



Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 10:52 pm BST

PDB ID : 7AK6 / pdb_00007ak6
EMDB ID : EMD-11811
Title : Cryo-EM structure of ND6-P25L mutant respiratory complex I from Mus musculus at 3.8 Å
Authors : Yin, Z.; Bridges, H.R.; Grba, D.; Hirst, J.
Deposited on : 2020-09-29
Resolution : 3.82 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

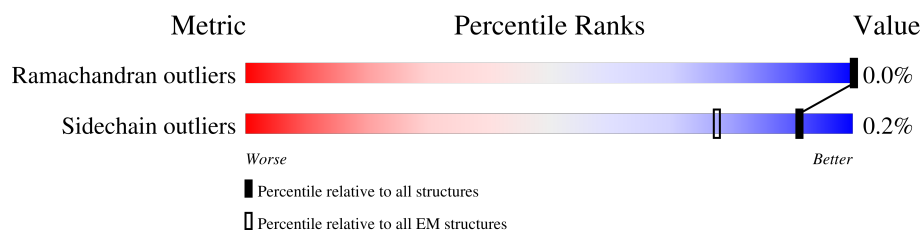
EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

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 3.82 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	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	115	<div> <div>52%</div> <div>79%</div> <div>19%</div> </div>
2	B	224	<div> <div>16%</div> <div>69%</div> <div>31%</div> </div>
3	C	263	<div> <div>19%</div> <div>78%</div> <div>21%</div> </div>
4	D	463	<div> <div>25%</div> <div>90%</div> <div>10%</div> </div>
5	E	248	<div> <div>55%</div> <div>85%</div> <div>15%</div> </div>
6	F	464	<div> <div>56%</div> <div>92%</div> <div>8%</div> </div>
7	G	727	<div> <div>41%</div> <div>94%</div> <div>6%</div> </div>
8	H	318	<div> <div>45%</div> <div>96%</div> <div>.</div> </div>
9	I	212	<div> <div>16%</div> <div>84%</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
10	J	172	68% 99% .
11	K	98	50% 99% .
12	L	607	61% 100%
13	M	459	36% 100%
14	N	345	32% 99%
15	O	355	50% 90% 10%
16	P	377	47% 76% 24%
17	Q	175	26% 71% 29%
18	R	116	34% 80% 19%
19	S	99	73% 83% 17%
20	T	156	44% 46% 54%
20	U	156	48% 56% 44%
21	V	116	62% 97% .
22	W	131	53% 86% 13%
23	X	172	59% 99% ..
24	Y	143	85% 98% .
25	Z	144	43% 97% .
26	a	68	46% 100%
27	b	84	60% 98% .
28	c	76	43% 61% 39%
29	d	120	49% 99% .
30	e	106	42% 97% ..
31	f	57	63% 89% 11%
32	g	151	40% 68% 32%
33	h	189	30% 72% 28%

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Mol	Chain	Length	Quality of chain
34	i	128	
35	j	105	
36	k	104	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	112	
44	s	104	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 65323 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	93	Total	C	N	O	S	0	0
			761	527	105	124	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	155	Total	C	N	O	S	0	0
			1241	793	222	212	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	207	Total	C	N	O	S	0	0
			1721	1111	296	311	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	417	Total	C	N	O	S	0	0
			3369	2155	576	614	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	210	Total	C	N	O	S	0	0
			1639	1043	275	310	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	428	Total	C	N	O	S	0	0
			3301	2080	590	609	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	686	Total	C	N	O	S	0	0
			5281	3313	917	1010	41		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	305	Total	C	N	O	S	0	0
			2441	1642	367	411	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	178	Total	C	N	O	S	0	0
			1408	885	243	268	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	171	Total	C	N	O	S	0	0
			1278	858	185	220	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			737	477	112	137	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			4800	3182	746	827	45		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3632	2408	567	617	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	344	Total	C	N	O	S	0	0
			2696	1791	416	452	37		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	319	Total	C	N	O	S	0	0
			2599	1668	430	491	10		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	288	Total	C	N	O	S	0	0
			2281	1453	412	409	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	125	Total	C	N	O	S	0	0
			1015	642	179	190	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	94	Total	C	N	O	S	0	0
			738	458	135	142	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	82	Total	C	N	O	S	0	0
			659	413	125	118	3		

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	72	Total	C	N	O	S	0	0
			584	376	86	117	5		
20	U	88	Total	C	N	O	S	0	0
			706	453	104	144	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	112	Total	C	N	O	S	0	0
			915	596	152	164	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	114	Total	C	N	O	S	0	0
			970	619	180	165	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	171	Total	C	N	O	S	0	0
			1396	889	250	247	10		

- Molecule 24 is a protein called MCG5603.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	140	Total	C	N	O	S	0	0
			1037	662	175	192	8		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	139	Total	C	N	O	S	0	0
			1152	741	204	199	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	68	Total	C	N	O	S	0	0
			556	360	99	93	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	82	Total	C	N	O	S	0	0
			643	422	104	113	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	46	Total	C	N	O	S	0	0
			381	249	66	65	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	119	Total	C	N	O	S	0	0
			985	645	167	164	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	104	Total	C	N	O	S	0	0
			870	550	161	151	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	51	Total	C	N	O	S	0	0
			433	278	78	75	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	102	Total	C	N	O	S	0	0
			858	555	137	162	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	137	Total	C	N	O	S	0	0
			1153	756	192	202	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	95	Total	C	N	O	S	0	0
			802	524	138	137	3		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	62	Total	C	N	O	S	0	0
			537	355	88	93	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	77	Total	C	N	O	S	0	0
			626	414	106	104	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	156	Total	C	N	O	S	0	0
			1312	846	219	236	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	125	Total	C	N	O		0	0
			1044	673	188	183			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	176	Total	C	N	O	S	0	0
			1527	976	274	266	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	114	Total	C	N	O	S	0	0
			984	620	185	171	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	168	Total	C	N	O	S	0	0
			1424	896	256	264	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	143	Total	C	N	O	S	0	0
			1192	766	212	210	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	96	Total	C	N	O	S	0	0
			776	490	145	138	3		

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

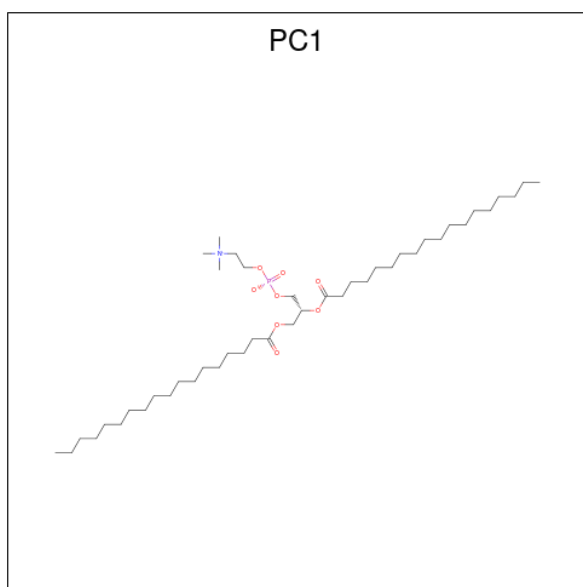
Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	39	Total	C	N	O	0	0
			329	207	59	63		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



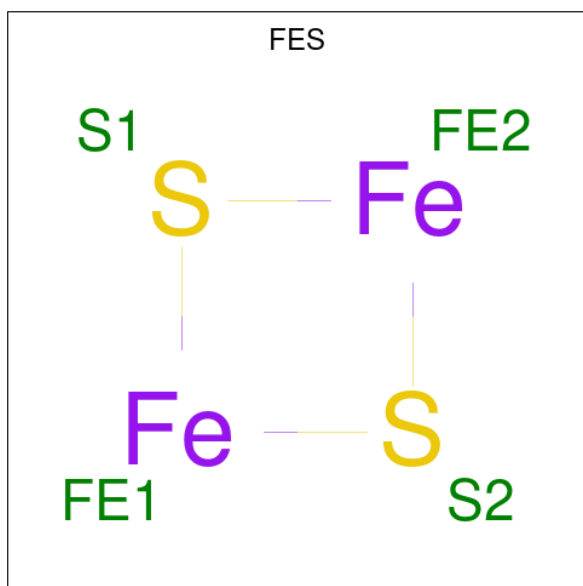
Mol	Chain	Residues	Atoms			AltConf
45	B	1	Total	Fe	S	0
			8	4	4	
45	F	1	Total	Fe	S	0
			8	4	4	
45	G	1	Total	Fe	S	0
			8	4	4	
45	G	1	Total	Fe	S	0
			8	4	4	
45	I	1	Total	Fe	S	0
			8	4	4	
45	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



