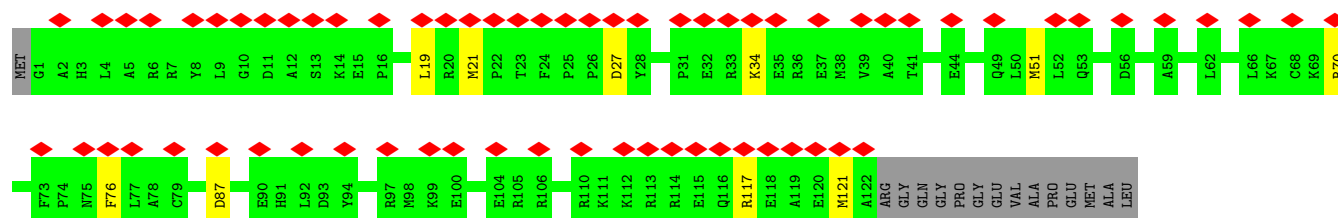
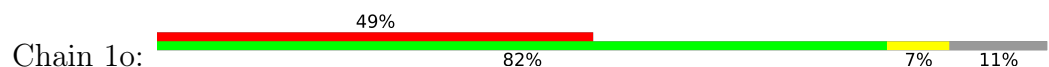




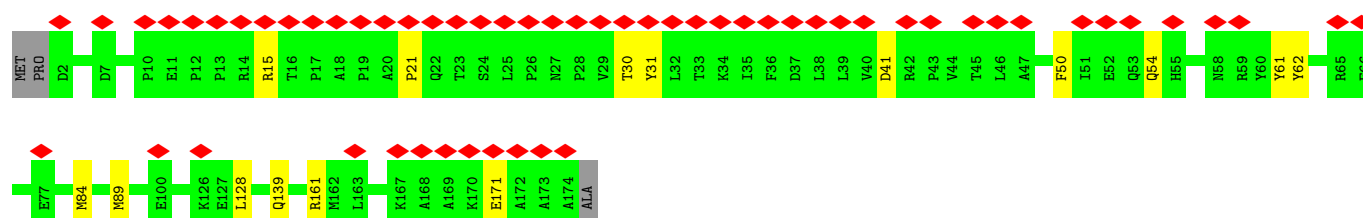
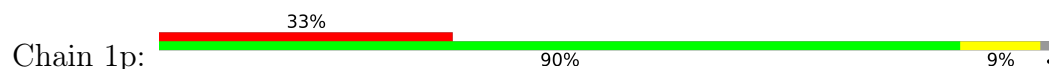
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



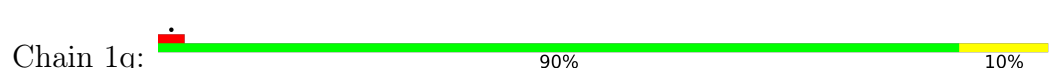
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



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



- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46000	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	1.011	Depositor
Minimum map value	-0.198	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	556.0, 556.0, 556.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, CDL, ZN, U10, FES, EHZ, FMN, K, MG, NDP, 3PE, GTP, SF4, SAC, MYR, FME, ACE

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	0.35	0/930	0.57	0/1271
2	1B	0.32	0/1273	0.56	0/1722
3	1C	0.29	0/1791	0.50	0/2439
4	1D	0.31	0/3545	0.53	1/4806 (0.0%)
5	1E	0.28	0/1698	0.49	0/2311
6	1F	0.59	5/3401 (0.1%)	0.88	6/4595 (0.1%)
7	1G	0.31	1/5451 (0.0%)	0.50	0/7387
8	1H	0.35	0/2566	0.52	1/3509 (0.0%)
9	1I	0.34	0/1443	0.52	0/1952
10	1J	0.35	0/1364	0.57	0/1850
11	1K	0.35	0/751	0.58	0/1018
12	1L	0.28	0/4939	0.57	1/6718 (0.0%)
13	1M	0.29	0/3713	0.54	0/5063
14	1N	0.32	1/2765 (0.0%)	0.57	2/3758 (0.1%)
15	1O	0.29	0/2650	0.55	0/3588
16	1P	0.29	0/2828	0.51	0/3834
17	1Q	0.31	0/1070	0.55	0/1446
18	1R	0.29	0/755	0.54	0/1018
19	1S	0.25	0/711	0.52	0/956
20	1T	0.39	0/701	0.55	0/946
20	1U	0.29	0/706	0.51	0/954
21	1V	0.34	0/946	0.59	0/1281
22	1W	0.30	0/995	0.55	0/1340
23	1X	0.53	1/1436 (0.1%)	0.49	0/1938
24	1Y	0.35	0/1037	0.56	0/1404
25	1Z	0.30	0/1199	0.52	0/1617
26	1a	0.29	0/577	0.47	0/777
27	1b	0.36	1/664 (0.2%)	0.54	0/912
28	1c	0.33	0/430	0.67	0/581
29	1d	0.30	0/1024	0.60	1/1383 (0.1%)
30	1e	0.27	0/836	0.51	0/1118
31	1f	0.28	0/499	0.68	2/673 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	1g	0.27	0/858	0.57	0/1165
33	1h	0.27	0/1184	0.51	0/1603
34	1i	0.30	0/1131	0.57	0/1541
35	1j	0.64	2/627 (0.3%)	0.58	0/858
36	1k	0.33	0/668	0.58	0/903
37	1l	0.27	0/1365	0.52	0/1867
38	1m	0.31	0/1092	0.56	0/1481
39	1n	0.25	0/1549	0.52	0/2098
40	1o	0.26	0/1069	0.56	0/1430
41	1p	0.25	0/1481	0.50	0/1997
42	1q	0.34	0/1253	0.57	0/1704
43	1r	0.30	0/782	0.57	0/1057
44	1s	0.97	5/394 (1.3%)	1.35	5/533 (0.9%)
All	All	0.34	16/68147 (0.0%)	0.57	19/92402 (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
2	1B	0	2
6	1F	0	2
8	1H	0	1
21	1V	0	1
31	1f	0	1
All	All	0	7

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1F	207	PRO	CG-CD	-24.61	0.69	1.50
23	1X	87	CYS	CB-SG	-17.34	1.52	1.82
44	1s	32	PRO	CG-CD	-11.48	1.12	1.50
6	1F	207	PRO	CB-CG	10.31	2.01	1.50
35	1j	71	GLU	CD-OE1	-10.11	1.14	1.25
7	1G	21	GLU	CD-OE2	-9.10	1.15	1.25
35	1j	71	GLU	CD-OE2	-8.25	1.16	1.25
44	1s	31	GLU	C-N	7.91	1.49	1.34
6	1F	206	LYS	C-N	7.67	1.48	1.34
6	1F	207	PRO	CA-CB	-6.83	1.39	1.53
44	1s	32	PRO	N-CD	6.82	1.57	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1F	207	PRO	C-N	6.61	1.46	1.34
14	1N	323	MET	SD-CE	-6.36	1.42	1.77
27	1b	81	LYS	CE-NZ	-5.72	1.34	1.49
44	1s	32	PRO	N-CA	-5.59	1.37	1.47
44	1s	32	PRO	CB-CG	5.33	1.76	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1F	207	PRO	CA-N-CD	-28.82	71.15	111.50
6	1F	207	PRO	CB-CG-CD	-27.30	0.04	106.50
44	1s	32	PRO	CA-N-CD	-19.47	84.24	111.50
6	1F	206	LYS	C-N-CD	16.44	162.92	128.40
6	1F	207	PRO	N-CA-CB	-14.12	86.35	103.30
44	1s	31	GLU	C-N-CD	13.52	156.80	128.40
6	1F	207	PRO	CA-CB-CG	-12.25	80.72	104.00
6	1F	207	PRO	N-CD-CG	-10.55	87.37	103.20
14	1N	323	MET	CA-CB-CG	8.08	127.04	113.30
12	1L	350	LEU	CA-CB-CG	7.42	132.35	115.30
29	1d	113	LEU	CA-CB-CG	6.90	131.18	115.30
44	1s	32	PRO	CA-CB-CG	-6.71	91.25	104.00
44	1s	32	PRO	N-CD-CG	-6.67	93.20	103.20
44	1s	34	ASP	CB-CG-OD1	6.54	124.18	118.30
31	1f	28	ARG	CA-CB-CG	6.00	126.61	113.40
4	1D	19	MET	CA-CB-CG	5.93	123.39	113.30
14	1N	323	MET	N-CA-CB	-5.57	100.57	110.60
31	1f	43	LEU	CA-CB-CG	5.48	127.90	115.30
8	1H	200	LEU	CA-CB-CG	5.39	127.70	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1B	108	PRO	Peptide
2	1B	109	GLU	Peptide
6	1F	206	LYS	Peptide
6	1F	207	PRO	Mainchain
8	1H	196	ALA	Peptide
21	1V	113	TRP	Peptide
31	1f	28	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	113/115 (98%)	103 (91%)	9 (8%)	1 (1%)	17	56
2	1B	153/258 (59%)	138 (90%)	15 (10%)	0	100	100
3	1C	207/264 (78%)	199 (96%)	8 (4%)	0	100	100
4	1D	427/476 (90%)	402 (94%)	25 (6%)	0	100	100
5	1E	212/249 (85%)	195 (92%)	16 (8%)	1 (0%)	29	68
6	1F	430/464 (93%)	414 (96%)	16 (4%)	0	100	100
7	1G	697/727 (96%)	655 (94%)	41 (6%)	1 (0%)	51	84
8	1H	316/318 (99%)	292 (92%)	21 (7%)	3 (1%)	17	56
9	1I	174/239 (73%)	168 (97%)	6 (3%)	0	100	100
10	1J	173/175 (99%)	160 (92%)	10 (6%)	3 (2%)	9	42
11	1K	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
12	1L	604/606 (100%)	552 (91%)	47 (8%)	5 (1%)	19	58
13	1M	457/459 (100%)	438 (96%)	19 (4%)	0	100	100
14	1N	345/347 (99%)	322 (93%)	22 (6%)	1 (0%)	41	75
15	1O	318/357 (89%)	298 (94%)	20 (6%)	0	100	100
16	1P	340/377 (90%)	324 (95%)	16 (5%)	0	100	100
17	1Q	127/175 (73%)	117 (92%)	10 (8%)	0	100	100
18	1R	94/123 (76%)	89 (95%)	5 (5%)	0	100	100
19	1S	85/99 (86%)	79 (93%)	6 (7%)	0	100	100
20	1T	83/156 (53%)	76 (92%)	7 (8%)	0	100	100
20	1U	84/156 (54%)	77 (92%)	7 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	1V	113/116 (97%)	106 (94%)	7 (6%)	0	100	100
22	1W	113/128 (88%)	107 (95%)	6 (5%)	0	100	100
23	1X	169/172 (98%)	164 (97%)	4 (2%)	1 (1%)	25	64
24	1Y	137/141 (97%)	132 (96%)	5 (4%)	0	100	100
25	1Z	139/144 (96%)	130 (94%)	9 (6%)	0	100	100
26	1a	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
27	1b	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
28	1c	47/76 (62%)	43 (92%)	4 (8%)	0	100	100
29	1d	117/123 (95%)	104 (89%)	12 (10%)	1 (1%)	17	56
30	1e	97/106 (92%)	88 (91%)	9 (9%)	0	100	100
31	1f	55/135 (41%)	49 (89%)	6 (11%)	0	100	100
32	1g	98/154 (64%)	83 (85%)	14 (14%)	1 (1%)	15	54
33	1h	136/189 (72%)	126 (93%)	10 (7%)	0	100	100
34	1i	124/128 (97%)	115 (93%)	9 (7%)	0	100	100
35	1j	69/105 (66%)	66 (96%)	3 (4%)	0	100	100
36	1k	79/98 (81%)	74 (94%)	5 (6%)	0	100	100
37	1l	154/186 (83%)	142 (92%)	12 (8%)	0	100	100
38	1m	126/129 (98%)	114 (90%)	12 (10%)	0	100	100
39	1n	170/179 (95%)	157 (92%)	13 (8%)	0	100	100
40	1o	120/137 (88%)	110 (92%)	10 (8%)	0	100	100
41	1p	171/176 (97%)	162 (95%)	9 (5%)	0	100	100
42	1q	143/145 (99%)	131 (92%)	12 (8%)	0	100	100
43	1r	90/114 (79%)	86 (96%)	4 (4%)	0	100	100
44	1s	43/471 (9%)	38 (88%)	4 (9%)	1 (2%)	6	36
All	All	8194/9744 (84%)	7656 (93%)	519 (6%)	19 (0%)	50	81

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1A	109	LYS
7	1G	652	VAL
8	1H	68	ILE
8	1H	92	PRO
10	1J	2	THR

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Mol	Chain	Res	Type
10	1J	85	SER
23	1X	28	ALA
29	1d	53	VAL
10	1J	116	ILE
8	1H	208	VAL
12	1L	4	PHE
12	1L	562	LEU
12	1L	549	ALA
5	1E	157	ASN
12	1L	484	LEU
12	1L	600	THR
14	1N	110	PRO
44	1s	32	PRO
32	1g	68	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	99/99 (100%)	88 (89%)	11 (11%)	6	28
2	1B	131/212 (62%)	121 (92%)	10 (8%)	13	43
3	1C	190/227 (84%)	177 (93%)	13 (7%)	16	48
4	1D	371/405 (92%)	338 (91%)	33 (9%)	9	37
5	1E	183/207 (88%)	172 (94%)	11 (6%)	19	52
6	1F	346/368 (94%)	324 (94%)	22 (6%)	17	50
7	1G	588/610 (96%)	531 (90%)	57 (10%)	8	33
8	1H	274/274 (100%)	250 (91%)	24 (9%)	10	38
9	1I	151/201 (75%)	137 (91%)	14 (9%)	9	35
10	1J	140/140 (100%)	114 (81%)	26 (19%)	1	8
11	1K	84/84 (100%)	72 (86%)	12 (14%)	3	19
12	1L	539/539 (100%)	467 (87%)	72 (13%)	4	21
13	1M	408/408 (100%)	366 (90%)	42 (10%)	7	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	1N	310/310 (100%)	280 (90%)	30 (10%)	8	33
15	1O	283/307 (92%)	247 (87%)	36 (13%)	4	22
16	1P	296/323 (92%)	272 (92%)	24 (8%)	11	41
17	1Q	117/152 (77%)	104 (89%)	13 (11%)	6	28
18	1R	79/97 (81%)	66 (84%)	13 (16%)	2	13
19	1S	77/82 (94%)	67 (87%)	10 (13%)	4	21
20	1T	79/133 (59%)	64 (81%)	15 (19%)	1	8
20	1U	79/133 (59%)	72 (91%)	7 (9%)	9	37
21	1V	100/101 (99%)	90 (90%)	10 (10%)	7	32
22	1W	107/112 (96%)	95 (89%)	12 (11%)	6	27
23	1X	153/154 (99%)	137 (90%)	16 (10%)	7	31
24	1Y	101/102 (99%)	93 (92%)	8 (8%)	12	41
25	1Z	123/124 (99%)	111 (90%)	12 (10%)	8	33
26	1a	58/58 (100%)	50 (86%)	8 (14%)	3	20
27	1b	69/70 (99%)	66 (96%)	3 (4%)	29	62
28	1c	45/66 (68%)	39 (87%)	6 (13%)	4	21
29	1d	107/109 (98%)	96 (90%)	11 (10%)	7	32
30	1e	87/94 (93%)	77 (88%)	10 (12%)	5	26
31	1f	54/113 (48%)	48 (89%)	6 (11%)	6	28
32	1g	92/129 (71%)	78 (85%)	14 (15%)	3	17
33	1h	121/158 (77%)	108 (89%)	13 (11%)	6	30
34	1i	119/120 (99%)	104 (87%)	15 (13%)	4	22
35	1j	62/84 (74%)	52 (84%)	10 (16%)	2	14
36	1k	63/76 (83%)	49 (78%)	14 (22%)	1	5
37	1l	141/161 (88%)	122 (86%)	19 (14%)	4	21
38	1m	113/114 (99%)	101 (89%)	12 (11%)	6	30
39	1n	156/160 (98%)	146 (94%)	10 (6%)	17	50
40	1o	110/120 (92%)	100 (91%)	10 (9%)	9	36
41	1p	154/156 (99%)	139 (90%)	15 (10%)	8	33
42	1q	131/131 (100%)	116 (88%)	15 (12%)	5	26
43	1r	85/98 (87%)	77 (91%)	8 (9%)	8	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	1s	44/351 (12%)	37 (84%)	7 (16%)	2	14
All	All	7219/8272 (87%)	6460 (90%)	759 (10%)	10	31

All (759) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	4	MET
1	1A	28	ASN
1	1A	30	TYR
1	1A	31	SER
1	1A	53	MET
1	1A	62	PHE
1	1A	71	LEU
1	1A	84	LEU
1	1A	87	MET
1	1A	93	PHE
1	1A	109	LYS
2	1B	30	VAL
2	1B	96	MET
2	1B	102	LYS
2	1B	107	MET
2	1B	109	GLU
2	1B	116	MET
2	1B	125	TYR
2	1B	152	THR
2	1B	157	LEU
2	1B	160	ILE
3	1C	7	THR
3	1C	8	ARG
3	1C	20	LYS
3	1C	33	LEU
3	1C	39	GLN
3	1C	43	SER
3	1C	69	ASN
3	1C	123	VAL
3	1C	129	TRP
3	1C	188	VAL
3	1C	196	LYS
3	1C	199	LEU
3	1C	201	SER
4	1D	14	PHE
4	1D	18	VAL

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Mol	Chain	Res	Type
4	1D	35	ASP
4	1D	61	VAL
4	1D	66	MET
4	1D	74	ARG
4	1D	76	CYS
4	1D	108	TYR
4	1D	152	MET
4	1D	167	PHE
4	1D	171	PHE
4	1D	183	ARG
4	1D	189	MET
4	1D	199	VAL
4	1D	215	SER
4	1D	219	SER
4	1D	220	PHE
4	1D	233	ARG
4	1D	246	THR
4	1D	256	SER
4	1D	282	GLU
4	1D	289	SER
4	1D	297	TYR
4	1D	312	SER
4	1D	323	ILE
4	1D	334	LYS
4	1D	339	LYS
4	1D	384	SER
4	1D	385	ARG
4	1D	407	LYS
4	1D	411	LEU
4	1D	414	VAL
4	1D	428	VAL
5	1E	11	ASP
5	1E	28	TYR
5	1E	36	LYS
5	1E	97	LYS
5	1E	105	THR
5	1E	121	GLN
5	1E	122	LYS
5	1E	141	GLU
5	1E	153	MET
5	1E	167	LYS
5	1E	183	LYS

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Mol	Chain	Res	Type
6	1F	20	ARG
6	1F	54	ASP
6	1F	63	SER
6	1F	66	ARG
6	1F	89	ARG
6	1F	105	CYS
6	1F	110	ILE
6	1F	119	VAL
6	1F	127	ARG
6	1F	150	GLN
6	1F	177	VAL
6	1F	207	PRO
6	1F	212	ASP
6	1F	218	CYS
6	1F	312	CYS
6	1F	355	LYS
6	1F	356	HIS
6	1F	359	CYS
6	1F	397	LYS
6	1F	399	ILE
6	1F	432	GLN
6	1F	435	LEU
7	1G	14	ASP
7	1G	32	LYS
7	1G	39	ARG
7	1G	53	ARG
7	1G	65	VAL
7	1G	69	CYS
7	1G	74	MET
7	1G	77	TRP
7	1G	83	SER
7	1G	88	LYS
7	1G	123	PHE
7	1G	131	LEU
7	1G	140	LYS
7	1G	148	THR
7	1G	161	ARG
7	1G	174	THR
7	1G	185	THR
7	1G	215	PHE
7	1G	222	THR
7	1G	223	ARG

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Mol	Chain	Res	Type
7	1G	224	LYS
7	1G	227	SER
7	1G	231	MET
7	1G	236	SER
7	1G	243	ARG
7	1G	248	MET
7	1G	287	GLU
7	1G	288	LYS
7	1G	323	VAL
7	1G	340	SER
7	1G	351	THR
7	1G	361	ASN
7	1G	365	ASN
7	1G	366	THR
7	1G	375	ASP
7	1G	398	SER
7	1G	420	ASP
7	1G	427	LYS
7	1G	467	LEU
7	1G	471	SER
7	1G	480	SER
7	1G	515	ARG
7	1G	523	PHE
7	1G	531	CYS
7	1G	532	ILE
7	1G	536	ASP
7	1G	548	HIS
7	1G	558	ASP
7	1G	583	THR
7	1G	609	MET
7	1G	620	ARG
7	1G	632	ARG
7	1G	650	LYS
7	1G	652	VAL
7	1G	662	VAL
7	1G	673	MET
7	1G	698	VAL
8	1H	3	MET
8	1H	14	LEU
8	1H	17	VAL
8	1H	35	LYS
8	1H	54	LYS

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Mol	Chain	Res	Type
8	1H	58	LYS
8	1H	68	ILE
8	1H	79	LEU
8	1H	85	MET
8	1H	111	LEU
8	1H	124	ASN
8	1H	183	MET
8	1H	195	ARG
8	1H	198	PHE
8	1H	202	GLU
8	1H	211	PHE
8	1H	212	ASN
8	1H	234	MET
8	1H	237	PHE
8	1H	241	LEU
8	1H	274	ARG
8	1H	276	SER
8	1H	291	LYS
8	1H	302	MET
9	1I	2	TYR
9	1I	3	LYS
9	1I	8	ARG
9	1I	14	MET
9	1I	15	LYS
9	1I	31	VAL
9	1I	36	MET
9	1I	40	TYR
9	1I	69	ARG
9	1I	97	GLU
9	1I	103	SER
9	1I	104	ARG
9	1I	129	ASP
9	1I	143	THR
10	1J	3	MET
10	1J	4	TYR
10	1J	7	PHE
10	1J	17	PHE
10	1J	20	PHE
10	1J	41	CYS
10	1J	47	PHE
10	1J	55	MET
10	1J	57	PHE

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Mol	Chain	Res	Type
10	1J	60	TYR
10	1J	64	MET
10	1J	66	VAL
10	1J	70	TYR
10	1J	78	MET
10	1J	90	PHE
10	1J	93	PHE
10	1J	98	MET
10	1J	101	PHE
10	1J	105	TYR
10	1J	111	GLU
10	1J	118	LYS
10	1J	130	THR
10	1J	132	ASP
10	1J	135	PHE
10	1J	165	VAL
10	1J	173	ARG
11	1K	10	MET
11	1K	31	LEU
11	1K	45	THR
11	1K	53	PHE
11	1K	54	THR
11	1K	59	MET
11	1K	69	CYS
11	1K	77	LEU
11	1K	83	ASN
11	1K	88	ASP
11	1K	89	TYR
11	1K	93	LEU
12	1L	12	LEU
12	1L	30	ASN
12	1L	31	LEU
12	1L	49	VAL
12	1L	53	MET
12	1L	61	MET
12	1L	71	LEU
12	1L	73	THR
12	1L	80	PHE
12	1L	82	MET
12	1L	86	SER
12	1L	88	MET
12	1L	101	MET

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Mol	Chain	Res	Type
12	1L	110	SER
12	1L	111	ASP
12	1L	125	LEU
12	1L	150	MET
12	1L	152	PHE
12	1L	176	ARG
12	1L	182	PHE
12	1L	186	MET
12	1L	206	ASN
12	1L	216	LEU
12	1L	227	PHE
12	1L	244	SER
12	1L	248	HIS
12	1L	253	VAL
12	1L	271	LYS
12	1L	276	MET
12	1L	277	THR
12	1L	278	LEU
12	1L	294	THR
12	1L	295	GLN
12	1L	298	ILE
12	1L	313	MET
12	1L	314	MET
12	1L	338	MET
12	1L	341	MET
12	1L	366	MET
12	1L	378	LEU
12	1L	383	MET
12	1L	401	MET
12	1L	405	ASN
12	1L	407	TRP
12	1L	425	ARG
12	1L	437	PHE
12	1L	455	LYS
12	1L	475	MET
12	1L	476	THR
12	1L	481	THR
12	1L	486	MET
12	1L	488	MET
12	1L	494	THR
12	1L	496	MET
12	1L	498	PHE

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Mol	Chain	Res	Type
12	1L	525	MET
12	1L	528	TYR
12	1L	533	MET
12	1L	544	MET
12	1L	553	LEU
12	1L	554	ASP
12	1L	556	ILE
12	1L	557	TRP
12	1L	565	THR
12	1L	571	MET
12	1L	573	MET
12	1L	574	SER
12	1L	576	MET
12	1L	581	LYS
12	1L	585	LYS
12	1L	599	MET
12	1L	605	HIS
13	1M	10	MET
13	1M	14	MET
13	1M	16	TRP
13	1M	38	SER
13	1M	41	LEU
13	1M	55	THR
13	1M	57	PHE
13	1M	62	SER
13	1M	76	MET
13	1M	80	SER
13	1M	88	THR
13	1M	116	ILE
13	1M	122	PHE
13	1M	123	GLU
13	1M	136	TRP
13	1M	148	TYR
13	1M	152	TYR
13	1M	183	SER
13	1M	212	LEU
13	1M	225	ILE
13	1M	229	MET
13	1M	244	MET
13	1M	245	ARG
13	1M	257	MET
13	1M	269	MET

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Mol	Chain	Res	Type
13	1M	271	MET
13	1M	296	LEU
13	1M	316	MET
13	1M	322	THR
13	1M	336	ARG
13	1M	346	ARG
13	1M	350	THR
13	1M	361	MET
13	1M	364	LEU
13	1M	373	ILE
13	1M	396	MET
13	1M	398	MET
13	1M	400	MET
13	1M	410	MET
13	1M	413	THR
13	1M	416	ARG
13	1M	421	HIS
14	1N	15	SER
14	1N	59	TYR
14	1N	96	THR
14	1N	100	MET
14	1N	117	GLU
14	1N	123	SER
14	1N	146	SER
14	1N	159	MET
14	1N	177	LYS
14	1N	178	ILE
14	1N	198	THR
14	1N	201	THR
14	1N	235	ASN
14	1N	241	THR
14	1N	242	SER
14	1N	267	ILE
14	1N	268	GLN
14	1N	270	MET
14	1N	277	ILE
14	1N	282	MET
14	1N	288	LEU
14	1N	291	TYR
14	1N	307	SER
14	1N	312	LYS
14	1N	313	MET

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Mol	Chain	Res	Type
14	1N	323	MET
14	1N	329	MET
14	1N	335	LEU
14	1N	337	LEU
14	1N	345	SER
15	1O	1	LEU
15	1O	24	VAL
15	1O	28	ASP
15	1O	35	LYS
15	1O	67	LYS
15	1O	70	ASP
15	1O	81	LYS
15	1O	82	PHE
15	1O	87	LYS
15	1O	88	SER
15	1O	101	TYR
15	1O	105	LEU
15	1O	108	TYR
15	1O	110	ASP
15	1O	129	TYR
15	1O	145	ARG
15	1O	146	LYS
15	1O	147	GLN
15	1O	150	GLU
15	1O	178	GLU
15	1O	192	MET
15	1O	206	TYR
15	1O	214	MET
15	1O	226	ARG
15	1O	232	GLU
15	1O	233	LYS
15	1O	235	VAL
15	1O	242	LYS
15	1O	250	ASP
15	1O	254	ARG
15	1O	258	ARG
15	1O	265	ASN
15	1O	283	THR
15	1O	305	SER
15	1O	314	ASP
15	1O	316	TRP
16	1P	32	ARG

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Mol	Chain	Res	Type
16	1P	43	SER
16	1P	50	ARG
16	1P	58	HIS
16	1P	101	THR
16	1P	102	LYS
16	1P	122	LYS
16	1P	140	LYS
16	1P	154	LYS
16	1P	170	ASP
16	1P	184	SER
16	1P	186	ARG
16	1P	220	ASP
16	1P	226	LYS
16	1P	242	VAL
16	1P	263	TYR
16	1P	268	ARG
16	1P	280	THR
16	1P	289	MET
16	1P	292	MET
16	1P	300	LEU
16	1P	319	ARG
16	1P	323	THR
16	1P	340	VAL
17	1Q	16	LYS
17	1Q	47	SER
17	1Q	49	VAL
17	1Q	56	LYS
17	1Q	58	GLU
17	1Q	70	MET
17	1Q	74	SER
17	1Q	80	SER
17	1Q	84	LEU
17	1Q	85	THR
17	1Q	116	LYS
17	1Q	117	SER
17	1Q	122	PHE
18	1R	3	ARG
18	1R	14	THR
18	1R	30	ASP
18	1R	31	ARG
18	1R	32	GLN
18	1R	58	SER

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Mol	Chain	Res	Type
18	1R	70	ARG
18	1R	71	VAL
18	1R	79	THR
18	1R	80	LYS
18	1R	81	THR
18	1R	84	CYS
18	1R	90	GLN
19	1S	25	ARG
19	1S	29	SER
19	1S	47	ASN
19	1S	59	ASP
19	1S	64	LEU
19	1S	74	LYS
19	1S	78	LEU
19	1S	84	ASP
19	1S	87	THR
19	1S	91	GLU
20	1T	6	LEU
20	1T	12	LYS
20	1T	14	ARG
20	1T	17	TYR
20	1T	19	LEU
20	1T	20	LYS
20	1T	22	TYR
20	1T	23	ASP
20	1T	29	LYS
20	1T	40	LEU
20	1T	54	MET
20	1T	60	PHE
20	1T	69	LYS
20	1T	71	MET
20	1T	79	TYR
20	1U	17	TYR
20	1U	37	MET
20	1U	60	PHE
20	1U	64	ASP
20	1U	69	LYS
20	1U	71	MET
20	1U	85	ASP
21	1V	6	LYS
21	1V	7	THR
21	1V	39	LYS

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Mol	Chain	Res	Type
21	1V	59	LYS
21	1V	65	LYS
21	1V	72	GLN
21	1V	84	GLU
21	1V	88	SER
21	1V	97	LYS
21	1V	99	TRP
22	1W	17	VAL
22	1W	40	TYR
22	1W	51	GLN
22	1W	64	ARG
22	1W	69	LYS
22	1W	83	VAL
22	1W	87	LYS
22	1W	88	MET
22	1W	95	ASN
22	1W	101	THR
22	1W	104	MET
22	1W	114	ARG
23	1X	4	VAL
23	1X	5	GLU
23	1X	9	LEU
23	1X	15	GLN
23	1X	18	LYS
23	1X	47	TRP
23	1X	53	ARG
23	1X	91	SER
23	1X	107	ASP
23	1X	118	ARG
23	1X	127	VAL
23	1X	156	ASP
23	1X	158	LYS
23	1X	164	SER
23	1X	170	THR
23	1X	171	MET
24	1Y	2	LYS
24	1Y	8	TYR
24	1Y	15	THR
24	1Y	57	ARG
24	1Y	90	PHE
24	1Y	91	ILE
24	1Y	105	ARG

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Mol	Chain	Res	Type
24	1Y	117	MET
25	1Z	4	SER
25	1Z	5	LYS
25	1Z	8	GLN
25	1Z	23	ARG
25	1Z	50	MET
25	1Z	55	ARG
25	1Z	68	ARG
25	1Z	79	LYS
25	1Z	100	ASP
25	1Z	113	THR
25	1Z	117	VAL
25	1Z	121	MET
26	1a	12	MET
26	1a	38	VAL
26	1a	50	ARG
26	1a	55	SER
26	1a	59	ARG
26	1a	60	TYR
26	1a	63	THR
26	1a	68	ASN
27	1b	39	ASN
27	1b	76	SER
27	1b	78	GLU
28	1c	2	PHE
28	1c	5	ARG
28	1c	21	LEU
28	1c	26	PHE
28	1c	43	LYS
28	1c	44	ARG
29	1d	3	SER
29	1d	13	PHE
29	1d	25	LYS
29	1d	39	TYR
29	1d	40	CYS
29	1d	54	VAL
29	1d	61	GLN
29	1d	70	PHE
29	1d	100	ASP
29	1d	105	ASP
29	1d	114	GLU
30	1e	9	LEU

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Mol	Chain	Res	Type
30	1e	18	THR
30	1e	37	LYS
30	1e	53	LYS
30	1e	69	GLN
30	1e	70	LYS
30	1e	83	ASP
30	1e	84	LYS
30	1e	87	LYS
30	1e	96	HIS
31	1f	1	MET
31	1f	8	ARG
31	1f	28	ARG
31	1f	31	ASP
31	1f	42	LEU
31	1f	49	ARG
32	1g	23	THR
32	1g	40	LYS
32	1g	50	ASP
32	1g	58	MET
32	1g	66	PHE
32	1g	74	SER
32	1g	85	MET
32	1g	91	ARG
32	1g	96	LEU
32	1g	98	LYS
32	1g	99	TYR
32	1g	103	ASN
32	1g	114	ASP
32	1g	116	ASN
33	1h	12	LYS
33	1h	18	ASP
33	1h	19	ARG
33	1h	21	PHE
33	1h	25	MET
33	1h	47	ILE
33	1h	59	TYR
33	1h	97	GLU
33	1h	123	TYR
33	1h	127	THR
33	1h	129	ASP
33	1h	138	LYS
33	1h	140	THR

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Mol	Chain	Res	Type
34	1i	10	ARG
34	1i	30	ARG
34	1i	33	VAL
34	1i	38	ARG
34	1i	40	TRP
34	1i	42	MET
34	1i	46	TRP
34	1i	48	LYS
34	1i	49	PHE
34	1i	50	LEU
34	1i	85	LEU
34	1i	99	ARG
34	1i	120	LYS
34	1i	126	HIS
34	1i	127	HIS
35	1j	10	ARG
35	1j	18	THR
35	1j	19	ARG
35	1j	32	MET
35	1j	33	TRP
35	1j	34	PHE
35	1j	40	PHE
35	1j	50	HIS
35	1j	63	GLU
35	1j	64	LEU
36	1k	12	LYS
36	1k	13	MET
36	1k	17	ASP
36	1k	38	ARG
36	1k	46	ARG
36	1k	51	ARG
36	1k	52	TYR
36	1k	59	ASN
36	1k	61	SER
36	1k	70	PHE
36	1k	72	TRP
36	1k	77	PHE
36	1k	85	TYR
36	1k	87	LEU
37	1l	3	HIS
37	1l	5	THR
37	1l	6	LYS

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Mol	Chain	Res	Type
37	1l	9	PHE
37	1l	16	THR
37	1l	27	TYR
37	1l	42	MET
37	1l	53	ARG
37	1l	79	TRP
37	1l	83	MET
37	1l	86	ARG
37	1l	88	ARG
37	1l	90	ASP
37	1l	97	SER
37	1l	108	PHE
37	1l	114	PHE
37	1l	115	MET
37	1l	156	TYR
37	1l	157	GLU
38	1m	2	PHE
38	1m	6	LYS
38	1m	9	ARG
38	1m	10	LEU
38	1m	27	GLU
38	1m	49	GLN
38	1m	65	ILE
38	1m	84	LYS
38	1m	91	LEU
38	1m	92	PHE
38	1m	99	PHE
38	1m	114	LEU
39	1n	8	TYR
39	1n	21	ARG
39	1n	47	PHE
39	1n	56	MET
39	1n	70	PHE
39	1n	98	VAL
39	1n	109	SER
39	1n	153	LEU
39	1n	157	ARG
39	1n	178	MET
40	1o	19	LEU
40	1o	21	MET
40	1o	27	ASP
40	1o	34	LYS