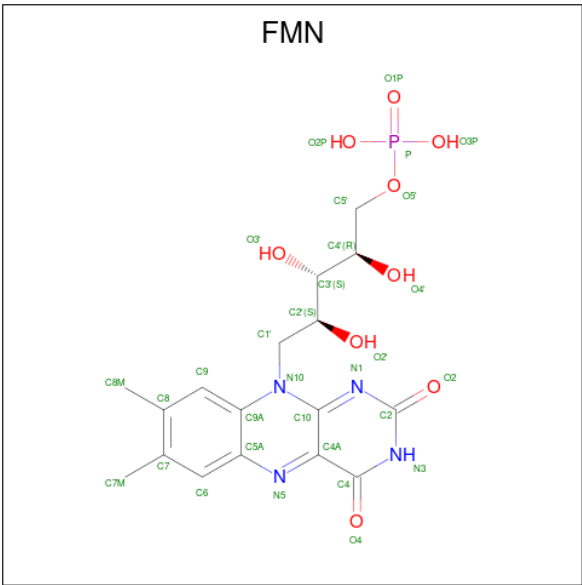
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	B	1	26	16	1	8	1	0

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



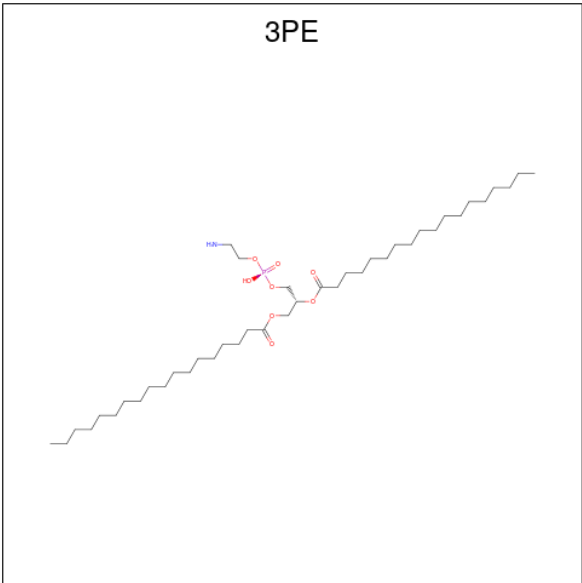
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	E	1	4	2	2	0
47	G	1	4	2	2	0

- Molecule 48 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).



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

- Molecule 49 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



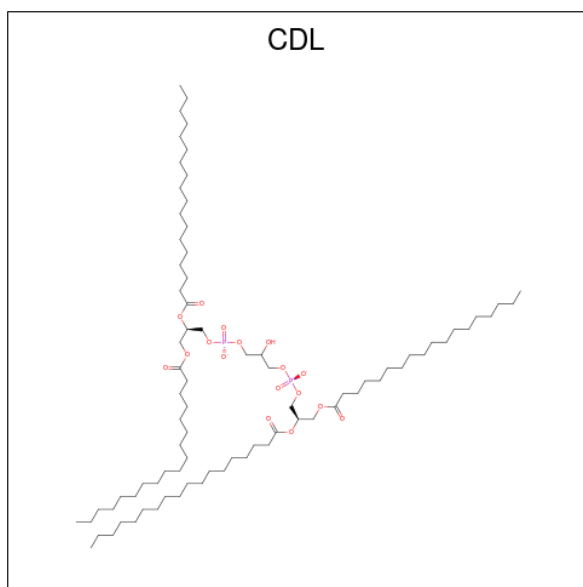
Mol	Chain	Residues	Atoms					AltConf
49	H	1	Total	C	N	O	P	0
			42	32	1	8	1	
49	J	1	Total	C	N	O	P	0
			38	28	1	8	1	

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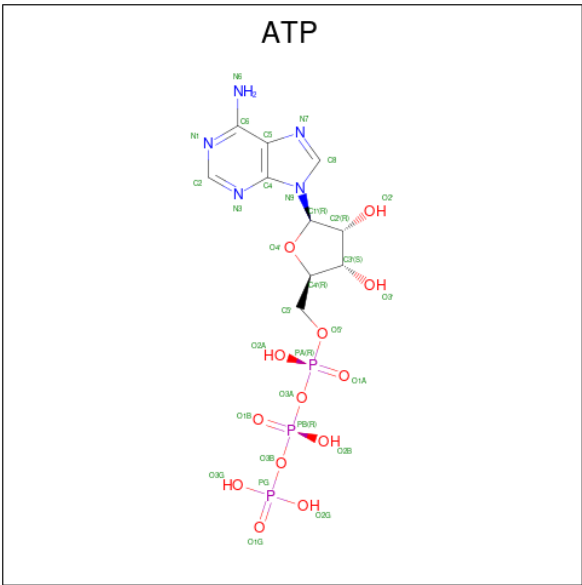
Mol	Chain	Residues	Atoms					AltConf
49	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
49	M	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 50 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



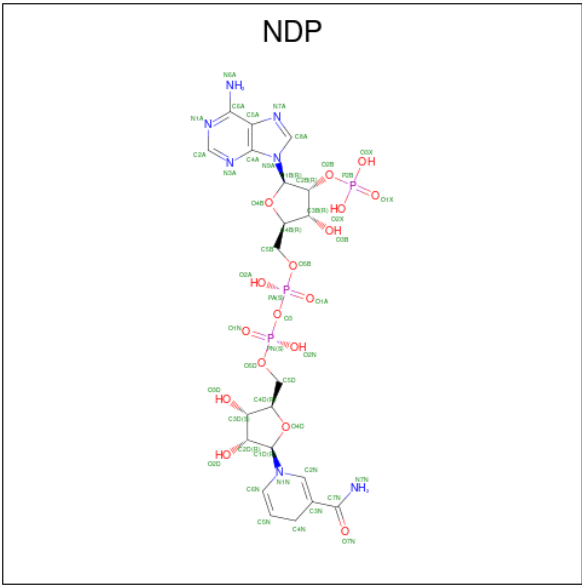
Mol	Chain	Residues	Atoms				AltConf
50	L	1	Total	C	O	P	0
			54	35	17	2	
50	d	1	Total	C	O	P	0
			50	31	17	2	

- Molecule 51 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

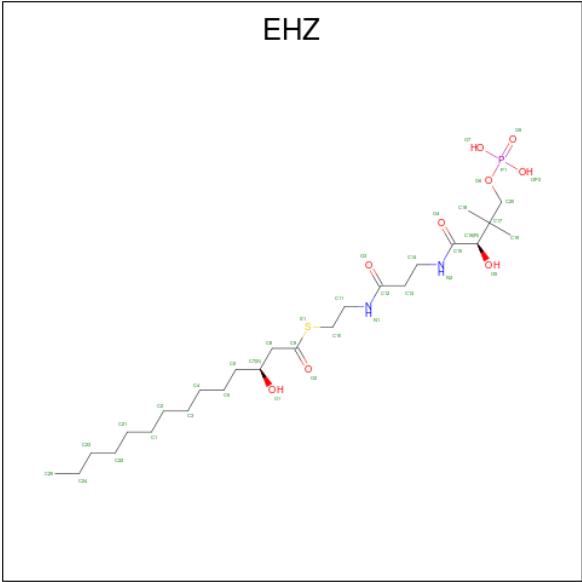


Mol	Chain	Residues	Atoms					AltConf
52	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

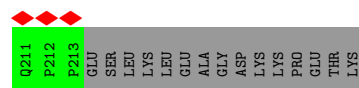
- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

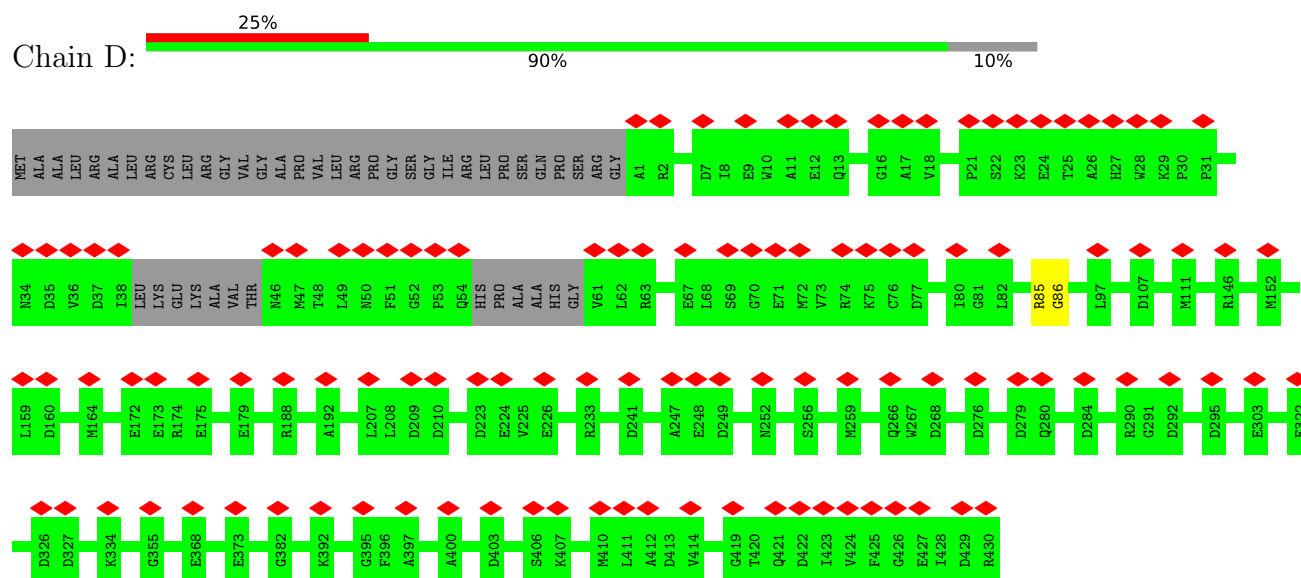
- Molecule 54 is {S}-[2-[3-[[2 {R}]-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).