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Mol	Chain	Res	Type
40	1o	51	MET
40	1o	70	ARG
40	1o	76	PHE
40	1o	87	ASP
40	1o	117	ARG
40	1o	121	MET
41	1p	15	ARG
41	1p	21	PRO
41	1p	30	THR
41	1p	31	TYR
41	1p	41	ASP
41	1p	50	PHE
41	1p	54	GLN
41	1p	61	TYR
41	1p	62	TYR
41	1p	84	MET
41	1p	89	MET
41	1p	128	LEU
41	1p	139	GLN
41	1p	161	ARG
41	1p	171	GLU
42	1q	12	GLN
42	1q	21	ARG
42	1q	32	ASP
42	1q	43	LYS
42	1q	50	GLU
42	1q	95	ASP
42	1q	104	THR
42	1q	115	PHE
42	1q	120	THR
42	1q	125	VAL
42	1q	128	SER
42	1q	129	THR
42	1q	131	ARG
42	1q	133	LYS
42	1q	144	TYR
43	1r	24	GLN
43	1r	39	LYS
43	1r	54	CYS
43	1r	63	MET
43	1r	91	LYS
43	1r	101	LYS

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Mol	Chain	Res	Type
43	1r	102	ARG
43	1r	106	SER
44	1s	39	ARG
44	1s	54	LEU
44	1s	58	LEU
44	1s	60	LYS
44	1s	63	MET
44	1s	72	SER
44	1s	74	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	10	ASN
7	1G	51	ASN
7	1G	237	ASN
7	1G	459	GLN
8	1H	47	GLN
9	1I	156	ASN
11	1K	57	ASN
12	1L	309	GLN
12	1L	405	ASN
12	1L	603	ASN
13	1M	213	HIS
13	1M	422	HIS
15	1O	72	GLN
15	1O	76	ASN
15	1O	107	GLN
15	1O	167	HIS
15	1O	184	GLN
15	1O	271	ASN
20	1T	35	HIS
21	1V	70	GLN
23	1X	15	GLN
29	1d	46	ASN
29	1d	61	GLN
30	1e	44	HIS
31	1f	13	HIS
32	1g	36	ASN
32	1g	41	ASN
32	1g	57	ASN
37	1l	78	HIS

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Mol	Chain	Res	Type
38	1m	78	ASN
39	1n	74	GLN
39	1n	77	GLN
40	1o	75	ASN
41	1p	133	GLN
42	1q	113	HIS
43	1r	46	HIS
43	1r	109	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\# Z  > 2$
1	FME	1A	1	1	8,9,10	0.49	0	7,9,11	1.07	1 (14%)
12	FME	1L	1	12	8,9,10	0.50	0	7,9,11	1.01	1 (14%)
34	SAC	1i	1	-	7,8,9	0.51	0	8,9,11	1.93	2 (25%)
13	FME	1M	1	13	8,9,10	0.51	0	7,9,11	1.02	1 (14%)
8	FME	1H	1	8	8,9,10	0.50	0	7,9,11	1.01	1 (14%)
10	FME	1J	1	10	8,9,10	0.51	0	7,9,11	1.18	1 (14%)
11	FME	1K	1	11	8,9,10	0.52	0	7,9,11	1.02	1 (14%)
14	FME	1N	1	14	8,9,10	0.50	0	7,9,11	0.99	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
1	FME	1A	1	1	-	0/7/9/11	-
12	FME	1L	1	12	-	0/7/9/11	-
34	SAC	1i	1	-	-	6/7/8/10	-
13	FME	1M	1	13	-	0/7/9/11	-
8	FME	1H	1	8	-	0/7/9/11	-
10	FME	1J	1	10	-	1/7/9/11	-
11	FME	1K	1	11	-	1/7/9/11	-
14	FME	1N	1	14	-	0/7/9/11	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1i	1	SAC	CA-N-C1A	3.70	129.98	123.15
34	1i	1	SAC	O-C-CA	-2.91	117.14	124.78
1	1A	1	FME	O-C-CA	-2.57	118.05	124.78
11	1K	1	FME	O-C-CA	-2.50	118.21	124.78
12	1L	1	FME	O-C-CA	-2.49	118.25	124.78
10	1J	1	FME	O-C-CA	-2.49	118.26	124.78
14	1N	1	FME	O-C-CA	-2.48	118.28	124.78
8	1H	1	FME	O-C-CA	-2.48	118.28	124.78
13	1M	1	FME	O-C-CA	-2.48	118.29	124.78

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	1J	1	FME	CB-CA-N-CN
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
11	1K	1	FME	N-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 29 ligands modelled in this entry, 3 are monoatomic - leaving 26 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
53	3PE	1M	502	-	37,37,50	0.30	0	40,42,55	0.41	0
51	CDL	1O	403	-	66,66,99	0.98	3 (4%)	72,78,111	1.38	5 (6%)
45	SF4	1F	502	6	0,12,12	-	-	-		
56	NDP	1P	501	-	45,52,52	0.63	0	53,80,80	0.75	2 (3%)
46	PC1	1L	702	-	45,45,53	0.29	0	51,53,61	0.33	0
58	EHZ	1n	201	-	29,36,37	0.21	0	35,44,47	0.94	1 (2%)
45	SF4	1B	201	2	0,12,12	-	-	-		
51	CDL	1a	101	-	60,60,99	0.33	0	66,72,111	0.43	0
47	FES	1E	301	5	0,4,4	-	-	-		
46	PC1	1q	201	-	47,47,53	0.29	0	53,55,61	0.31	0
46	PC1	1f	101	-	24,24,53	0.36	0	30,32,61	0.65	0
53	3PE	1Y	201	-	34,34,50	0.46	0	37,39,55	0.88	2 (5%)
45	SF4	1G	801	7	0,12,12	-	-	-		
45	SF4	1G	802	7	0,12,12	-	-	-		
46	PC1	1M	501	-	34,34,53	0.32	0	40,42,61	0.37	0
45	SF4	1I	201	9	0,12,12	-	-	-		
45	SF4	1I	202	9	0,12,12	-	-	-		
51	CDL	1H	702	-	50,50,99	0.36	0	56,62,111	0.59	1 (1%)
52	MYR	1L	701	-	14,14,15	0.32	0	13,13,15	0.40	0
54	GTP	1O	401	55	26,34,34	0.96	2 (7%)	32,54,54	0.90	1 (3%)
46	PC1	1B	202	-	33,33,53	0.32	0	39,41,61	0.34	0
58	EHZ	1W	201	-	29,36,37	0.16	0	35,44,47	1.02	1 (2%)
48	FMN	1F	501	-	33,33,33	0.60	0	48,50,50	0.67	1 (2%)
47	FES	1G	804	7	0,4,4	-	-	-		
46	PC1	1d	201	-	38,38,53	0.32	0	44,46,61	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
50	U10	1H	701	-	63,63,63	0.59	1 (1%)	76,79,79	0.74	4 (5%)

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
53	3PE	1M	502	-	-	5/41/41/54	-
51	CDL	1O	403	-	-	15/76/76/110	-
56	NDP	1P	501	-	-	5/30/77/77	0/5/5/5
45	SF4	1F	502	6	-	-	0/6/5/5
46	PC1	1L	702	-	-	9/49/49/57	-
58	EHZ	1n	201	-	-	10/42/44/45	-
45	SF4	1B	201	2	-	-	0/6/5/5
51	CDL	1a	101	-	-	6/71/71/110	-
47	FES	1E	301	5	-	-	0/1/1/1
46	PC1	1q	201	-	-	11/51/51/57	-
46	PC1	1f	101	-	-	5/27/27/57	-
53	3PE	1Y	201	-	-	12/38/38/54	-
45	SF4	1G	801	7	-	-	0/6/5/5
45	SF4	1G	802	7	-	-	0/6/5/5
46	PC1	1M	501	-	-	4/38/38/57	-
52	MYR	1L	701	-	-	2/11/12/13	-
45	SF4	1I	201	9	-	-	0/6/5/5
51	CDL	1H	702	-	-	10/61/61/110	-
54	GTP	1O	401	55	-	0/18/38/38	0/3/3/3
45	SF4	1I	202	9	-	-	0/6/5/5
46	PC1	1B	202	-	-	14/37/37/57	-
58	EHZ	1W	201	-	-	5/42/44/45	-
48	FMN	1F	501	-	-	1/18/18/18	0/3/3/3
47	FES	1G	804	7	-	-	0/1/1/1
46	PC1	1d	201	-	-	13/42/42/57	-
50	U10	1H	701	-	-	22/63/87/87	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	1O	403	CDL	C71-CB7	5.23	1.66	1.50
51	1O	403	CDL	OB9-CB7	4.75	1.36	1.22
54	1O	401	GTP	C5-C6	-2.60	1.42	1.47
50	1H	701	U10	C4-C5	-2.60	1.41	1.48
51	1O	403	CDL	OB8-CB7	2.06	1.39	1.33
54	1O	401	GTP	C8-N7	-2.04	1.31	1.35

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	1O	403	CDL	OB8-CB7-C71	-7.06	89.76	111.91
58	1W	201	EHZ	C10-S1-C9	5.55	119.14	101.87
51	1O	403	CDL	OB8-CB7-OB9	5.54	137.58	123.59
51	1O	403	CDL	OB8-CB6-CB4	5.11	123.31	108.43
58	1n	201	EHZ	C10-S1-C9	5.09	117.73	101.87
53	1Y	201	3PE	O21-C21-C22	3.35	118.73	111.50
51	1O	403	CDL	CB6-OB8-CB7	3.24	129.11	117.12
54	1O	401	GTP	O4'-C1'-C2'	-2.83	102.79	106.93
56	1P	501	NDP	O4D-C1D-C2D	-2.73	100.70	106.64
50	1H	701	U10	O4-C4-C5	-2.67	107.54	116.56
50	1H	701	U10	O3-C3-C2	2.57	125.25	116.56
51	1H	702	CDL	OB6-CB5-C51	2.55	117.00	111.50
53	1Y	201	3PE	O13-C11-C12	-2.39	100.14	109.10
51	1O	403	CDL	OB9-CB7-C71	2.29	132.66	123.73
50	1H	701	U10	O4-C4-C3	2.28	132.24	123.64
56	1P	501	NDP	C5A-C6A-N6A	2.21	123.72	120.35
50	1H	701	U10	C4-C3-C2	-2.15	116.46	120.68
48	1F	501	FMN	C4-N3-C2	-2.01	121.93	125.64

There are no chirality outliers.

All (149) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	1B	202	PC1	C11-O13-P-O14
46	1B	202	PC1	C2-C1-O11-P
46	1B	202	PC1	O32-C31-O31-C3
46	1B	202	PC1	C32-C31-O31-C3
46	1L	702	PC1	C11-O13-P-O14
46	1L	702	PC1	C1-O11-P-O14
46	1M	501	PC1	O11-C1-C2-O21
46	1d	201	PC1	C11-O13-P-O12
46	1d	201	PC1	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
46	1d	201	PC1	O13-C11-C12-N
46	1d	201	PC1	O22-C21-O21-C2
46	1d	201	PC1	C22-C21-O21-C2
46	1d	201	PC1	O32-C31-O31-C3
46	1d	201	PC1	C32-C31-O31-C3
46	1f	101	PC1	C2-C1-O11-P
46	1q	201	PC1	C11-O13-P-O14
50	1H	701	U10	C45-C44-C46-C47
51	1H	702	CDL	C1-CA2-OA2-PA1
51	1H	702	CDL	CA3-OA5-PA1-OA2
51	1H	702	CDL	CA3-OA5-PA1-OA3
51	1H	702	CDL	OB7-CB5-OB6-CB4
51	1H	702	CDL	C51-CB5-OB6-CB4
53	1Y	201	3PE	O22-C21-O21-C2
53	1Y	201	3PE	C22-C21-O21-C2
58	1W	201	EHZ	O2-C9-S1-C10
58	1W	201	EHZ	C8-C9-S1-C10
58	1n	201	EHZ	C7-C8-C9-O2
58	1n	201	EHZ	C12-C13-C14-N2
50	1H	701	U10	C15-C14-C16-C17
50	1H	701	U10	C25-C24-C26-C27
50	1H	701	U10	C35-C34-C36-C37
50	1H	701	U10	C50-C49-C51-C52
50	1H	701	U10	C13-C14-C16-C17
50	1H	701	U10	C23-C24-C26-C27
50	1H	701	U10	C33-C34-C36-C37
50	1H	701	U10	C43-C44-C46-C47
50	1H	701	U10	C48-C49-C51-C52
46	1q	201	PC1	C37-C38-C39-C3A
50	1H	701	U10	C4-C3-O3-C3M
46	1B	202	PC1	C1-O11-P-O13
46	1d	201	PC1	C11-O13-P-O11
51	1O	403	CDL	CA2-OA2-PA1-OA5
46	1d	201	PC1	C35-C36-C37-C38
50	1H	701	U10	C14-C16-C17-C18
46	1q	201	PC1	C3A-C3B-C3C-C3D
53	1Y	201	3PE	C31-C32-C33-C34
58	1n	201	EHZ	C1-C2-C3-C4
58	1n	201	EHZ	O3-C12-C13-C14
46	1q	201	PC1	C35-C36-C37-C38
58	1n	201	EHZ	C5-C6-C7-O1
58	1n	201	EHZ	C18-C17-C20-O6

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Mol	Chain	Res	Type	Atoms
46	1L	702	PC1	C33-C34-C35-C36
51	1O	403	CDL	C56-C57-C58-C59
58	1n	201	EHZ	C5-C6-C7-C8
46	1M	501	PC1	O11-C1-C2-C3
53	1Y	201	3PE	C32-C33-C34-C35
46	1d	201	PC1	C2-C1-O11-P
48	1F	501	FMN	C4'-C5'-O5'-P
51	1O	403	CDL	CA4-CA3-OA5-PA1
46	1q	201	PC1	C31-C32-C33-C34
46	1B	202	PC1	C1-C2-C3-O31
53	1Y	201	3PE	C1-O11-P-O13
56	1P	501	NDP	C2D-C1D-N1N-C6N
46	1L	702	PC1	C27-C28-C29-C2A
50	1H	701	U10	C2-C3-O3-C3M
53	1Y	201	3PE	O21-C2-C3-O31
46	1q	201	PC1	C39-C3A-C3B-C3C
51	1H	702	CDL	CA4-CA3-OA5-PA1
53	1M	502	3PE	O31-C31-C32-C33
53	1M	502	3PE	C34-C35-C36-C37
51	1O	403	CDL	CB7-C71-C72-C73
51	1O	403	CDL	C1-CA2-OA2-PA1
51	1a	101	CDL	C12-C13-C14-C15
46	1B	202	PC1	C11-O13-P-O11
46	1f	101	PC1	C11-O13-P-O11
46	1q	201	PC1	C11-O13-P-O11
46	1B	202	PC1	C1-O11-P-O14
51	1H	702	CDL	CA2-OA2-PA1-OA4
51	1O	403	CDL	CA2-OA2-PA1-OA3
46	1B	202	PC1	C12-C11-O13-P
46	1L	702	PC1	C12-C11-O13-P
46	1q	201	PC1	C12-C11-O13-P
53	1Y	201	3PE	C12-C11-O13-P
46	1B	202	PC1	C31-C32-C33-C34
56	1P	501	NDP	C2D-C1D-N1N-C2N
46	1L	702	PC1	O13-C11-C12-N
46	1f	101	PC1	O13-C11-C12-N
46	1B	202	PC1	O21-C2-C3-O31
56	1P	501	NDP	O4D-C1D-N1N-C6N
58	1n	201	EHZ	C19-C17-C20-O6
50	1H	701	U10	C5-C6-C7-C8
58	1n	201	EHZ	N1-C12-C13-C14
53	1Y	201	3PE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
46	1L	702	PC1	C11-O13-P-O11
46	1L	702	PC1	C1-O11-P-O13
46	1M	501	PC1	C1-O11-P-O13
51	1O	403	CDL	CB2-OB2-PB2-OB5
51	1a	101	CDL	CA3-OA5-PA1-OA2
51	1a	101	CDL	CB2-OB2-PB2-OB5
53	1M	502	3PE	C1-O11-P-O13
53	1M	502	3PE	C11-O13-P-O11
46	1B	202	PC1	O22-C21-C22-C23
51	1O	403	CDL	C55-C56-C57-C58
52	1L	701	MYR	C4-C5-C6-C7
50	1H	701	U10	C30-C29-C31-C32
53	1Y	201	3PE	C2-C1-O11-P
58	1W	201	EHZ	N2-C15-C16-C17
50	1H	701	U10	C40-C39-C41-C42
46	1B	202	PC1	O21-C21-C22-C23
50	1H	701	U10	C5-C4-O4-C4M
58	1W	201	EHZ	C11-C10-S1-C9
51	1O	403	CDL	OB6-CB4-CB6-OB8
50	1H	701	U10	C28-C29-C31-C32
46	1d	201	PC1	C39-C3A-C3B-C3C
46	1f	101	PC1	C11-C12-N-C15
50	1H	701	U10	C38-C39-C41-C42
56	1P	501	NDP	O4D-C1D-N1N-C2N
46	1q	201	PC1	C33-C34-C35-C36
46	1L	702	PC1	C24-C25-C26-C27
53	1Y	201	3PE	C1-C2-C3-O31
51	1H	702	CDL	OB5-CB3-CB4-OB6
50	1H	701	U10	C41-C42-C43-C44
52	1L	701	MYR	C11-C10-C9-C8
46	1f	101	PC1	C11-C12-N-C14
46	1M	501	PC1	C31-C32-C33-C34
58	1n	201	EHZ	C4-C5-C6-C7
50	1H	701	U10	C51-C52-C53-C54
51	1O	403	CDL	C72-C71-CB7-OB8
51	1O	403	CDL	C53-C54-C55-C56
51	1O	403	CDL	C12-C11-CA5-OA6
51	1O	403	CDL	CB3-CB4-CB6-OB8
46	1B	202	PC1	C1-O11-P-O12
51	1H	702	CDL	CA2-OA2-PA1-OA3
53	1M	502	3PE	C11-O13-P-O14
53	1Y	201	3PE	C11-O13-P-O14