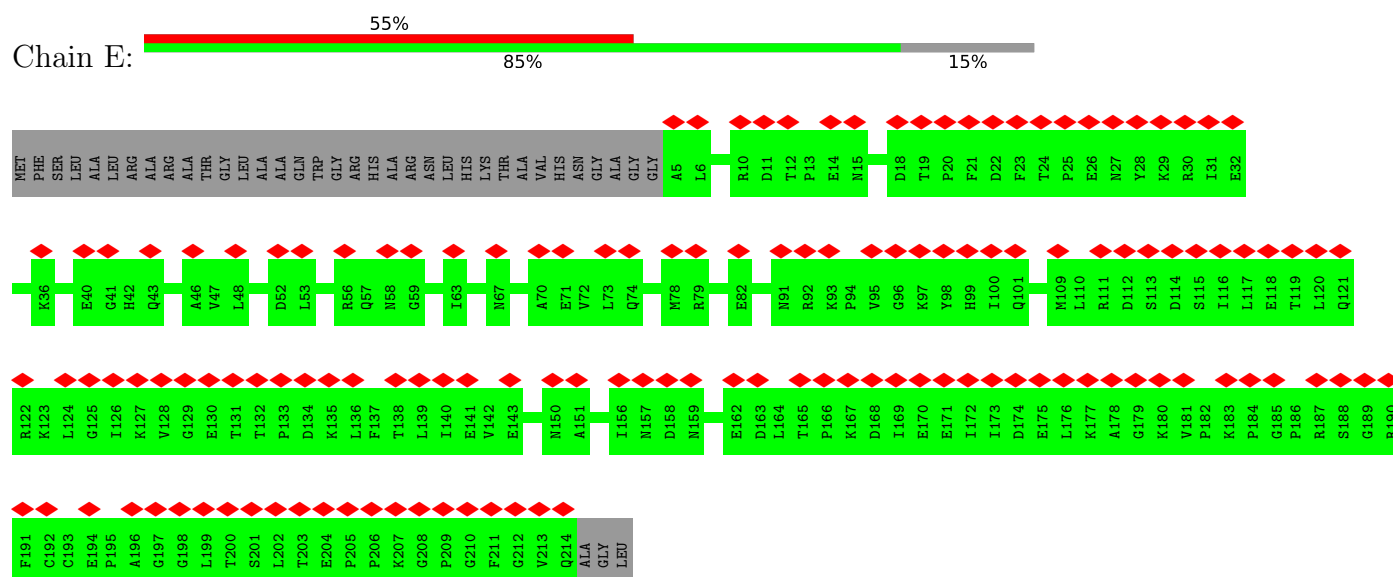
Mol	Chain	Residues	Atoms						AltConf
54	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
54	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	



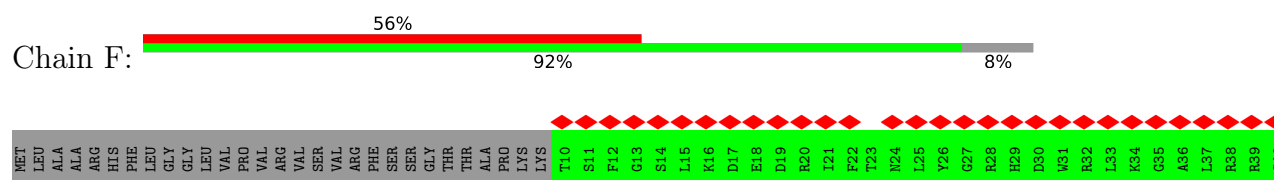
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

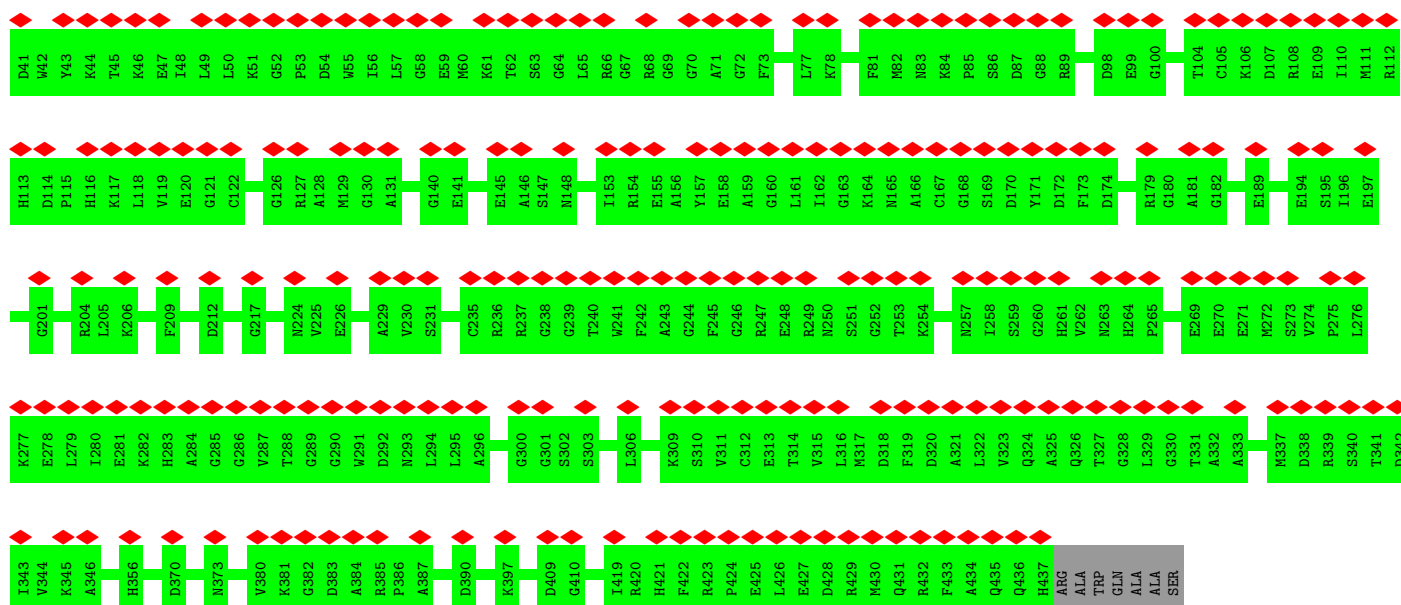


- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

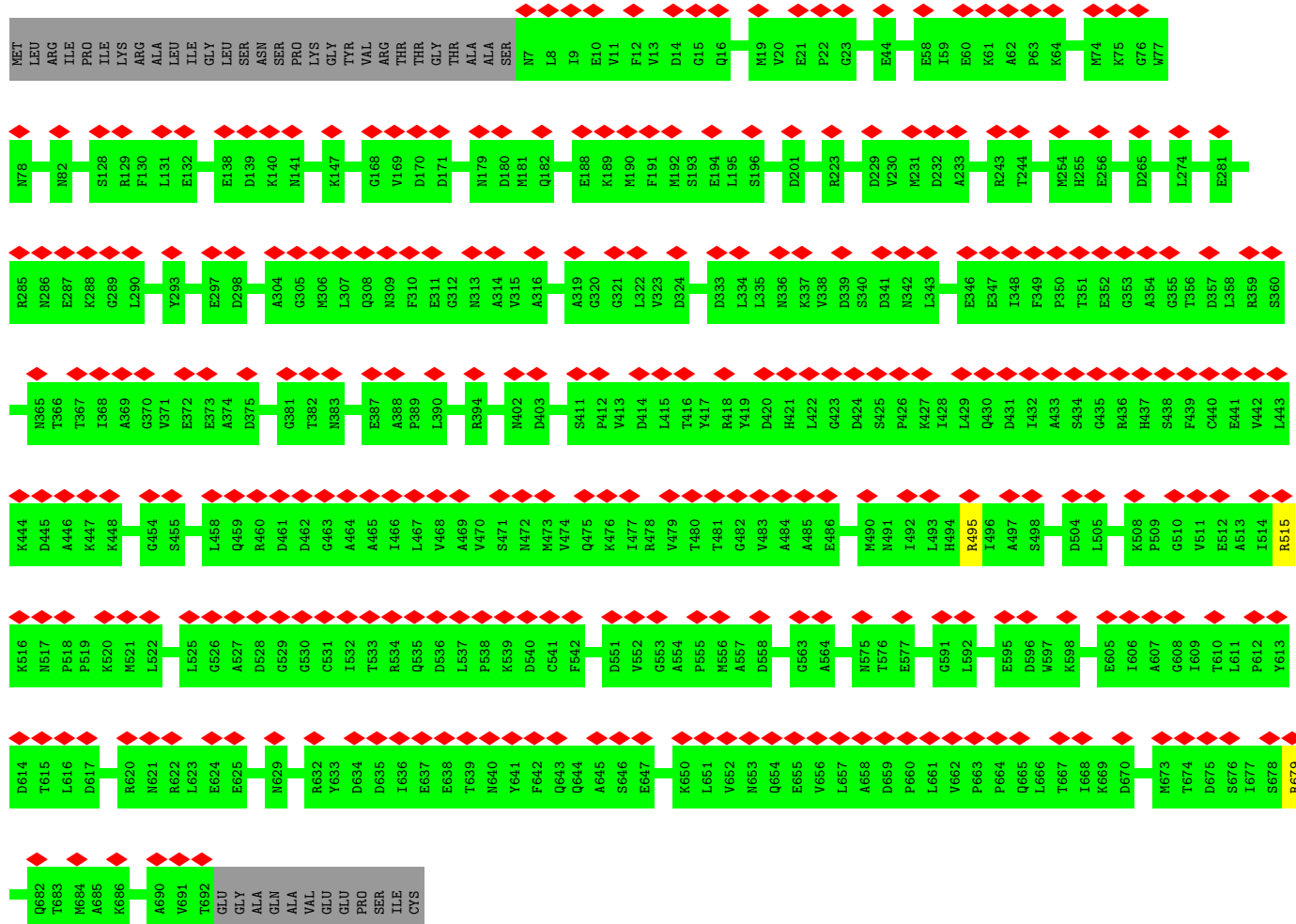
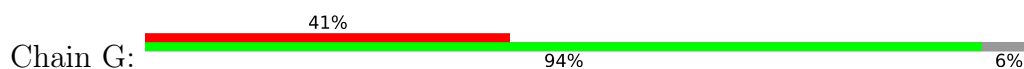


- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

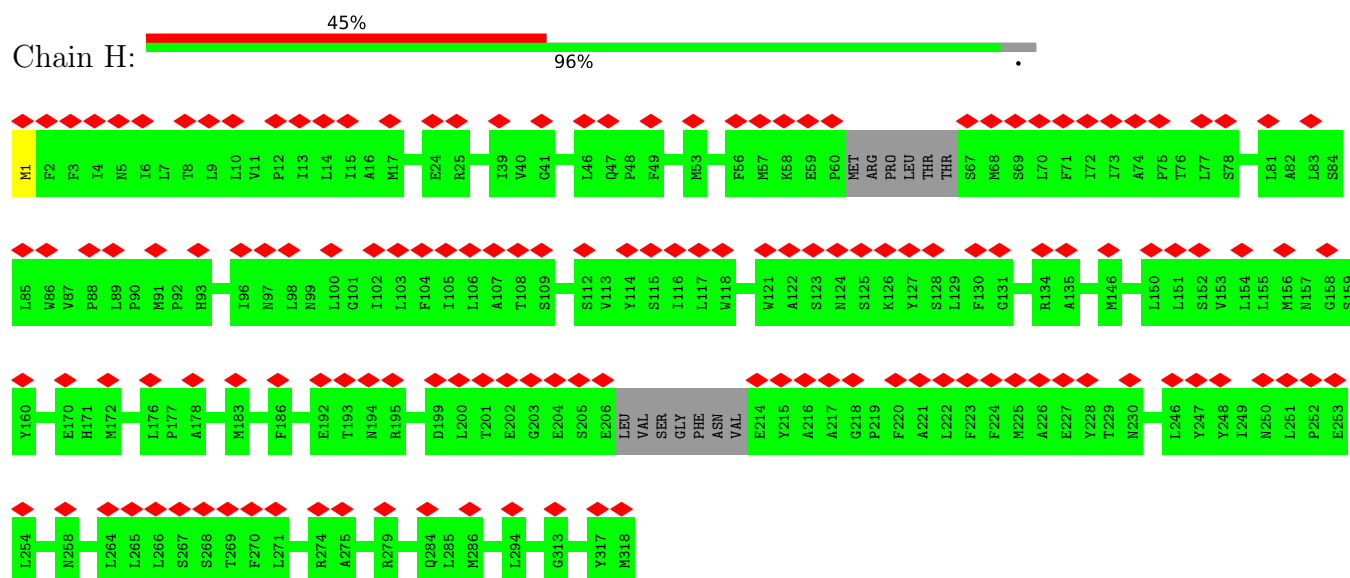




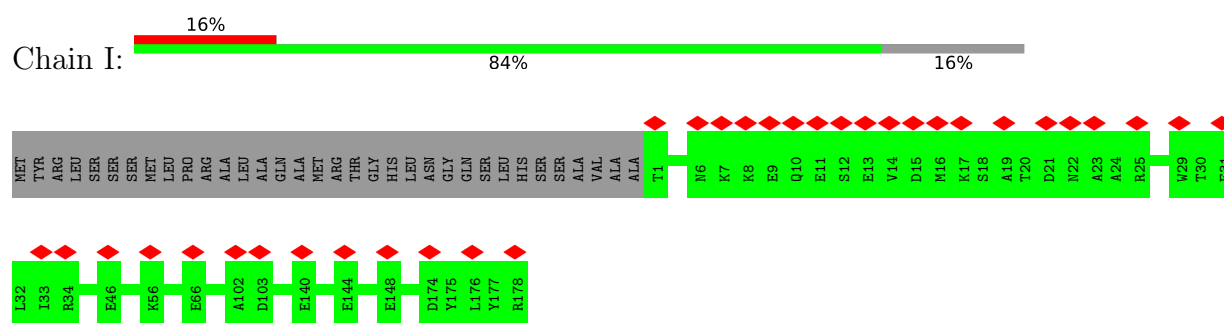
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



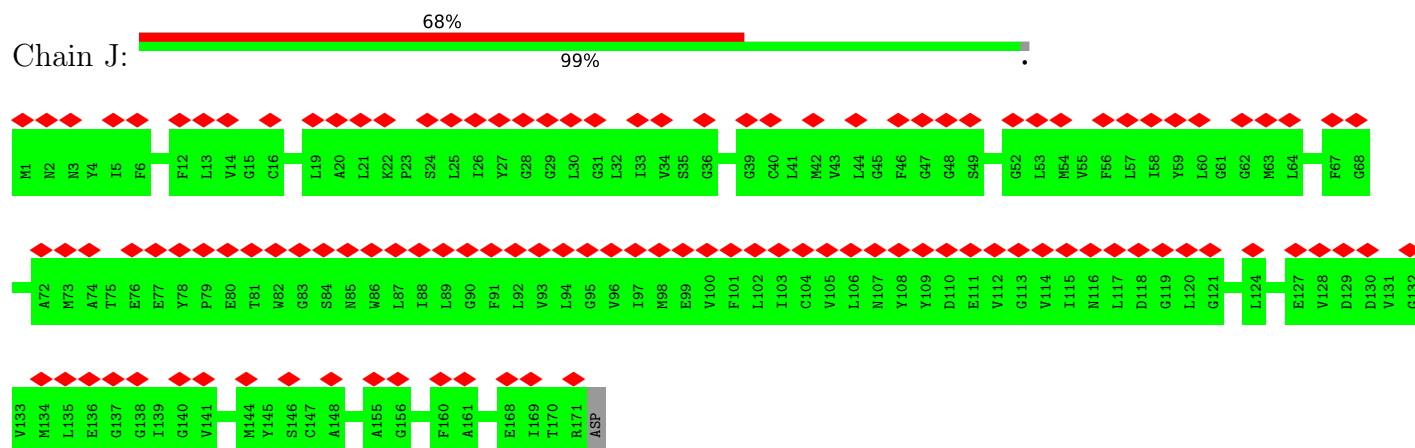
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