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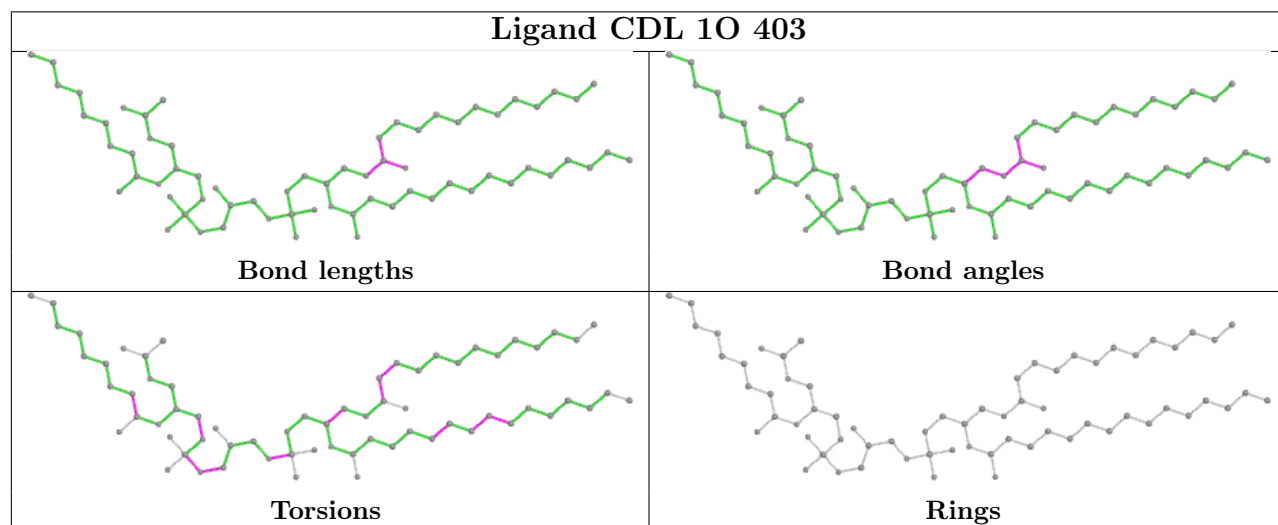
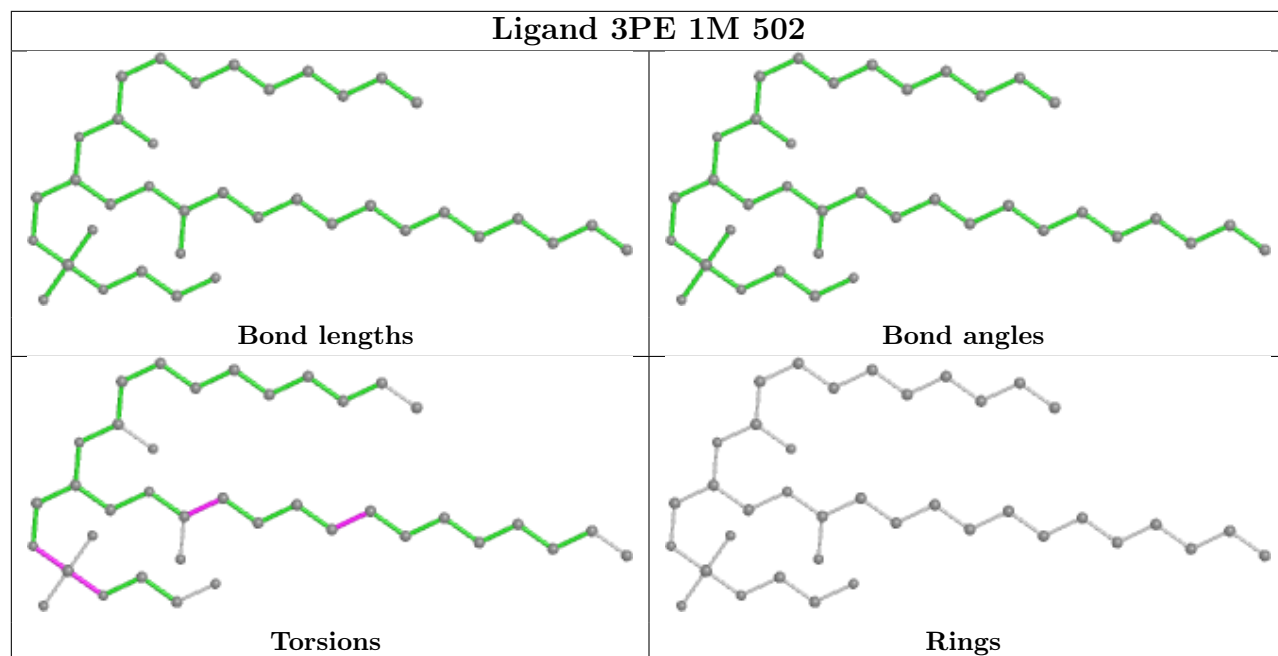
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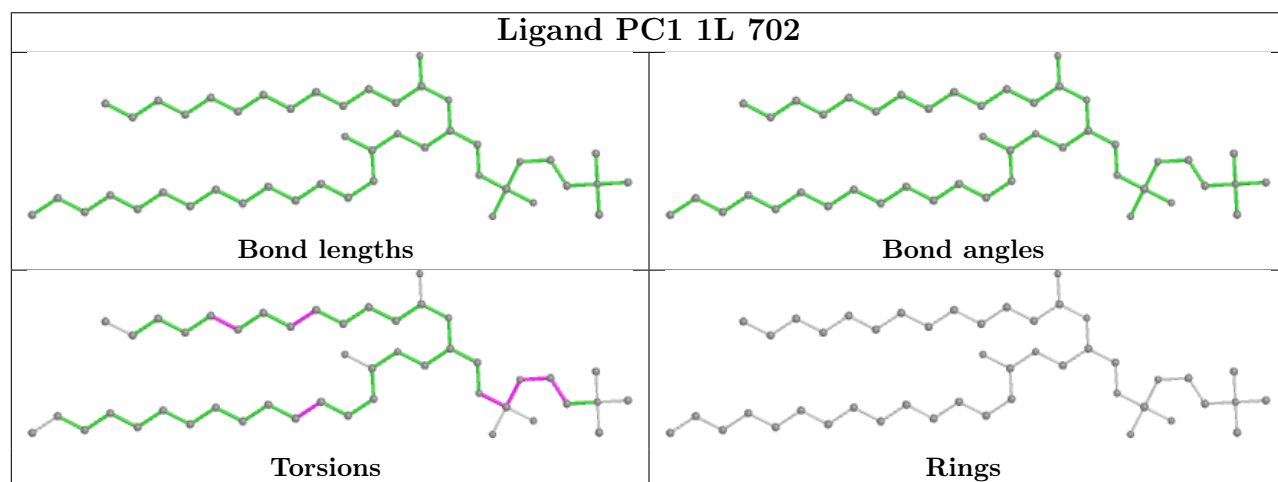
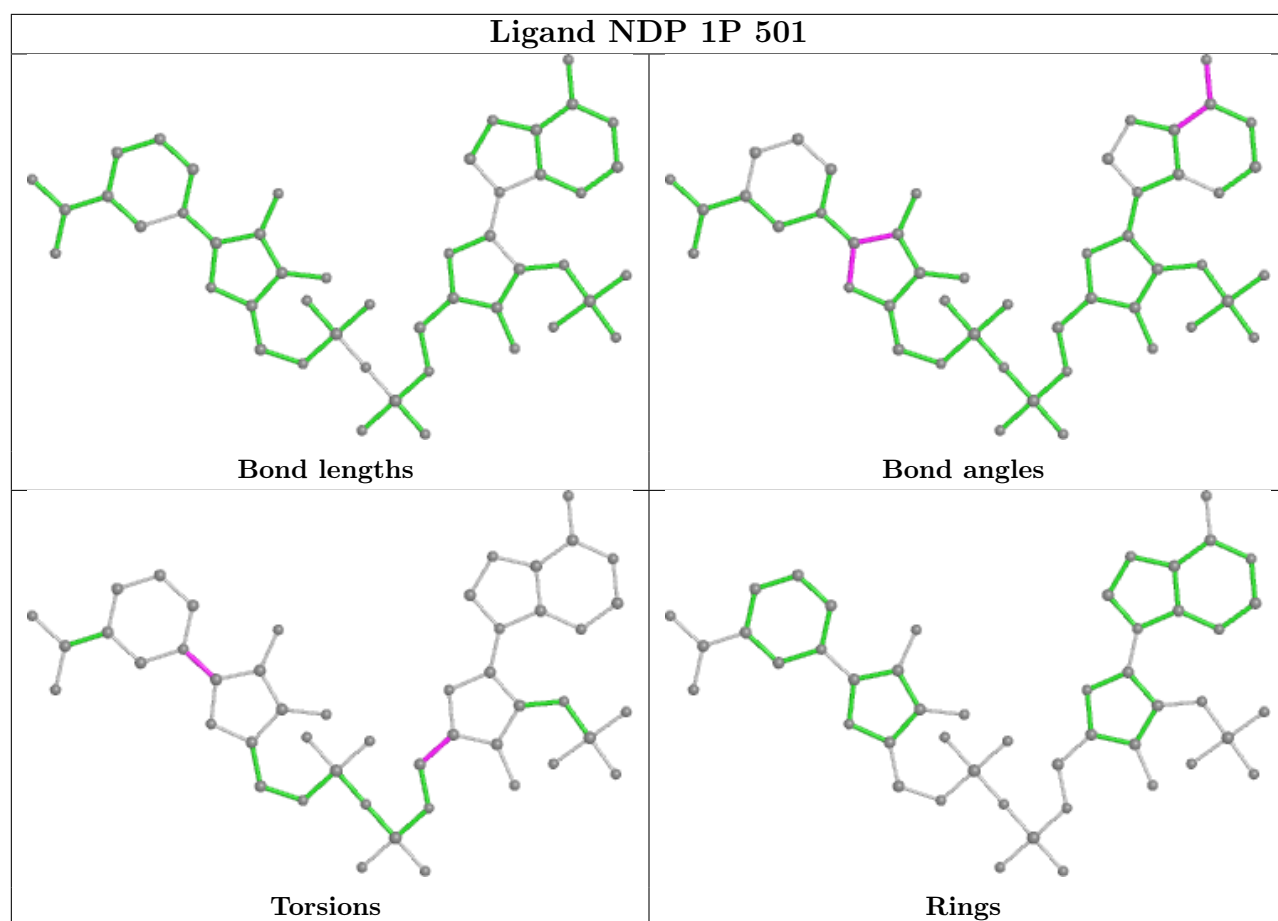
Mol	Chain	Res	Type	Atoms
56	1P	501	NDP	O4B-C4B-C5B-O5B
51	1O	403	CDL	C72-C71-CB7-OB9
50	1H	701	U10	C16-C17-C18-C19
58	1W	201	EHZ	O4-C15-C16-C17
51	1a	101	CDL	C12-C11-CA5-OA6
51	1H	702	CDL	C32-C31-CA7-OA8
46	1d	201	PC1	O31-C31-C32-C33
51	1a	101	CDL	C72-C71-CB7-OB8
53	1Y	201	3PE	O21-C21-C22-C23
51	1O	403	CDL	C12-C11-CA5-OA7
46	1q	201	PC1	O21-C21-C22-C23
46	1q	201	PC1	C23-C24-C25-C26
51	1a	101	CDL	C72-C71-CB7-OB9
46	1d	201	PC1	O32-C31-C32-C33

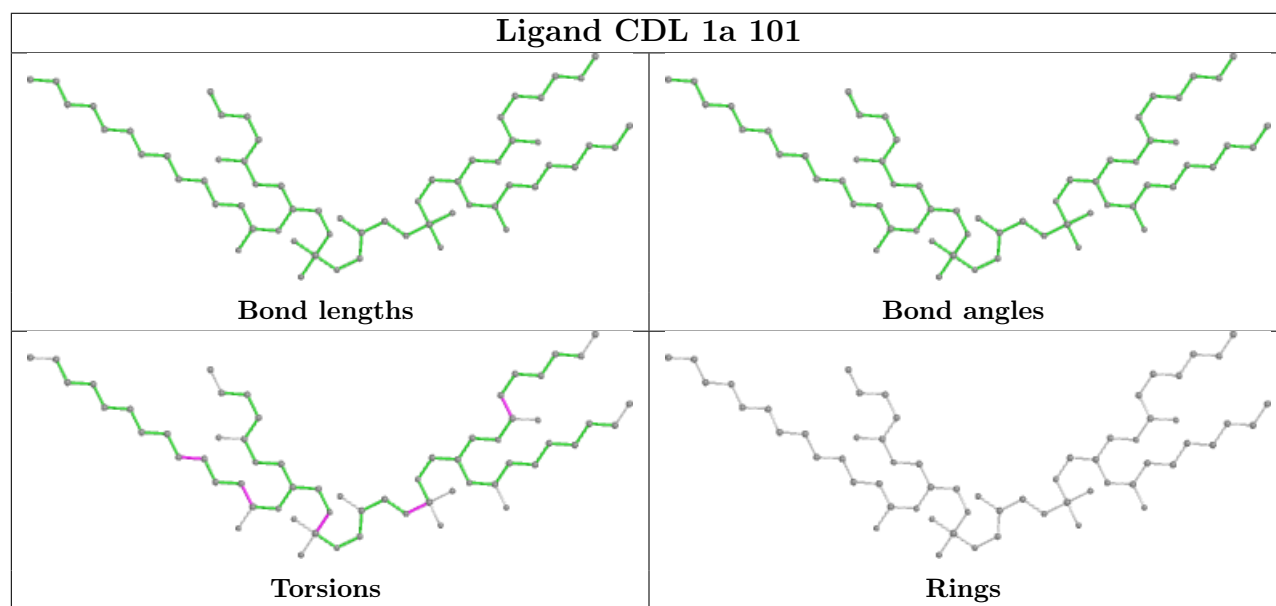
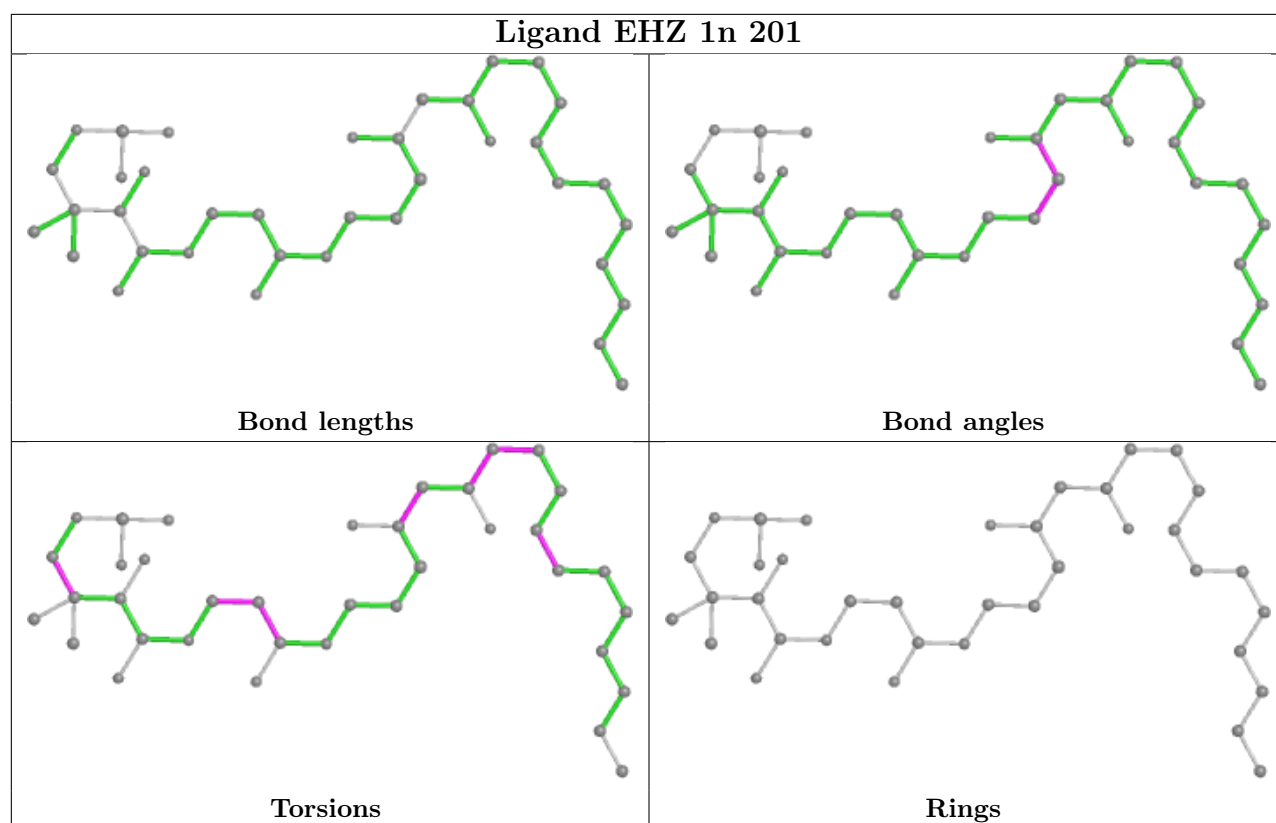
There are no ring outliers.