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

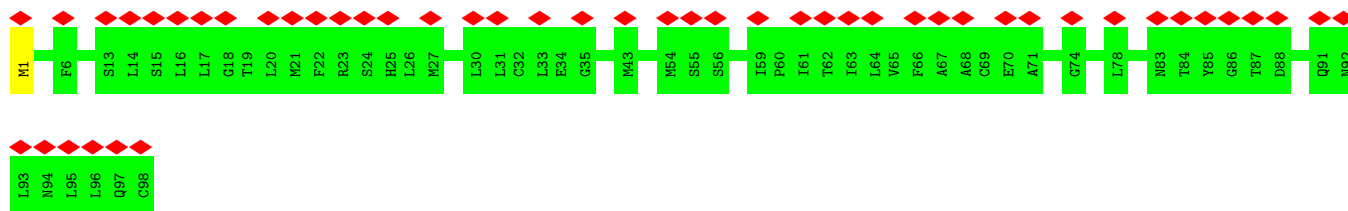


- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

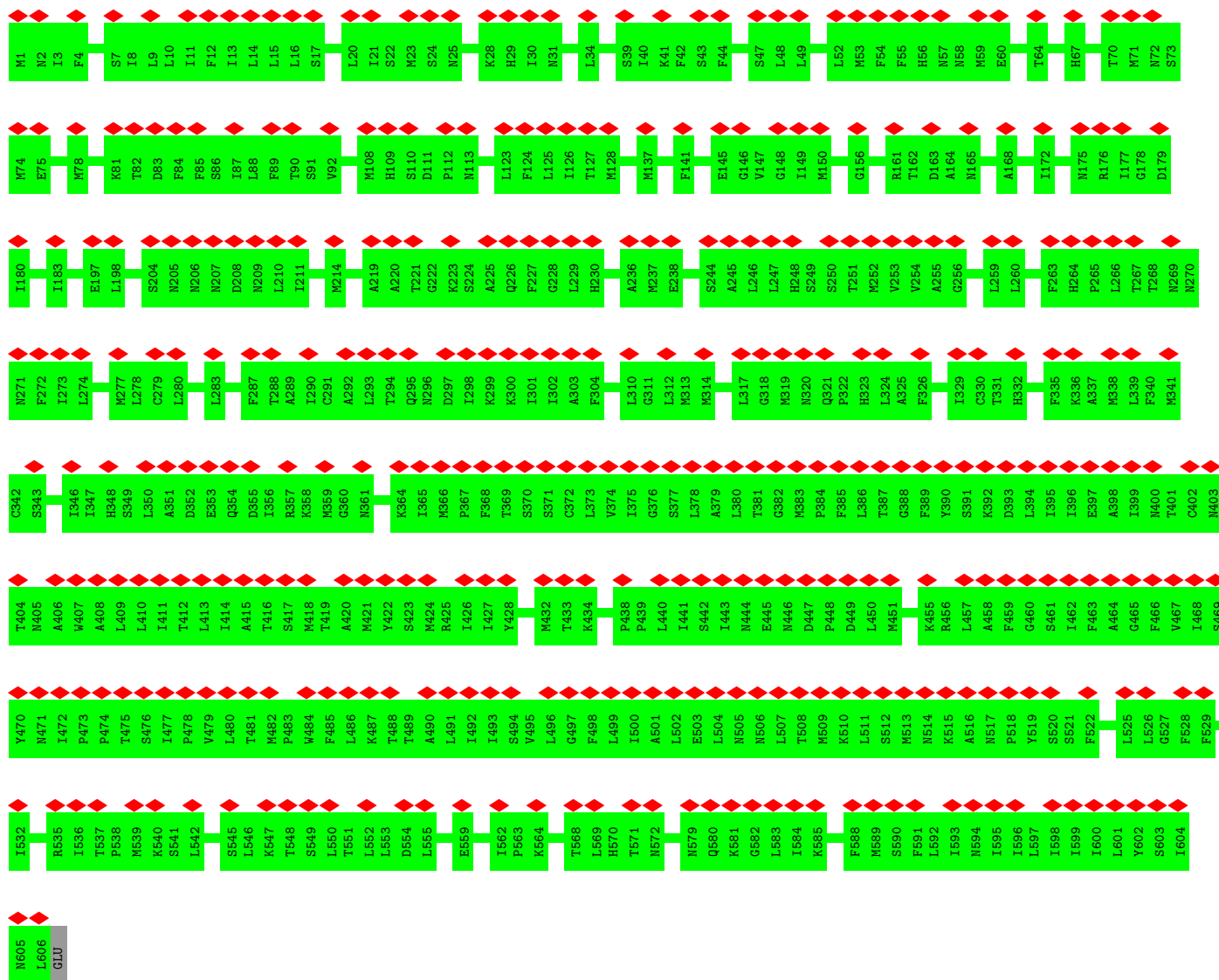


- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

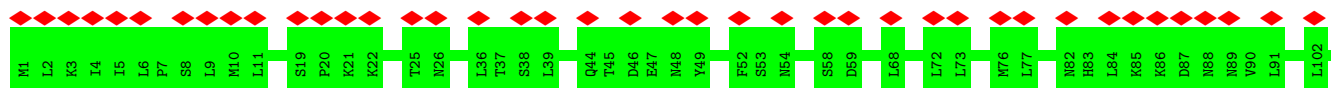


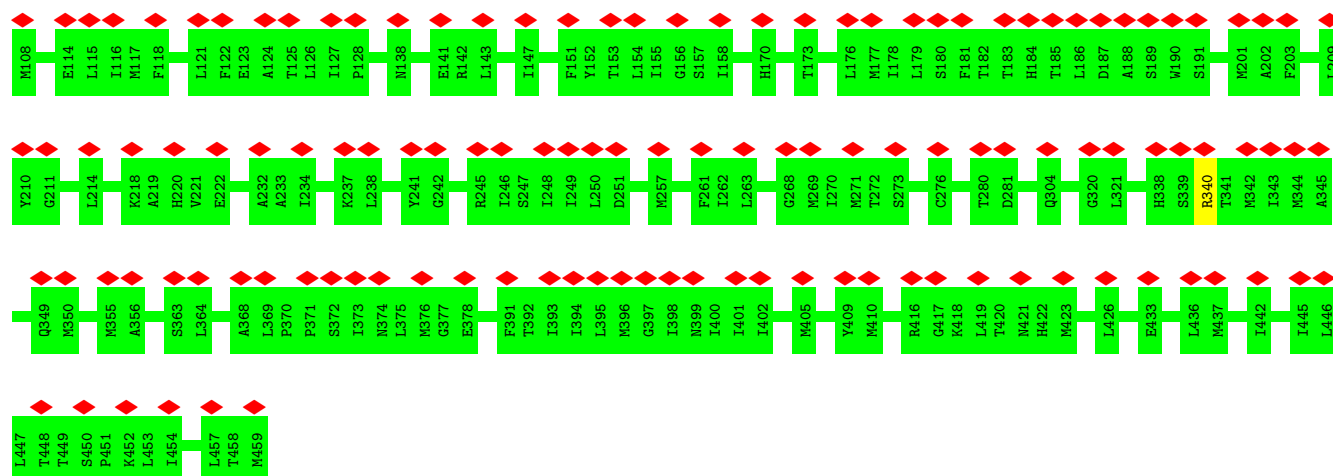


• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

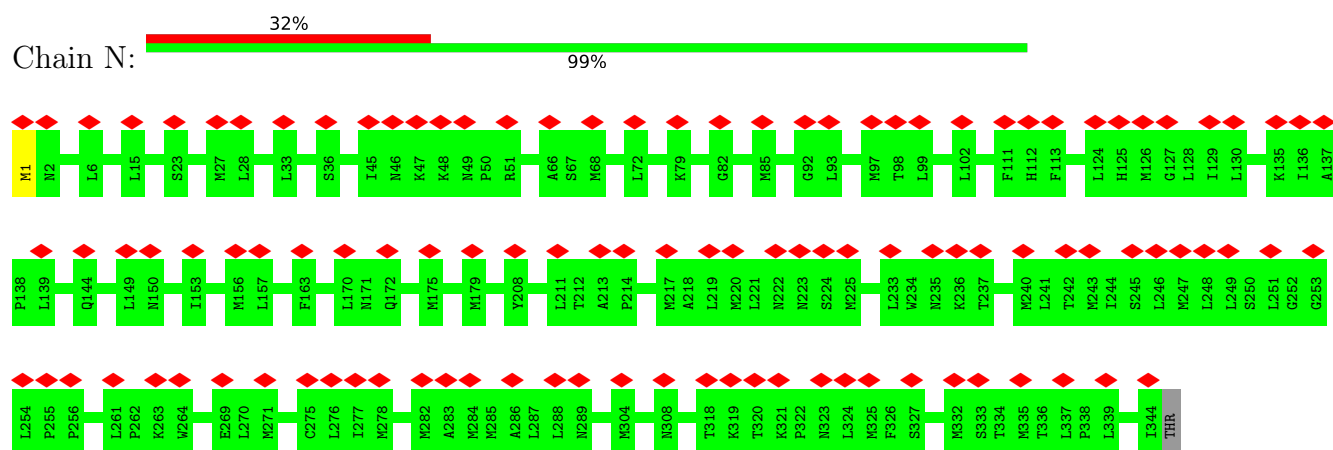


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



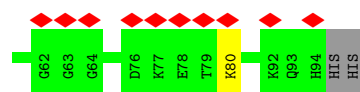


- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

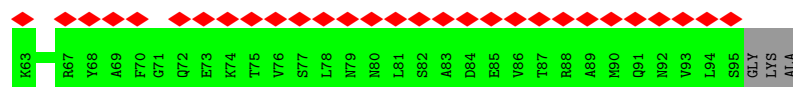
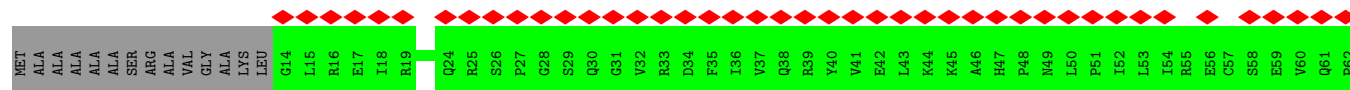
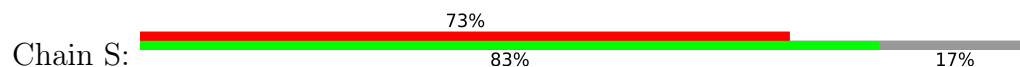