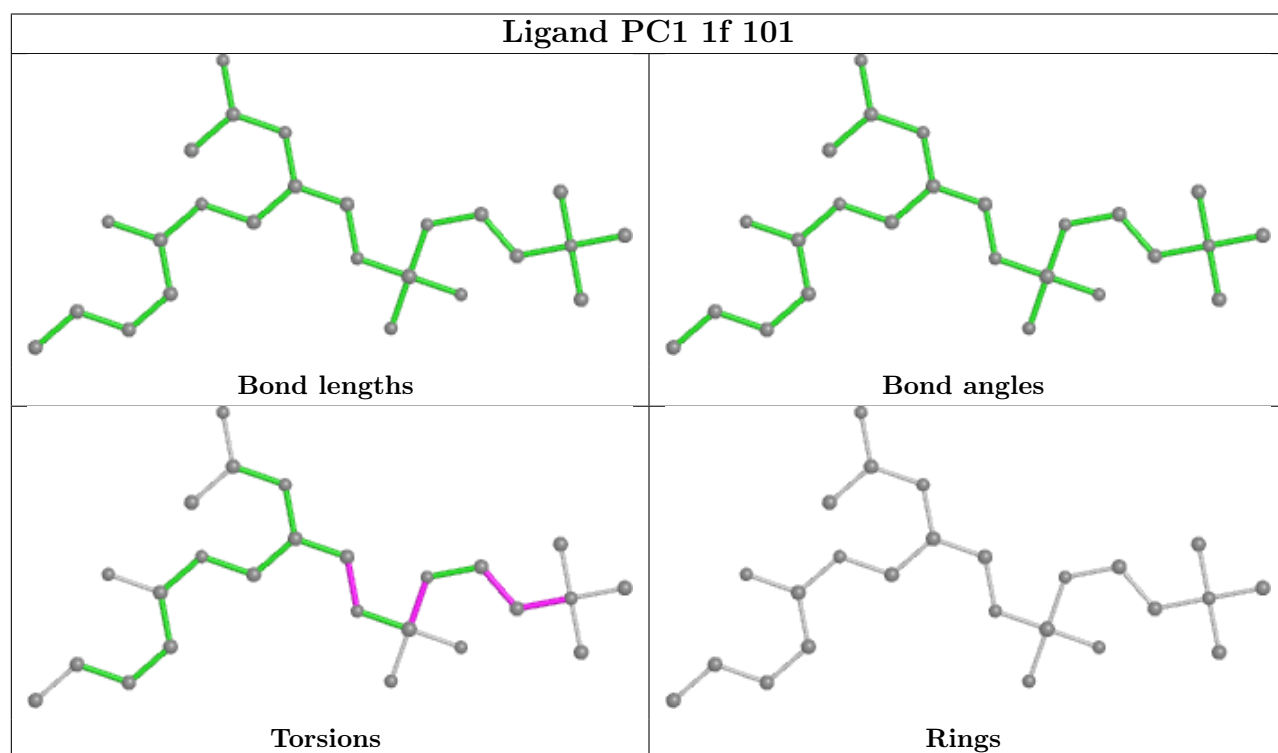
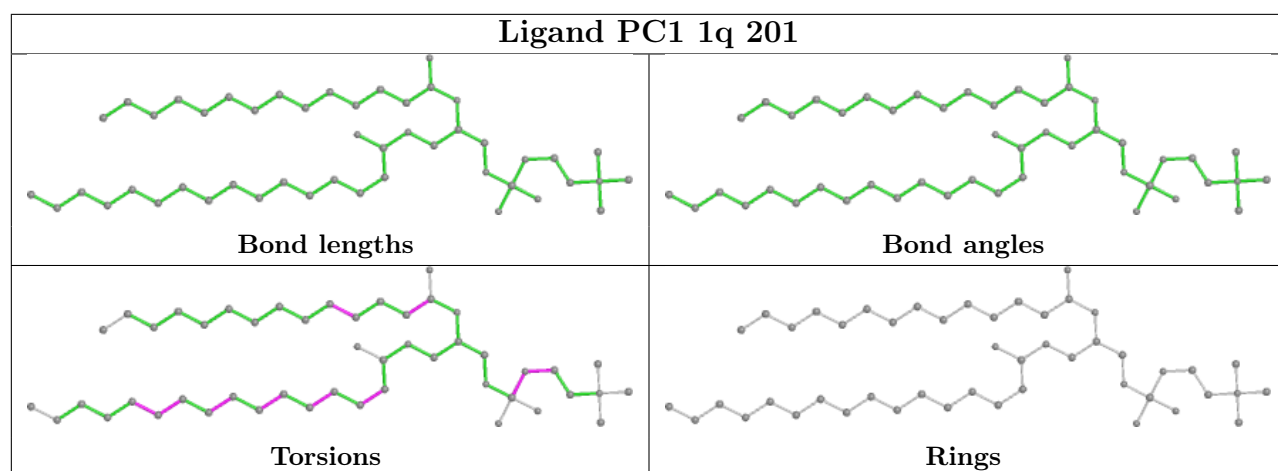
No monomer is involved in short contacts.

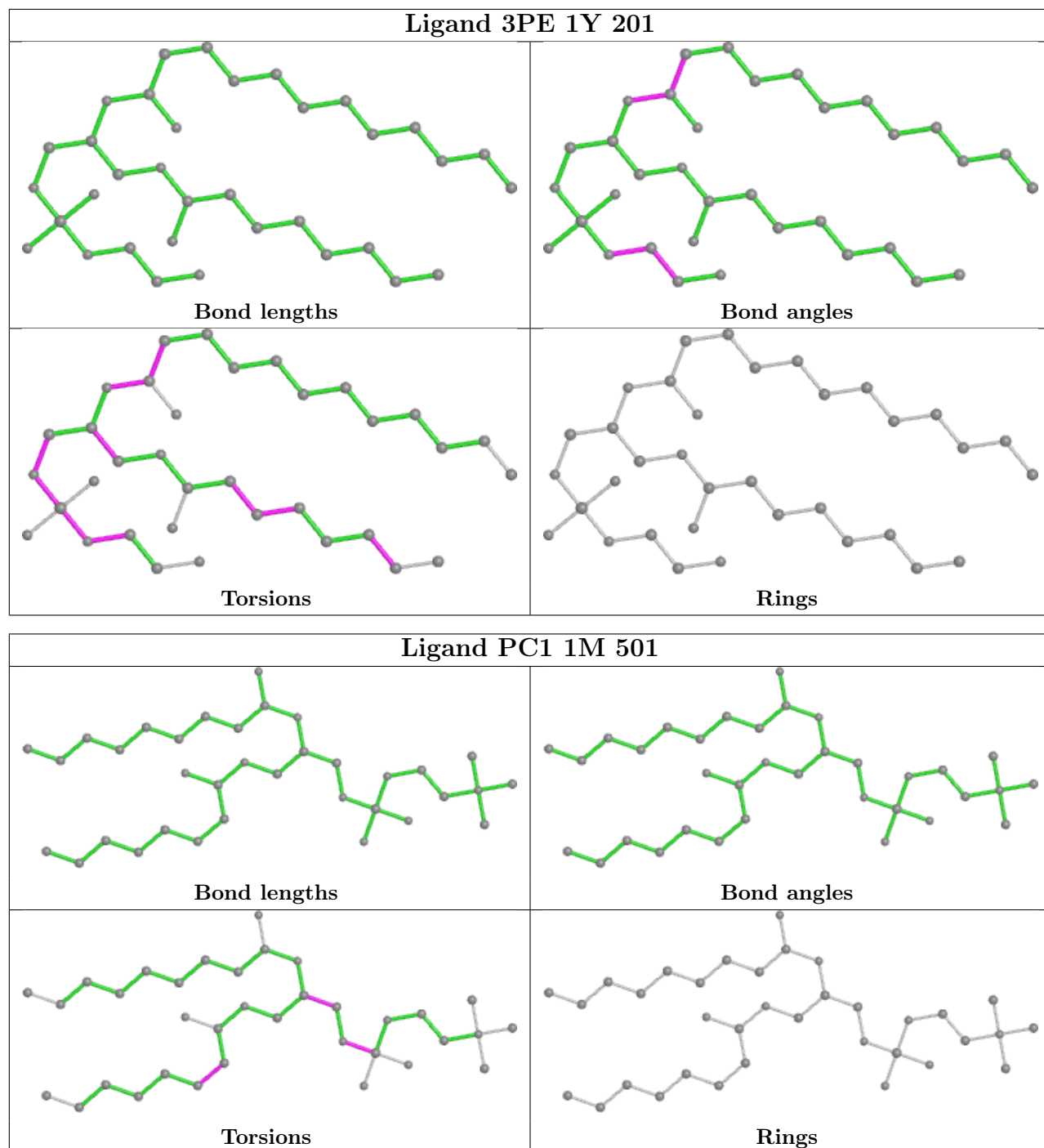
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



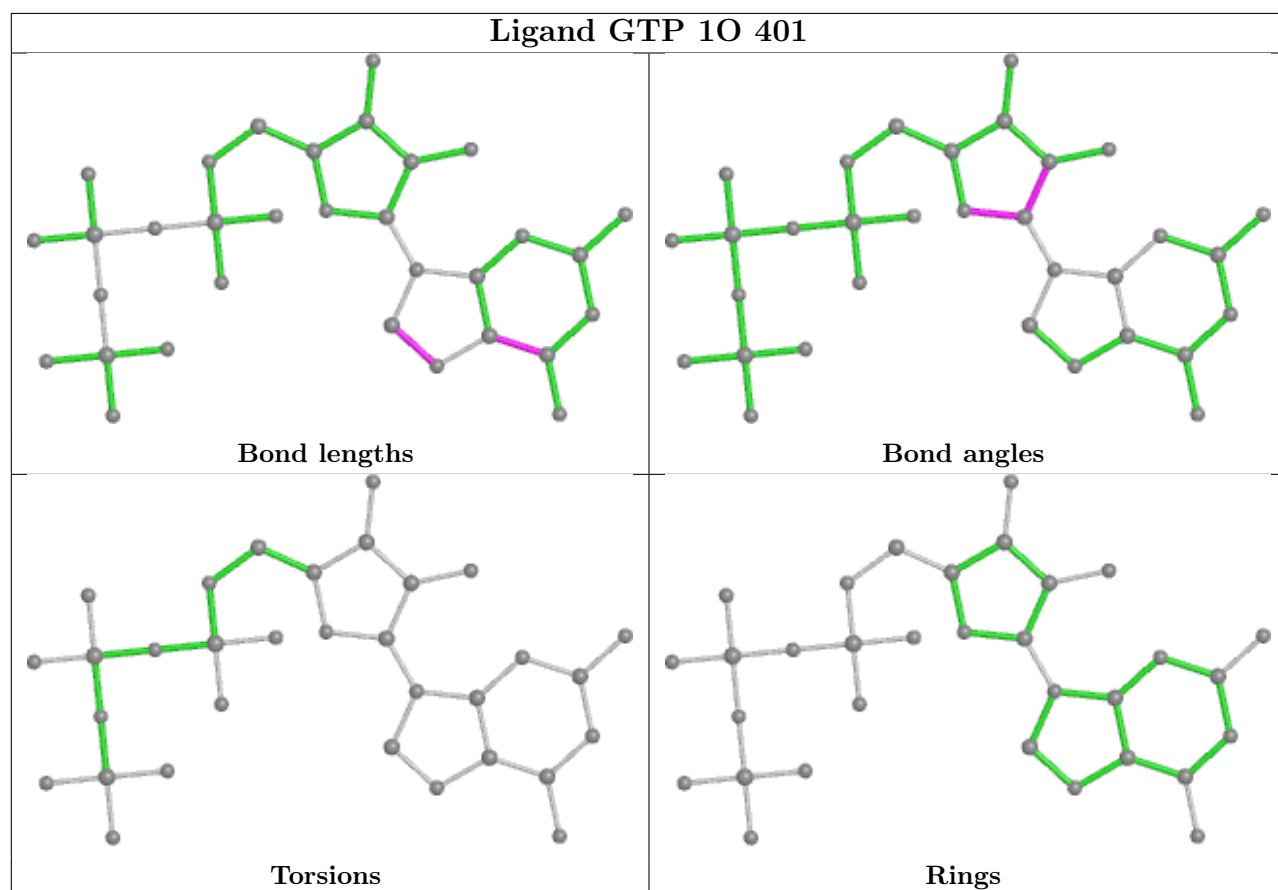
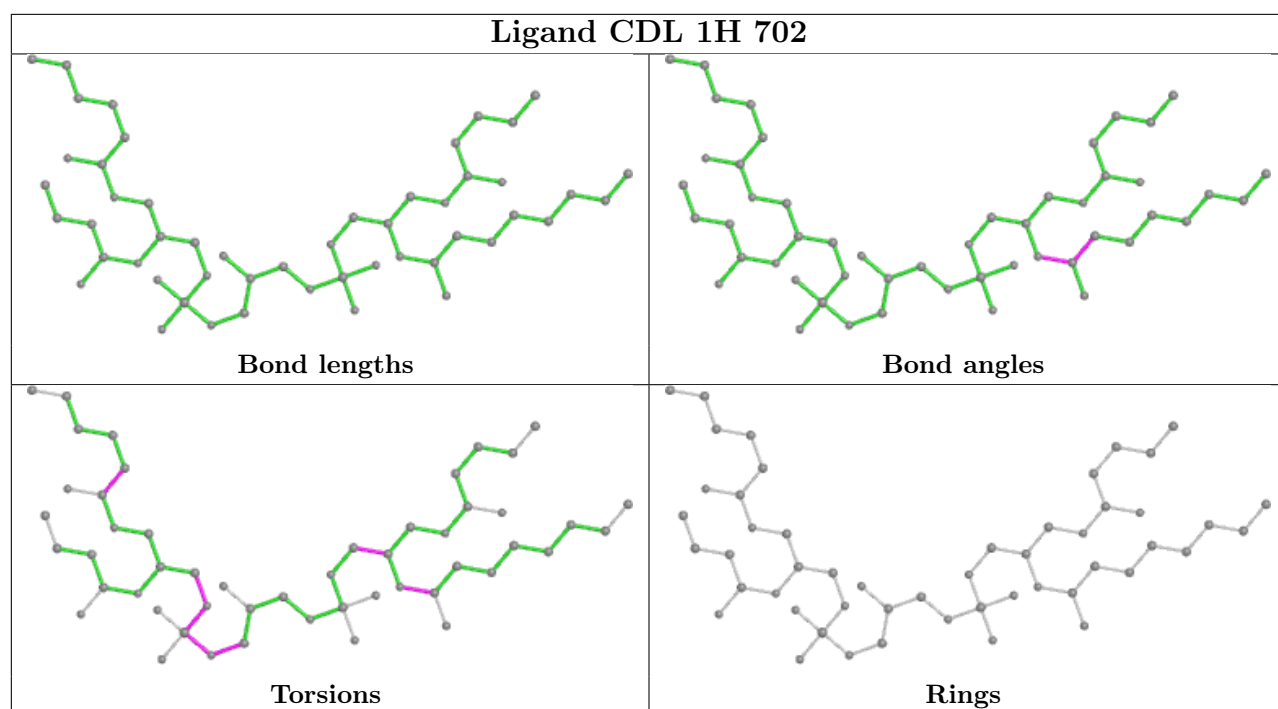


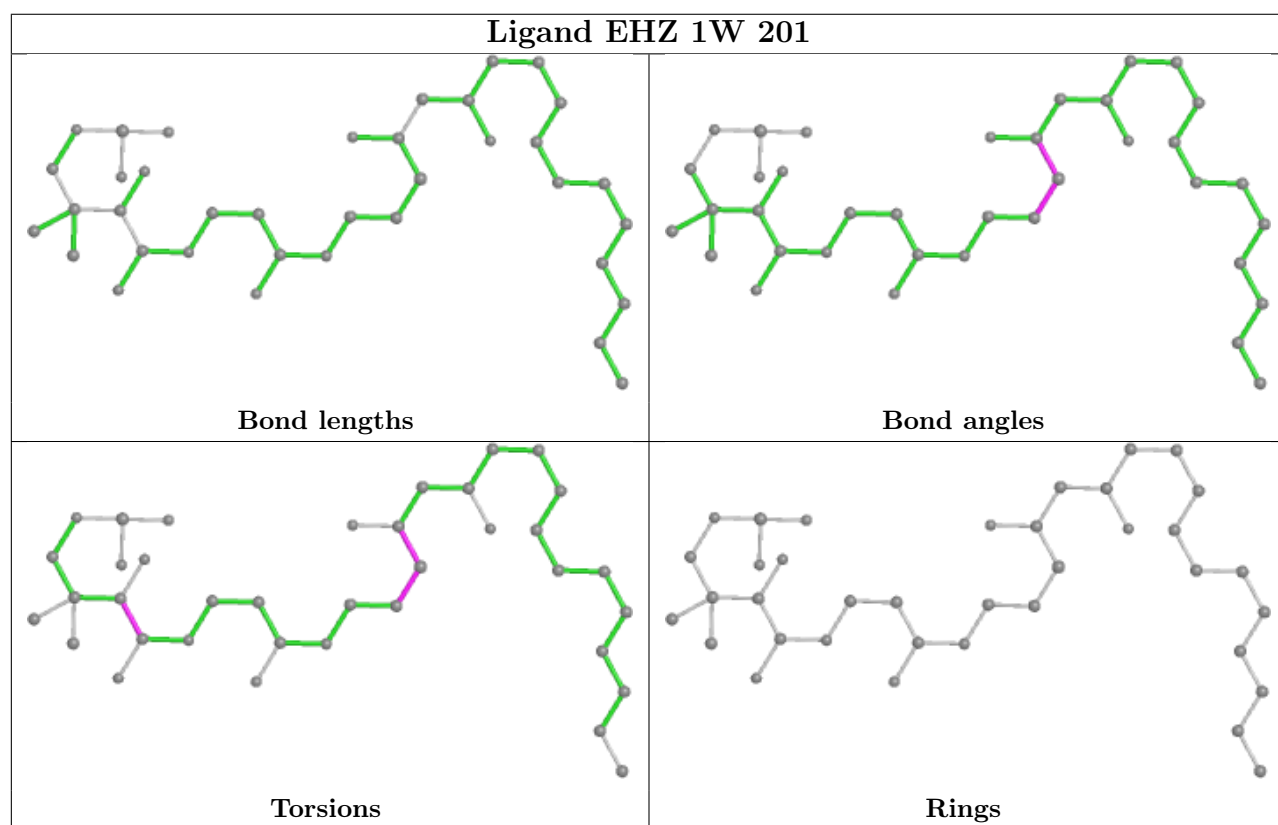
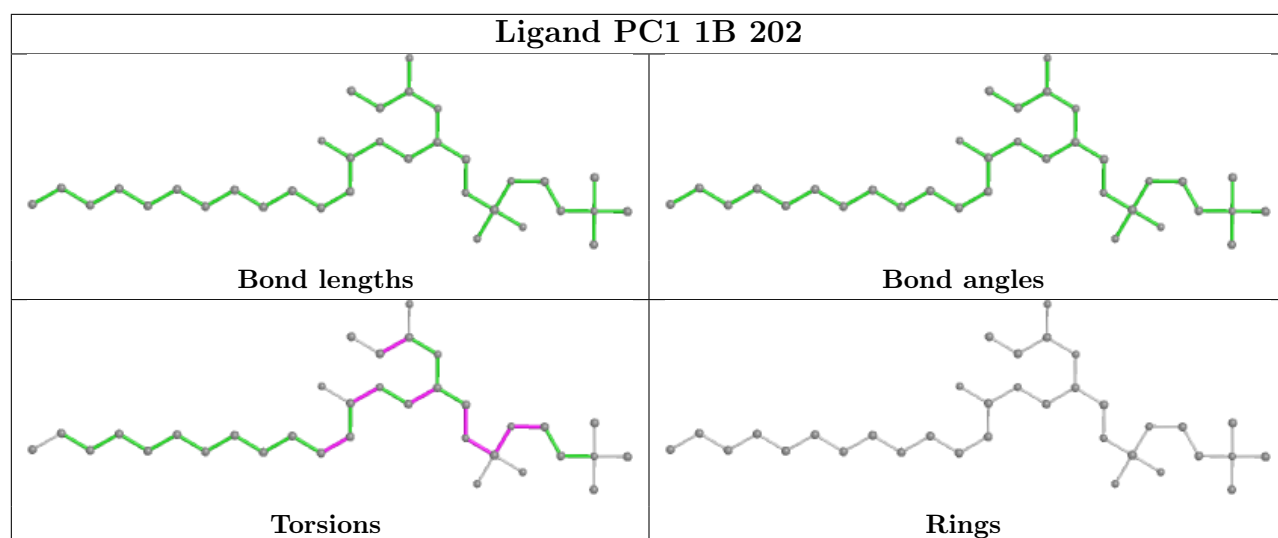


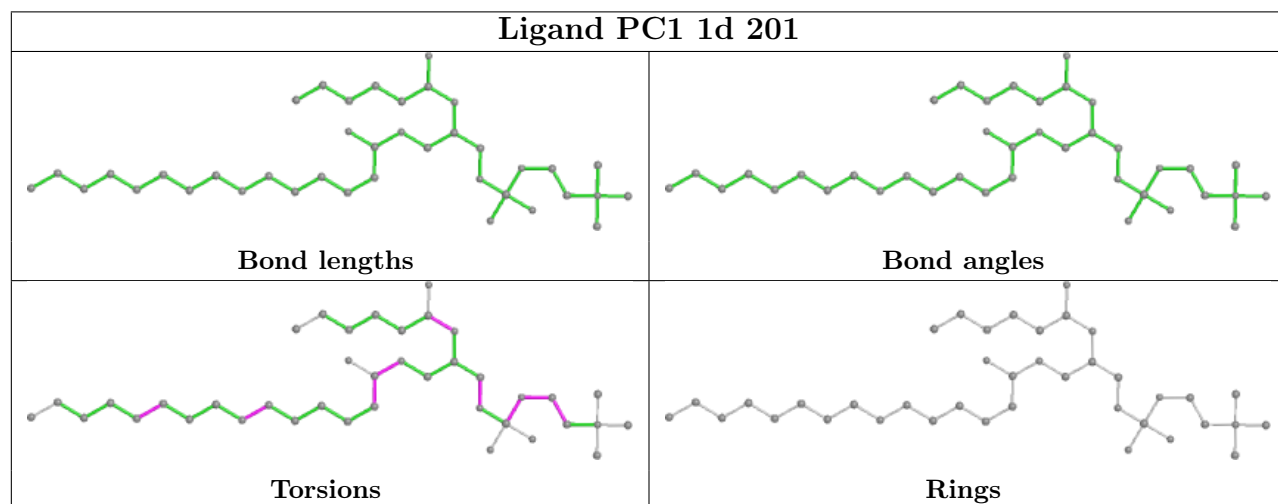
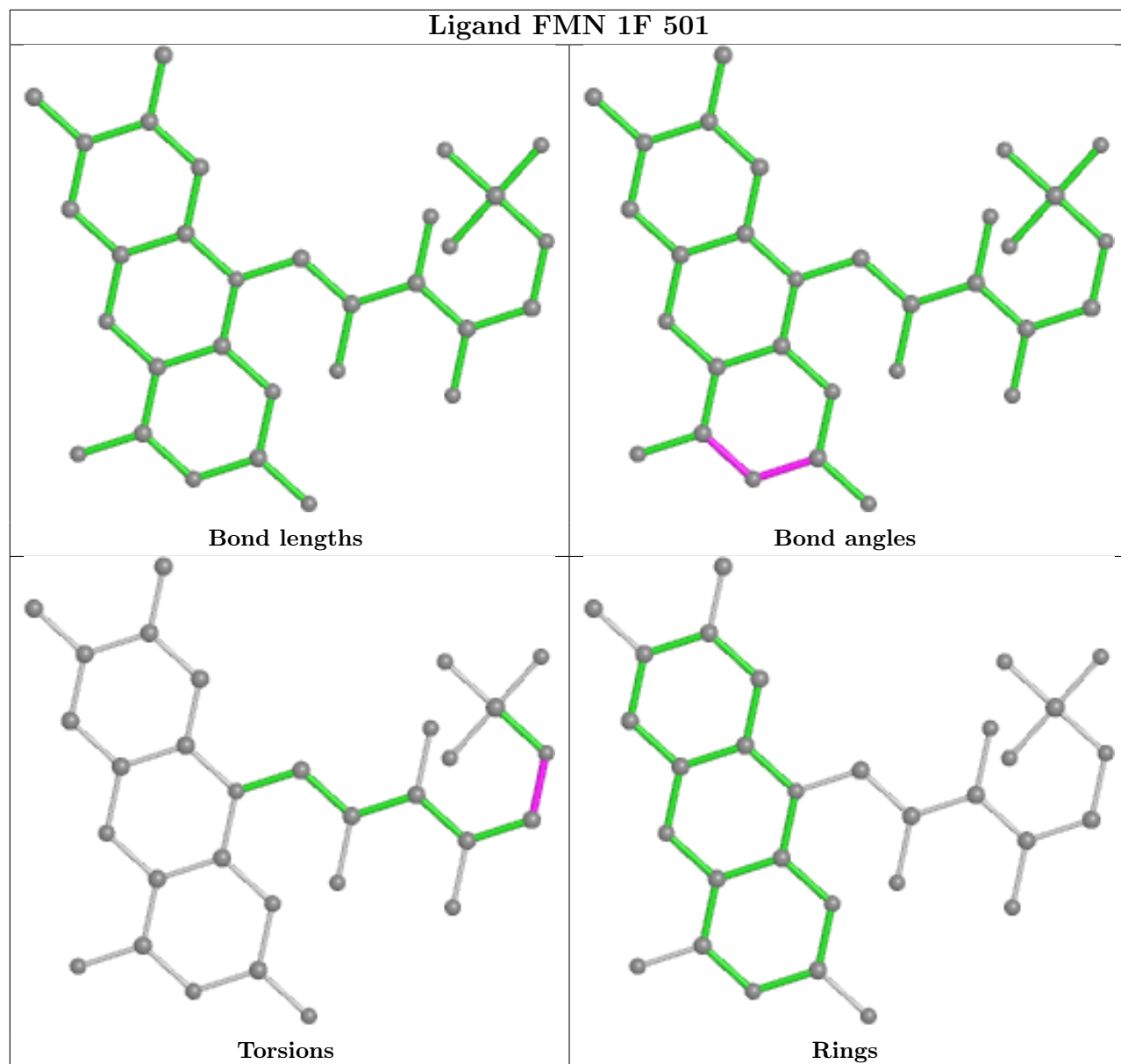


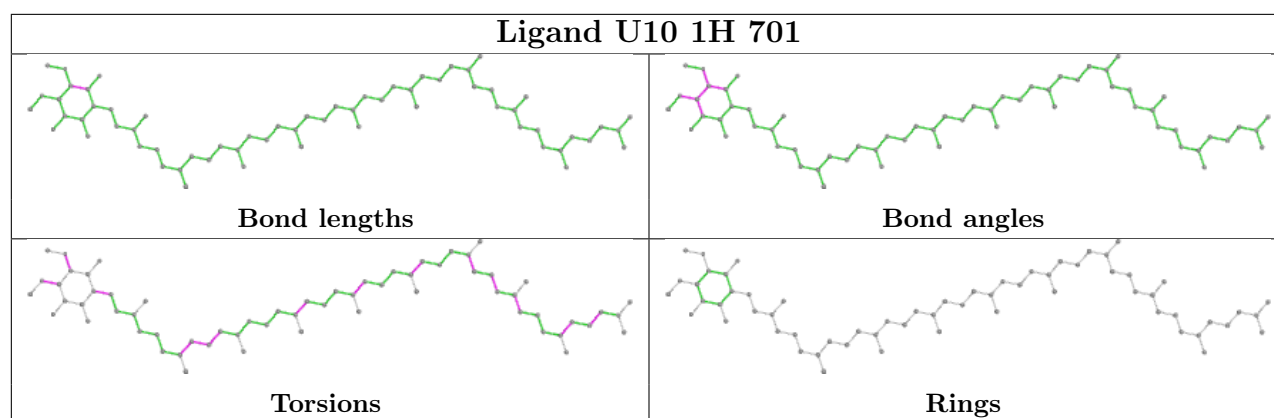












## 5.7 Other polymers [i](#)

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
43	1r	1
34	1i	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1r	1:ALA	C	2:SER	N	6.44
1	1i	1:SAC	C	2:GLY	N	3.63

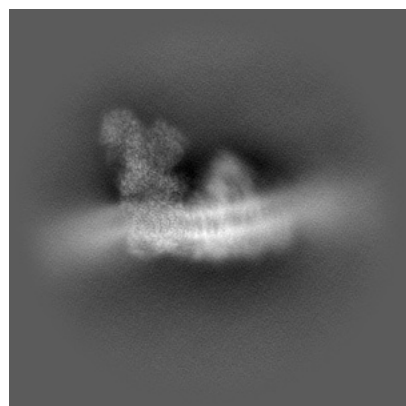
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42176. These allow visual inspection of the internal detail of the map and identification of artifacts.

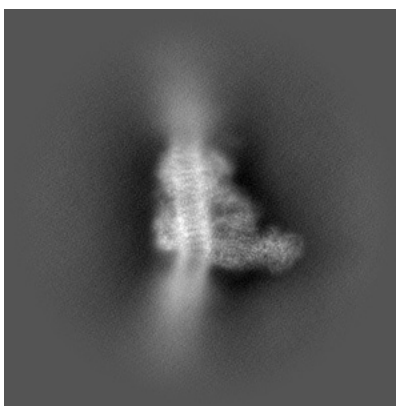
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

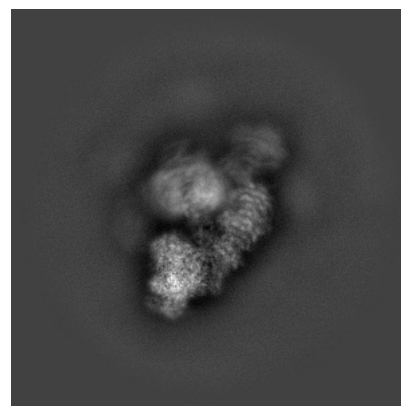
#### 6.1.1 Primary map



X

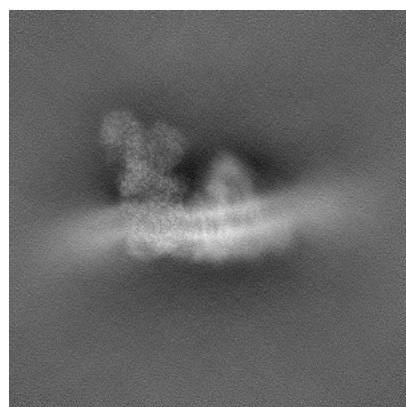


Y

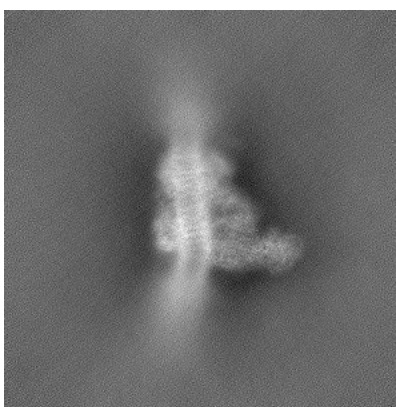


Z

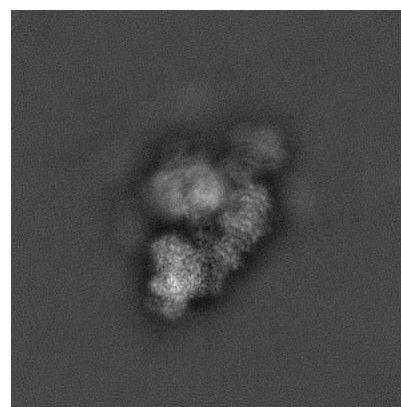
#### 6.1.2 Raw map



X



Y

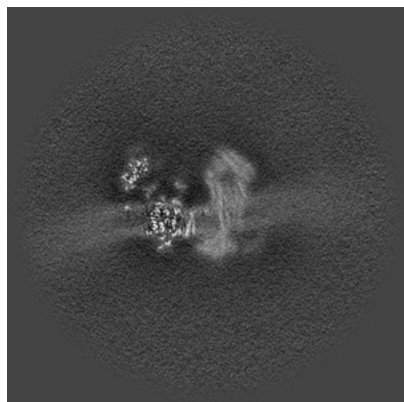


Z

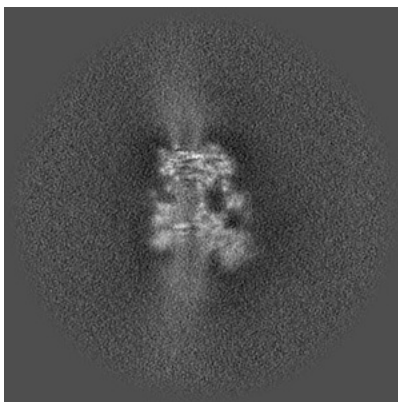
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