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

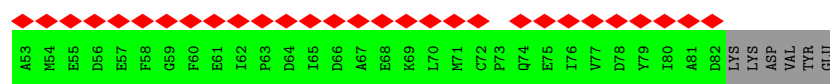
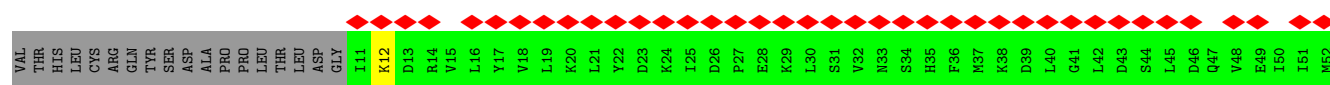
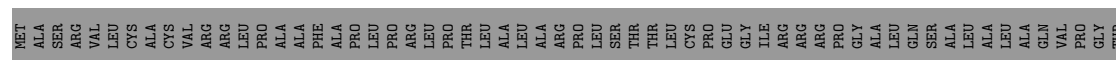
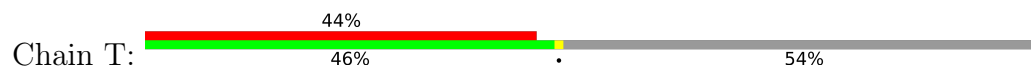




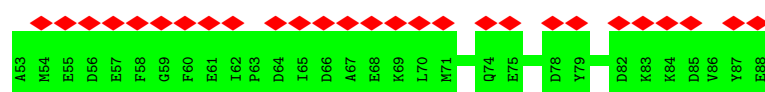
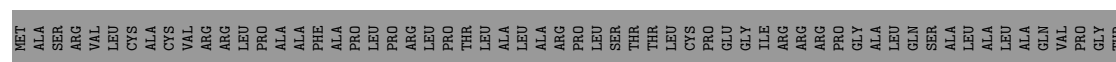
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



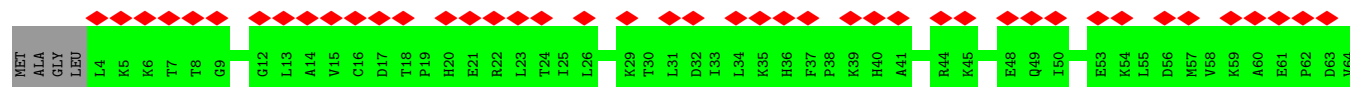
- Molecule 20: Acyl carrier protein, mitochondrial

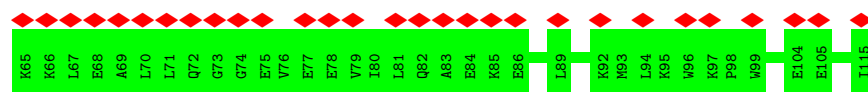


- Molecule 20: Acyl carrier protein, mitochondrial

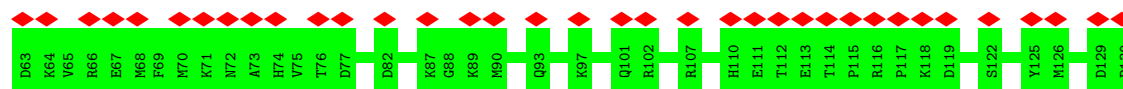
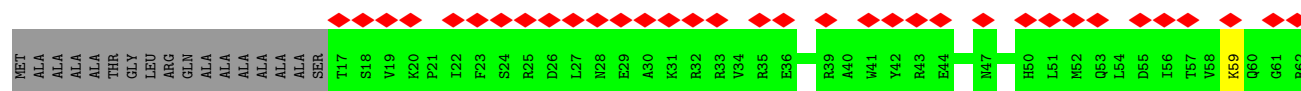
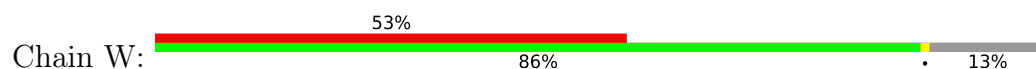


- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

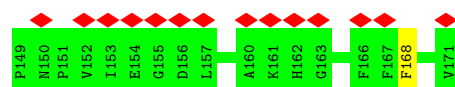
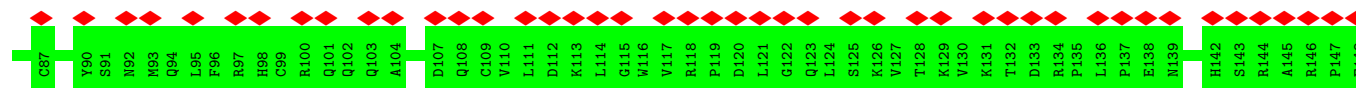
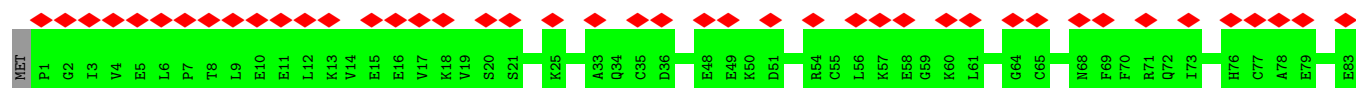




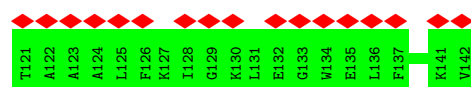
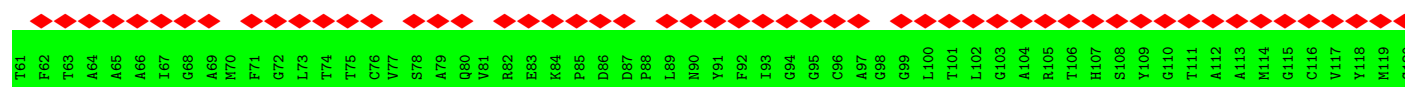
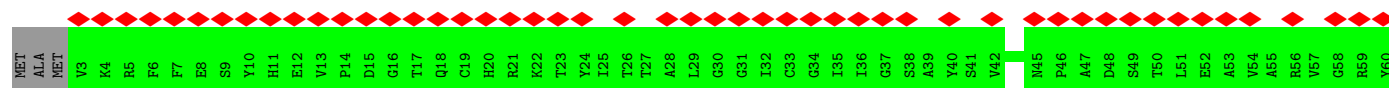
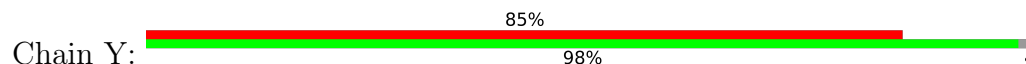
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



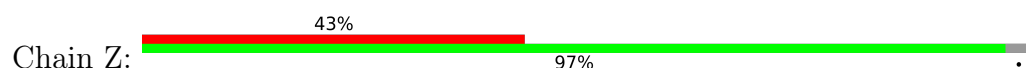
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

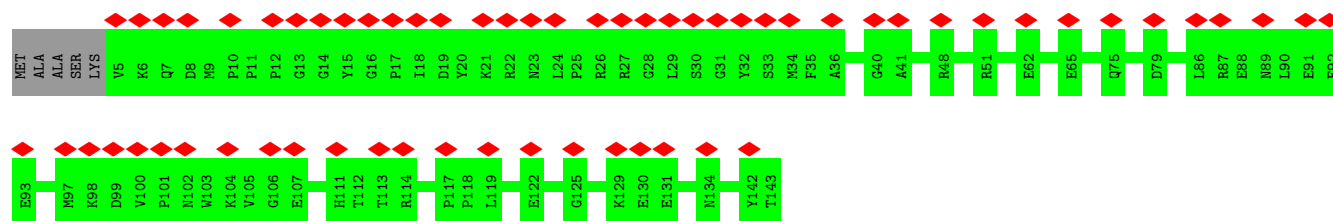


- Molecule 24: MCG5603

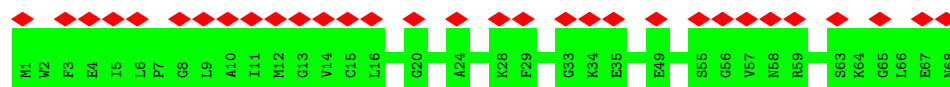


- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

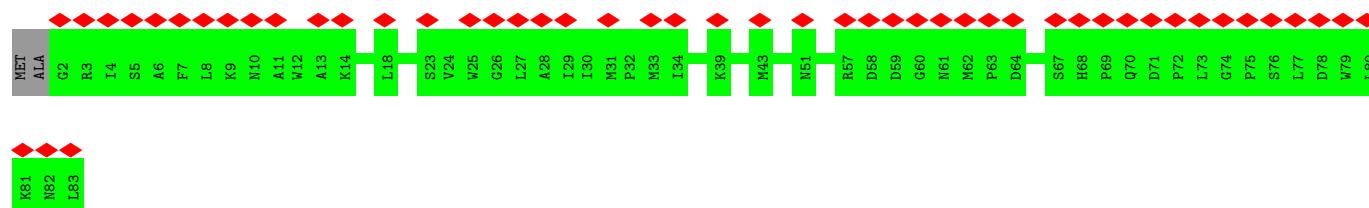




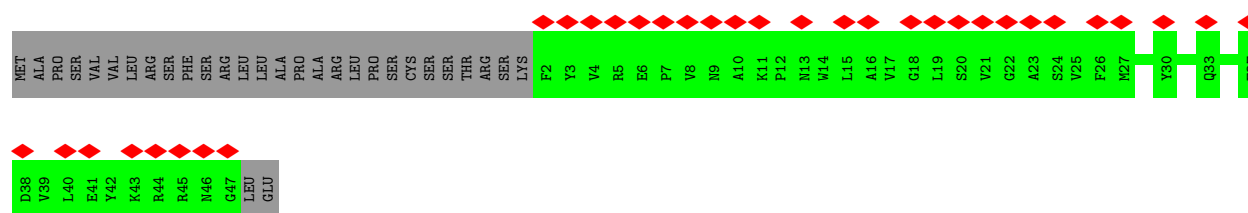
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



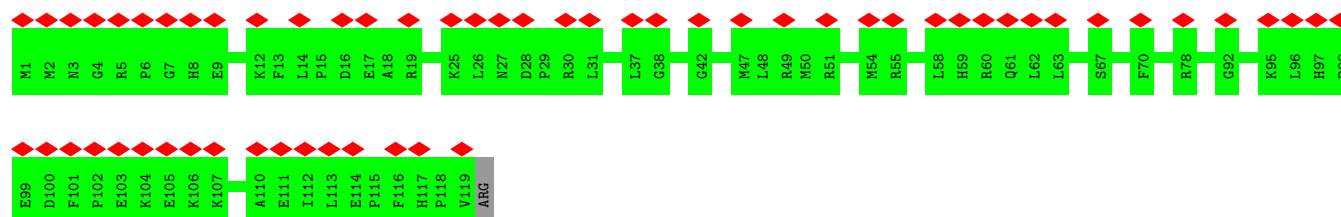
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



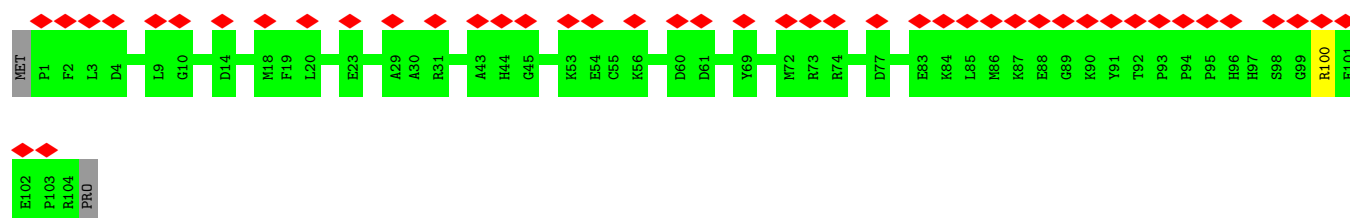
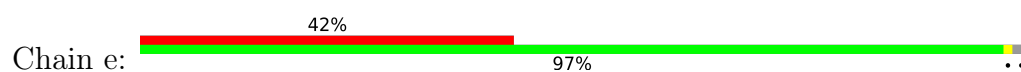
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



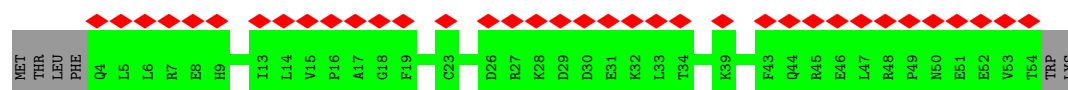
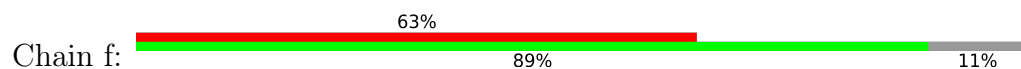
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



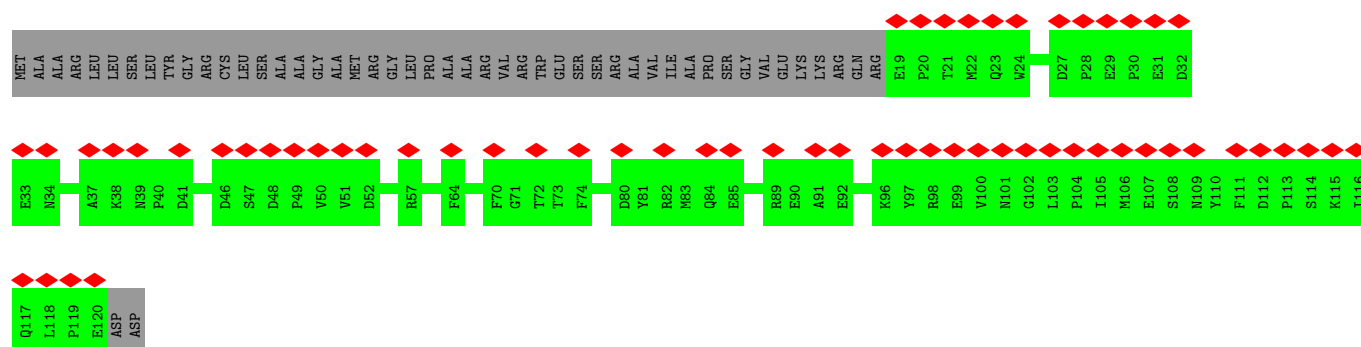
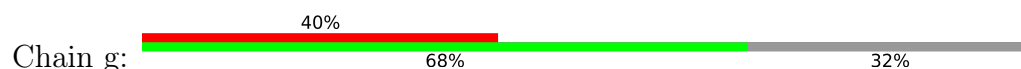
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



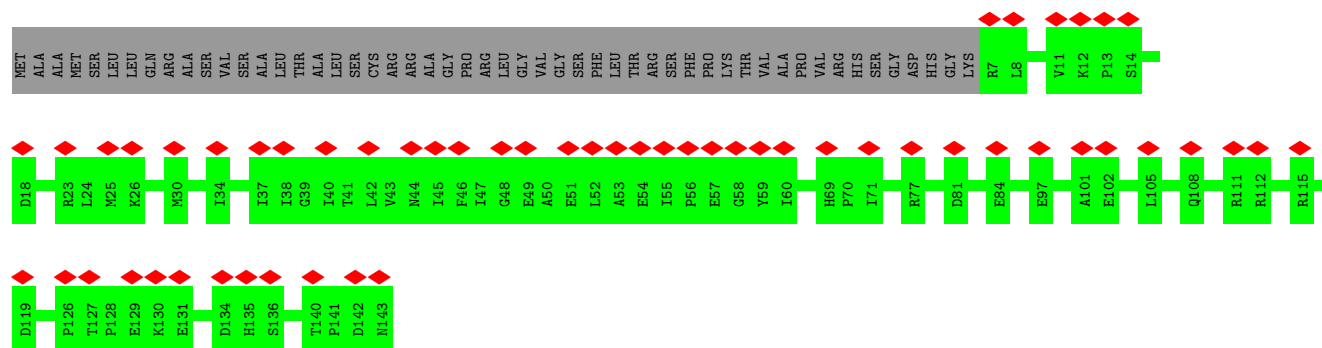
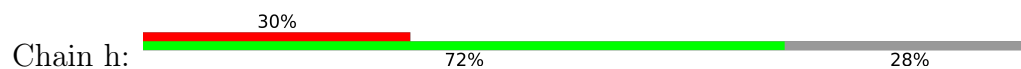
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



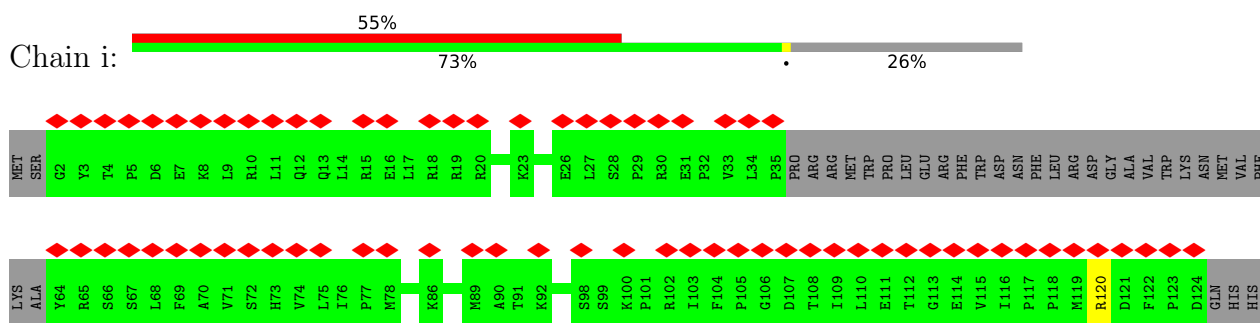
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