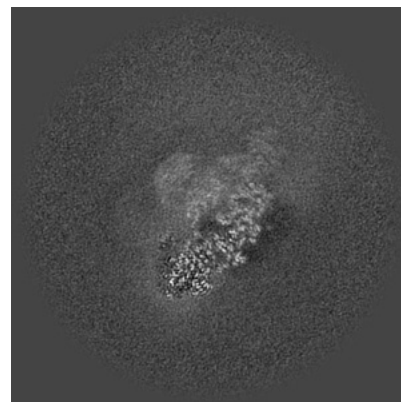
### 6.2.1 Primary map



X Index: 200

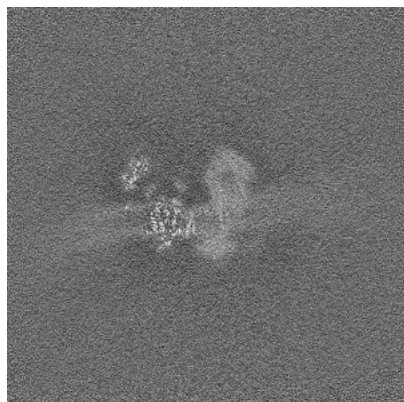


Y Index: 200

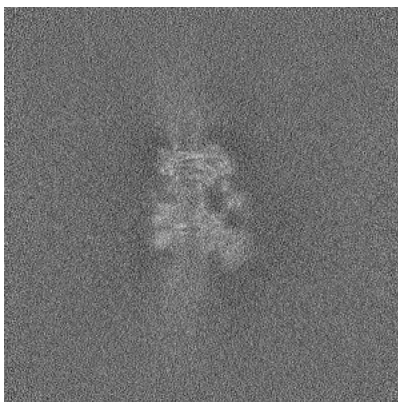


Z Index: 200

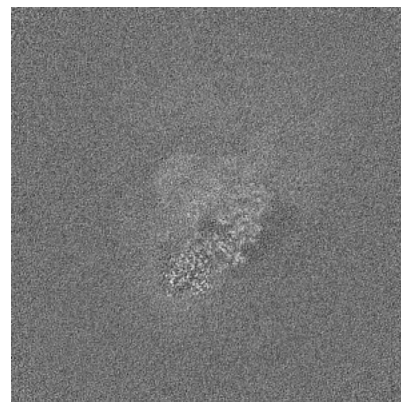
### 6.2.2 Raw map



X Index: 200



Y Index: 200



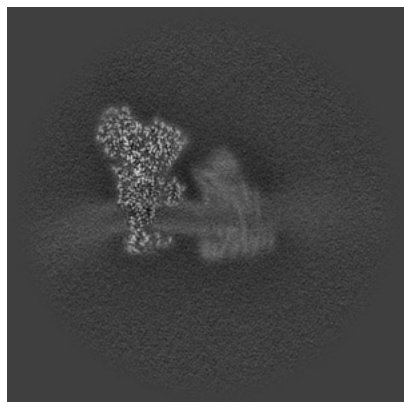
Z Index: 200

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

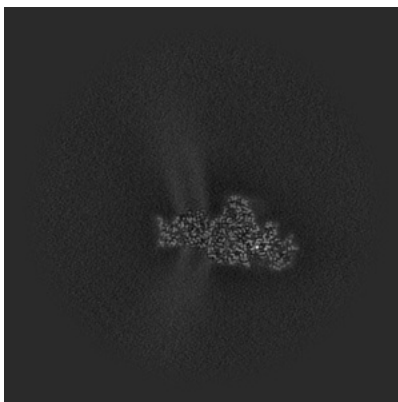


## 6.3 Largest variance slices [i](#)

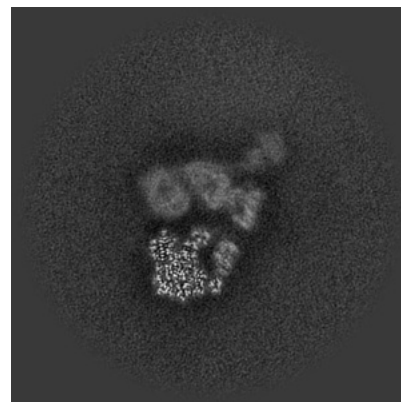
### 6.3.1 Primary map



X Index: 163

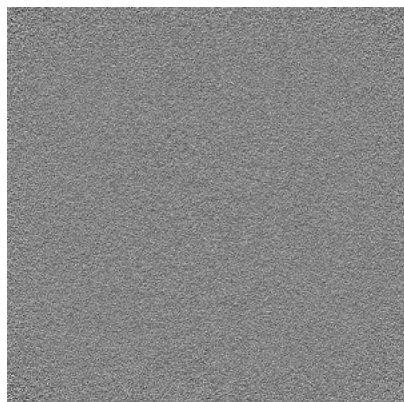


Y Index: 127

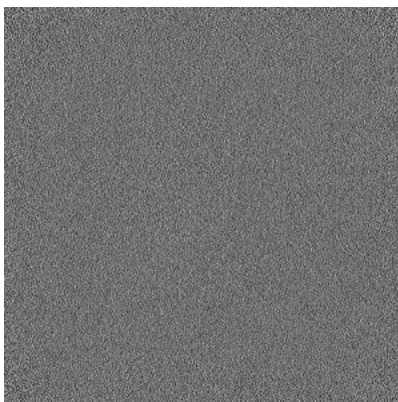


Z Index: 225

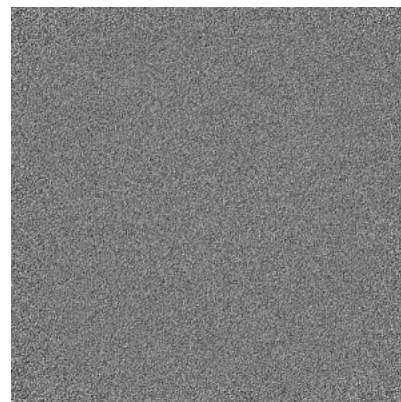
### 6.3.2 Raw map



X Index: 0



Y Index: 0

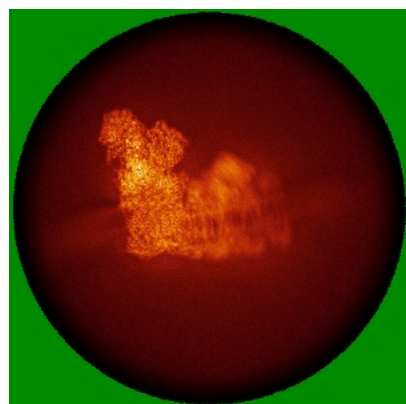


Z Index: 0

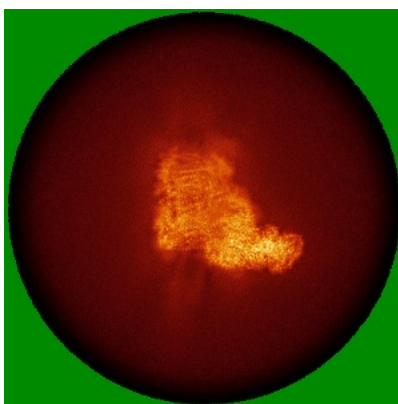
The images above show the largest variance slices of the map in three orthogonal directions.

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

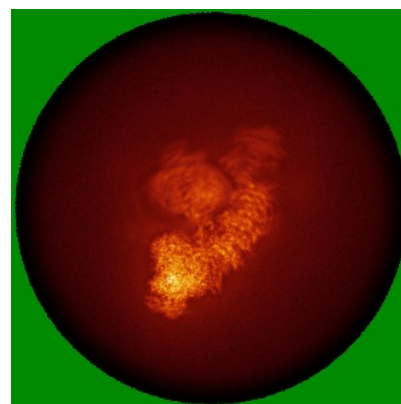
### 6.4.1 Primary map



X

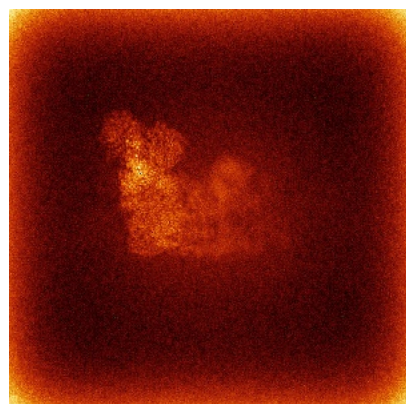


Y

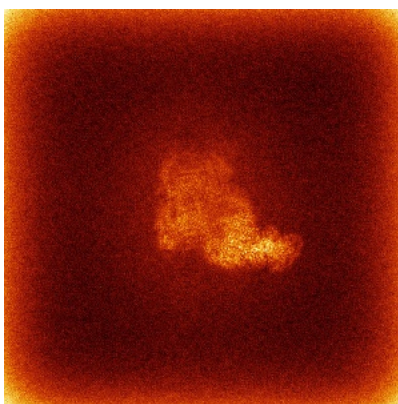


Z

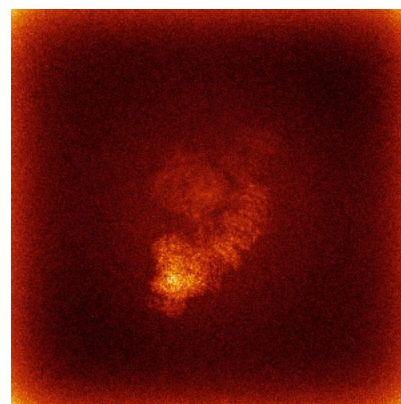
### 6.4.2 Raw map



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.



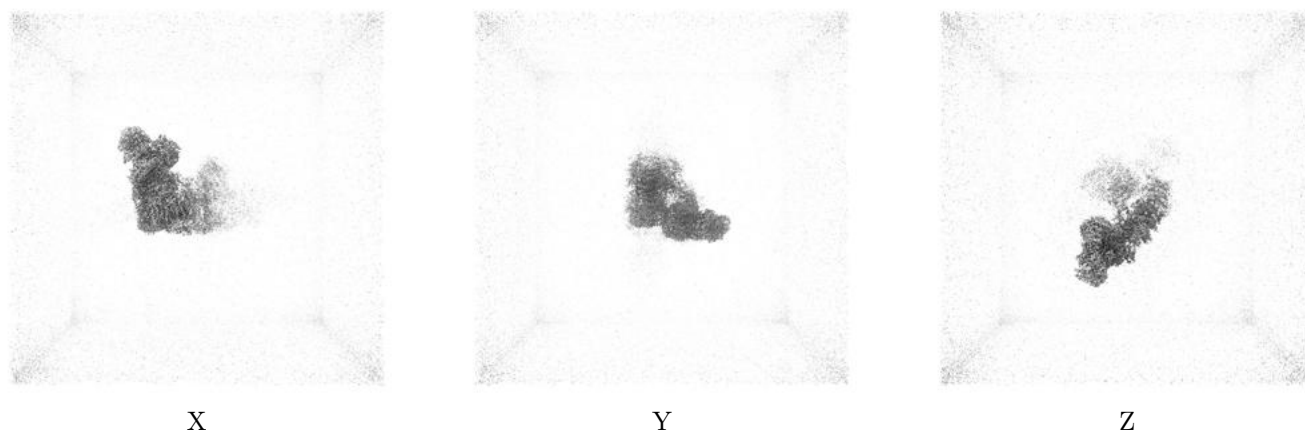
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

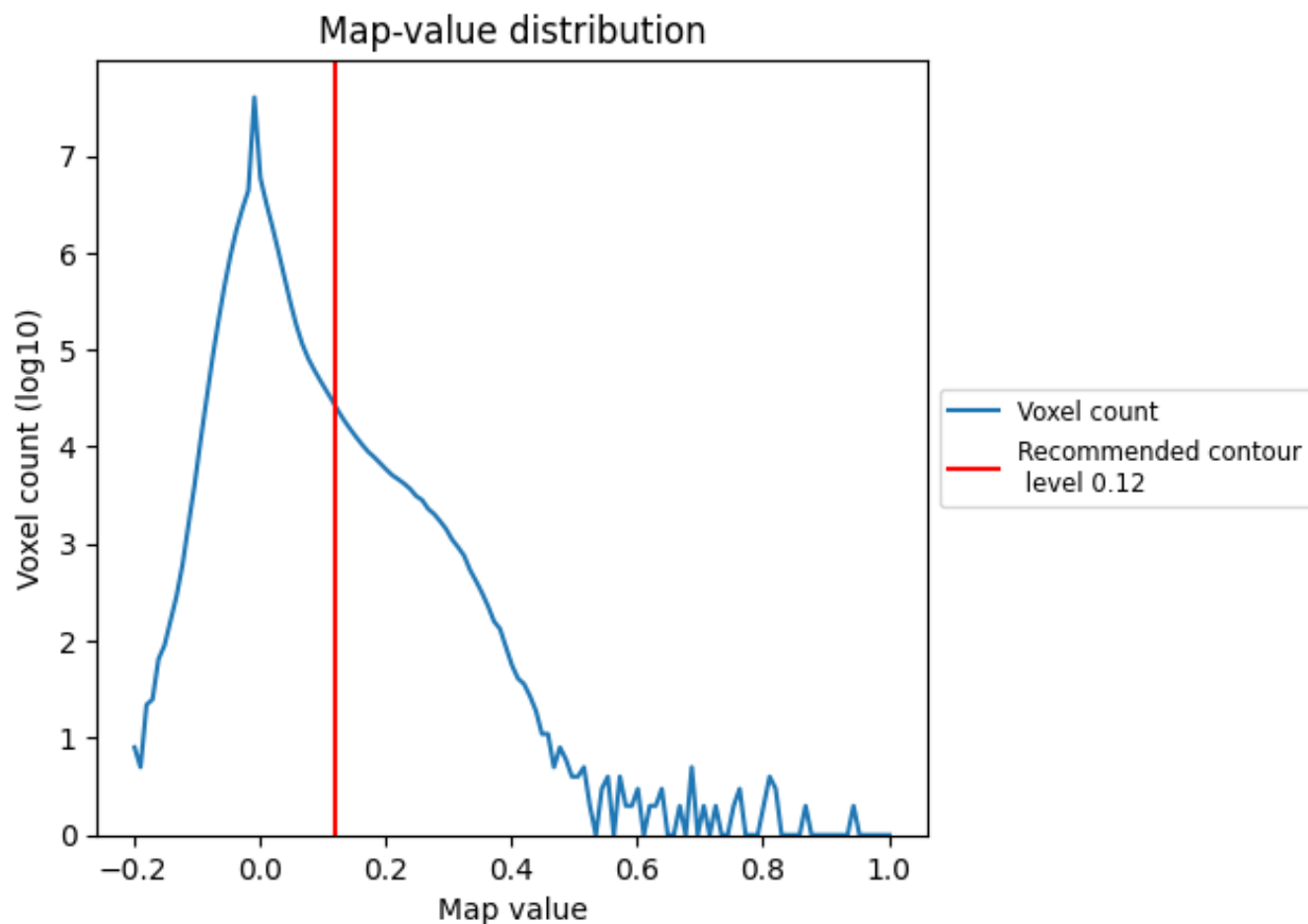
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

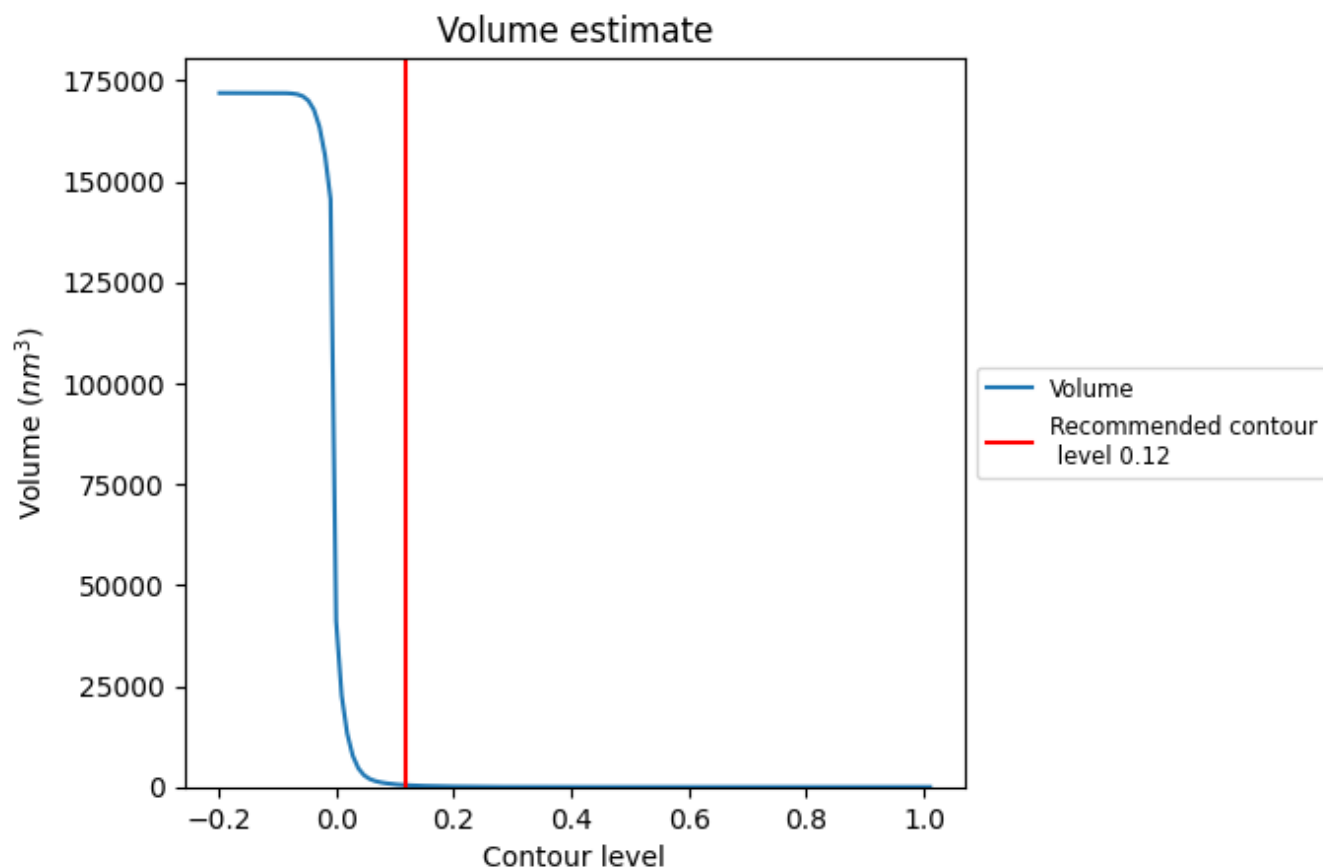
This section contains the results of statistical analysis of the map.

### 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.

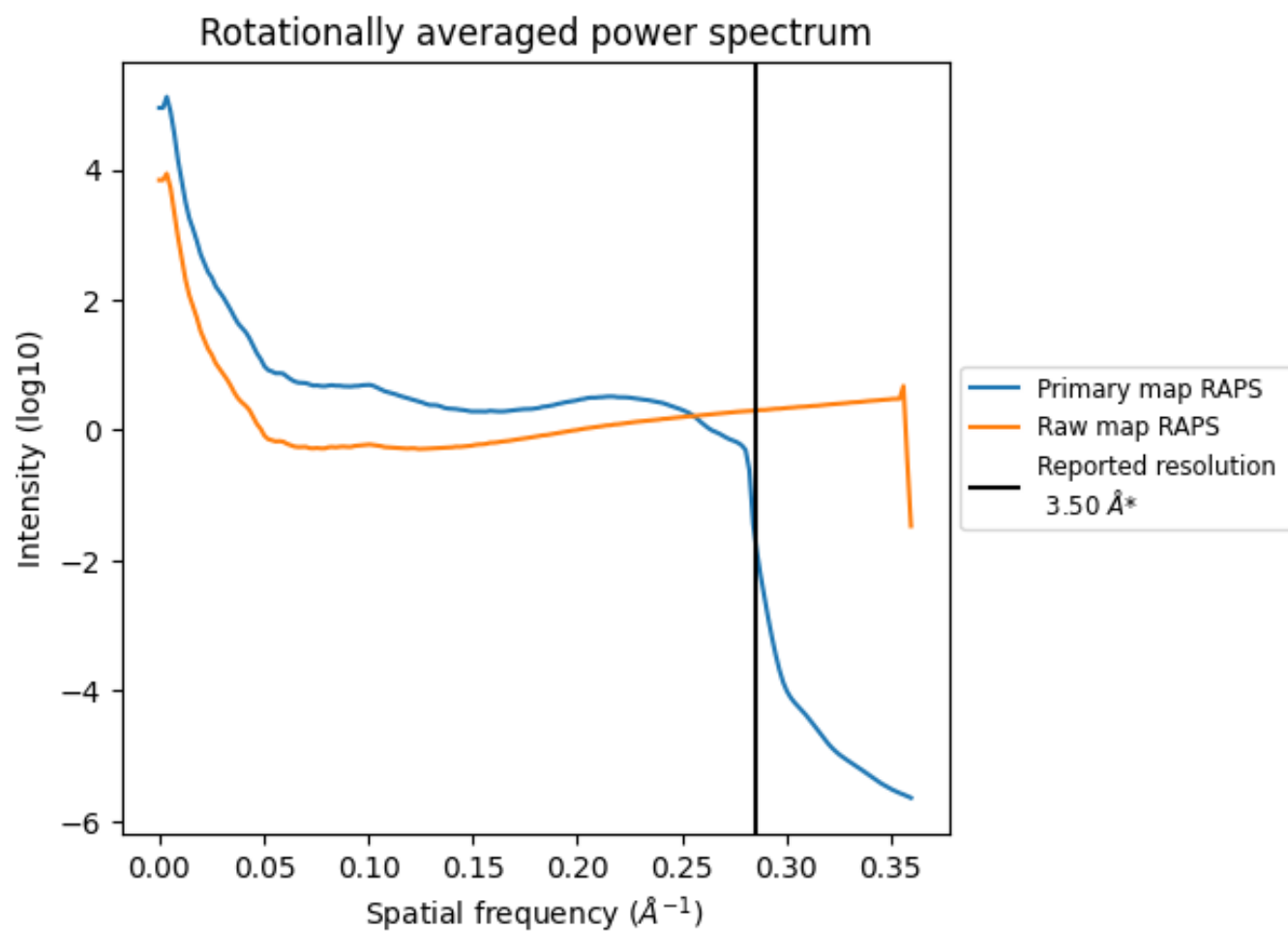
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 437  $\text{nm}^3$ ; this corresponds to an approximate mass of 394 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](#)

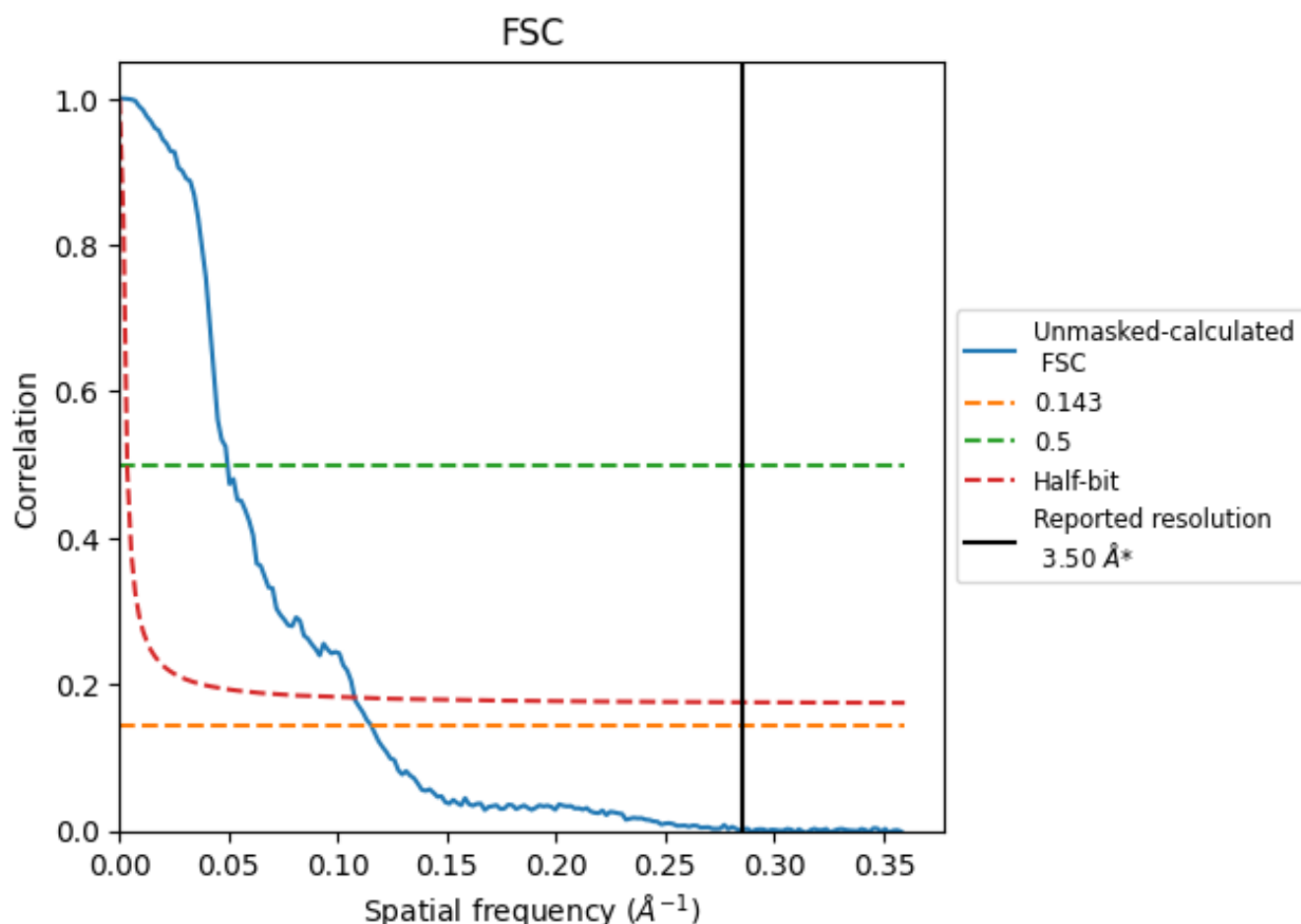


\*Reported resolution corresponds to spatial frequency of 0.286  $\text{\AA}^{-1}$

## 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 0.286  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

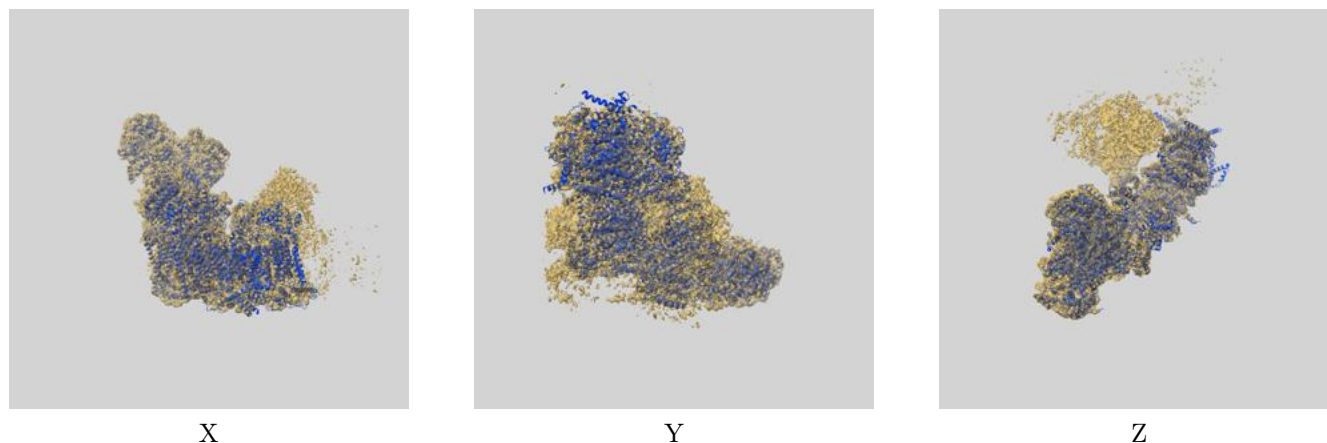
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.67	20.24	9.29

\*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 8.67 differs from the reported value 3.5 by more than 10 %

## 9 Map-model fit [i](#)

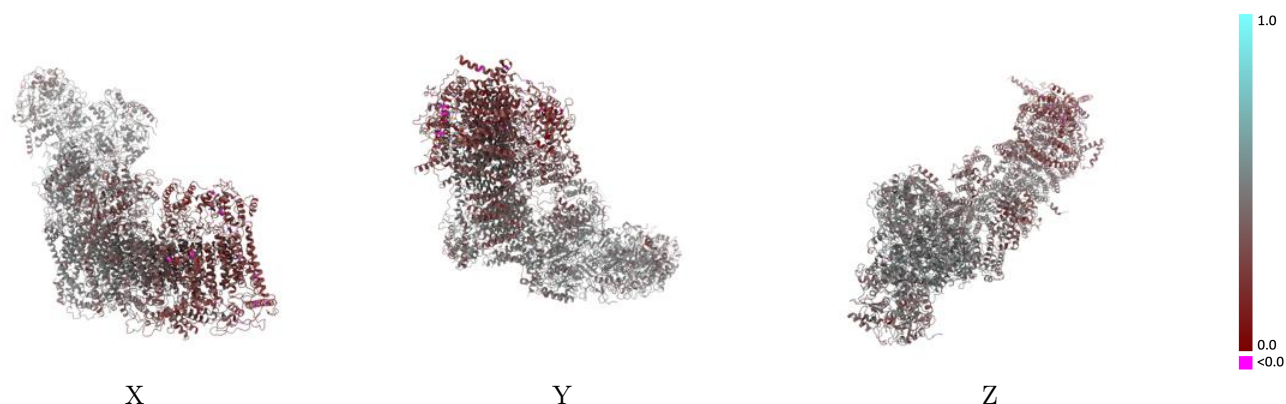
This section contains information regarding the fit between EMDB map EMD-42176 and PDB model 8UEZ. Per-residue inclusion information can be found in section 3 on page 21.

### 9.1 Map-model overlay [i](#)



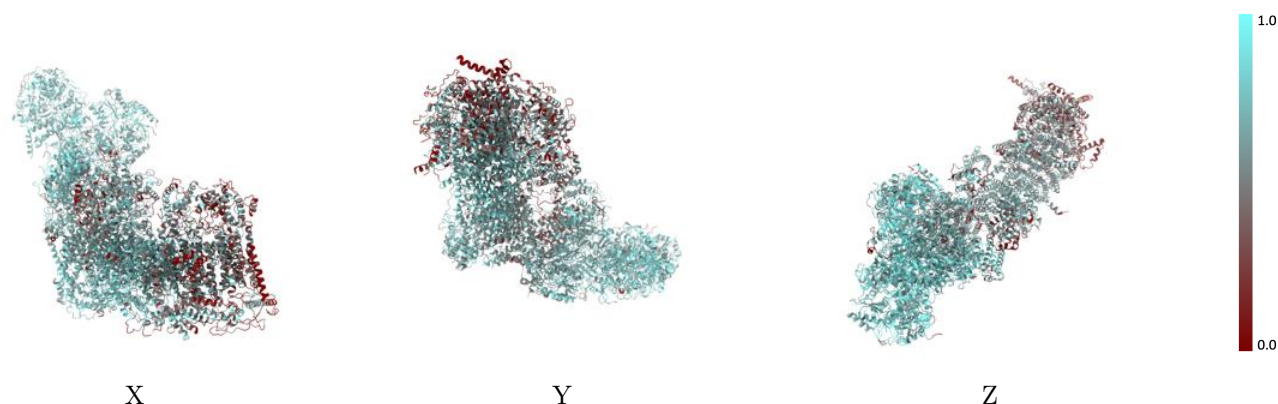
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



The images above show the model with each residue coloured according 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.

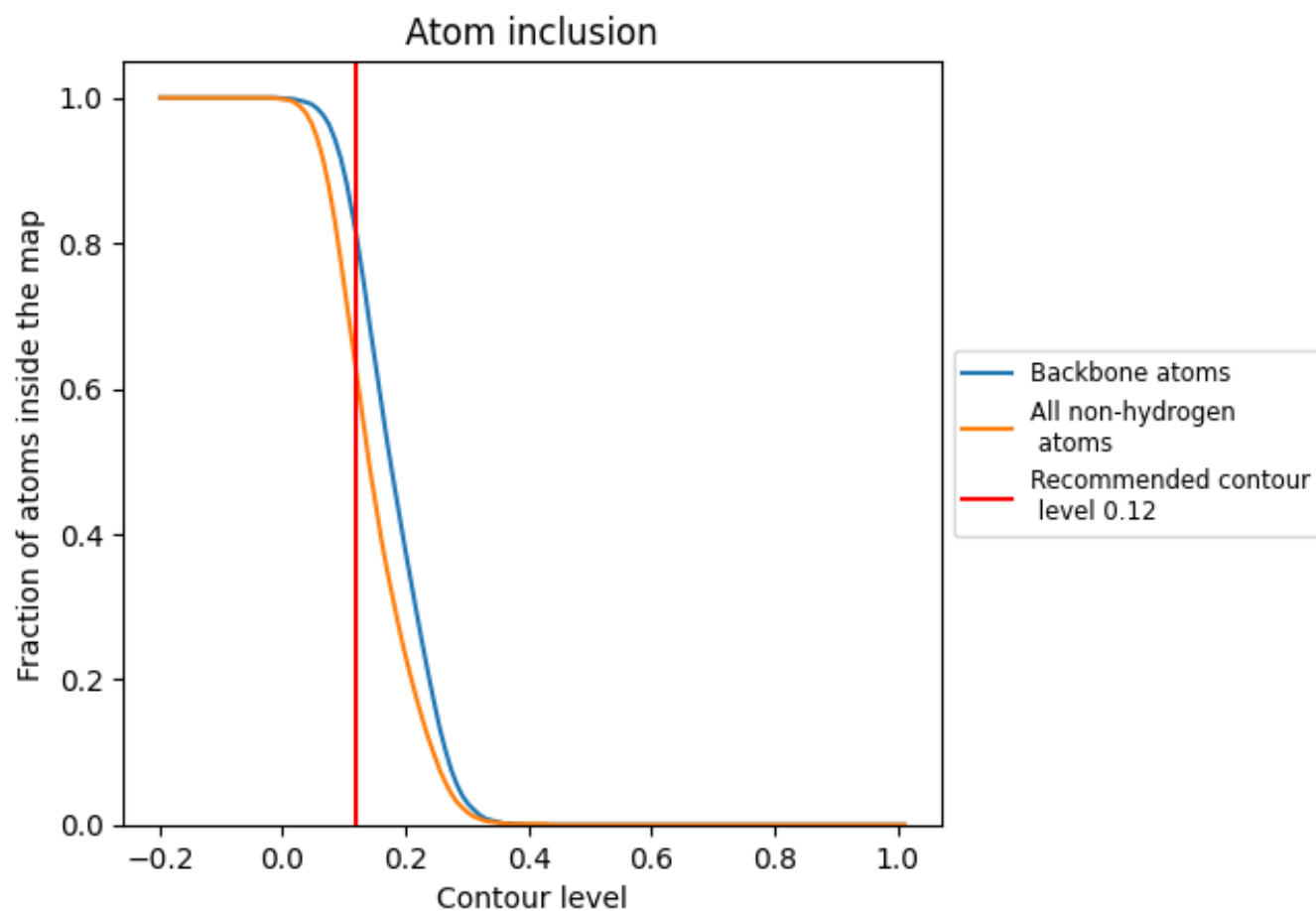
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.12).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ























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

Chain	Atom inclusion	Q-score
All	 0.6230	 0.4010
1A	 0.5080	 0.4400
1B	 0.6810	 0.4650
1C	 0.7470	 0.4810
1D	 0.6960	 0.4630
1E	 0.7530	 0.4310
1F	 0.7600	 0.4330
1G	 0.7680	 0.4620
1H	 0.6370	 0.4520
1I	 0.7930	 0.4780
1J	 0.5660	 0.4110
1K	 0.6560	 0.4220
1L	 0.4650	 0.2850
1M	 0.6410	 0.3930
1N	 0.7170	 0.4480
1O	 0.4580	 0.3360
1P	 0.6340	 0.4620
1Q	 0.6640	 0.4610
1R	 0.7260	 0.4720
1S	 0.7300	 0.4200
1T	 0.4410	 0.3560
1U	 0.3490	 0.2370
1V	 0.6490	 0.4250
1W	 0.6380	 0.4360
1X	 0.7470	 0.4320
1Y	 0.6080	 0.3420
1Z	 0.7450	 0.4470
1a	 0.7460	 0.4700
1b	 0.6920	 0.4520
1c	 0.4900	 0.3690
1d	 0.6970	 0.4220
1e	 0.7200	 0.4420
1f	 0.4750	 0.3600
1g	 0.5180	 0.3530
1h	 0.6120	 0.3860



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Chain	Atom inclusion	Q-score
1i	 0.2920	 0.2750
1j	 0.2660	 0.2590
1k	 0.2150	 0.2400
1l	 0.4720	 0.2970
1m	 0.4870	 0.2980
1n	 0.4540	 0.2740
1o	 0.4030	 0.2470
1p	 0.5130	 0.3290
1q	 0.7440	 0.4730
1r	 0.7510	 0.4730
1s	 0.7090	 0.4110