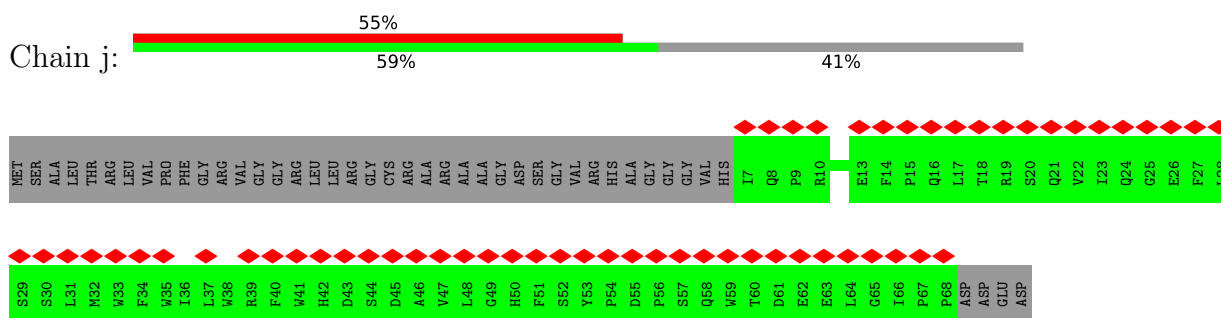
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



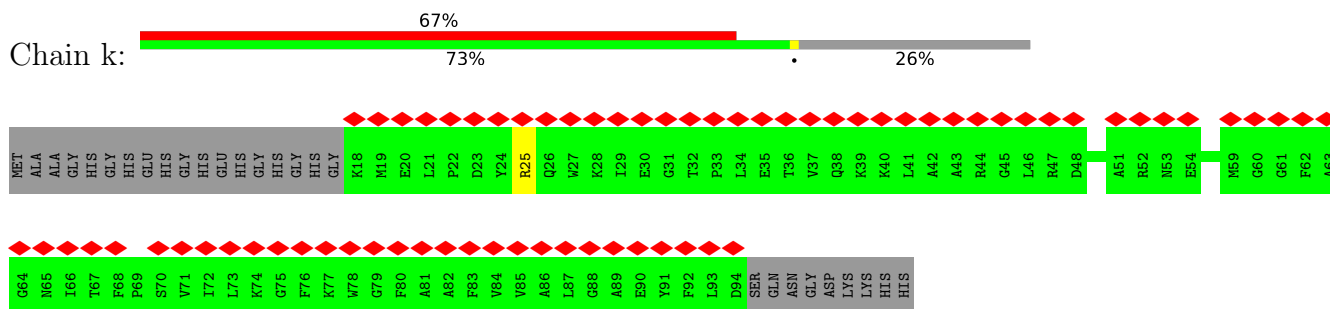
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



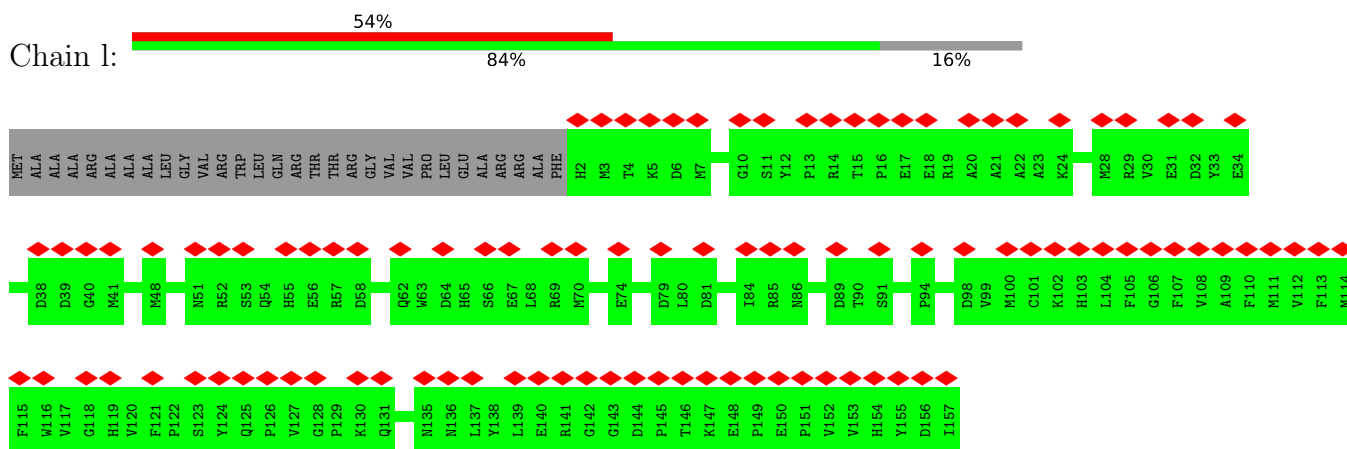
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



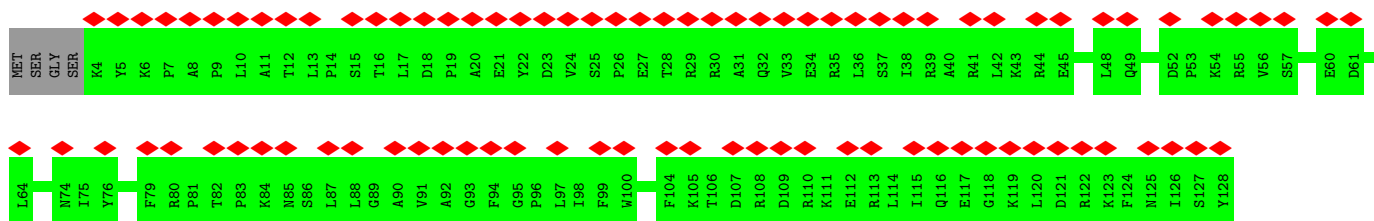
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



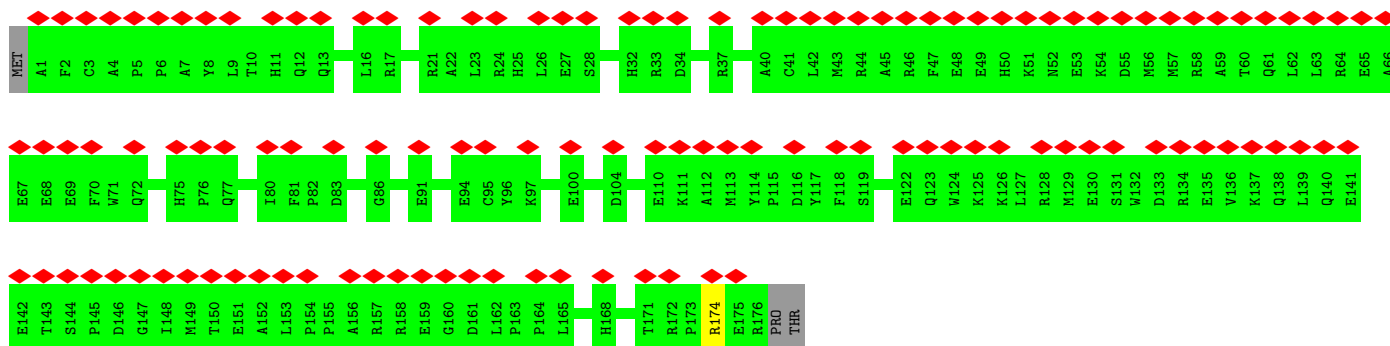
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



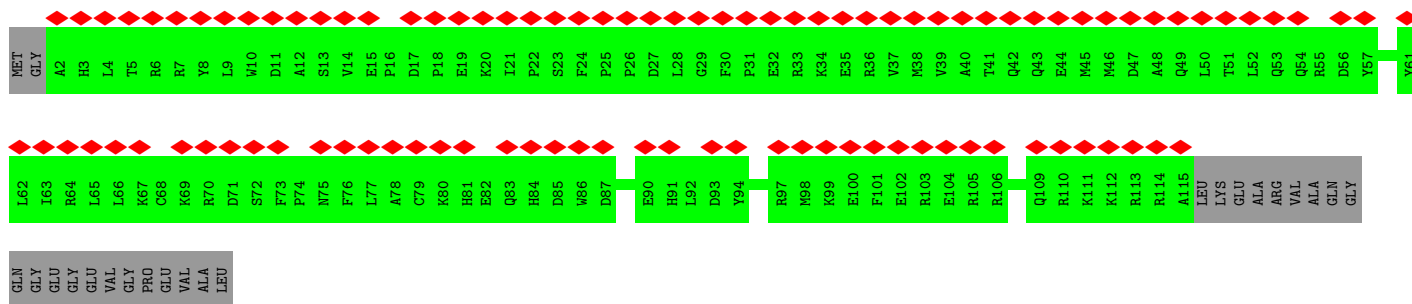
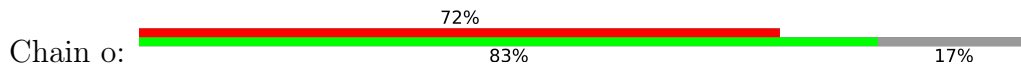
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



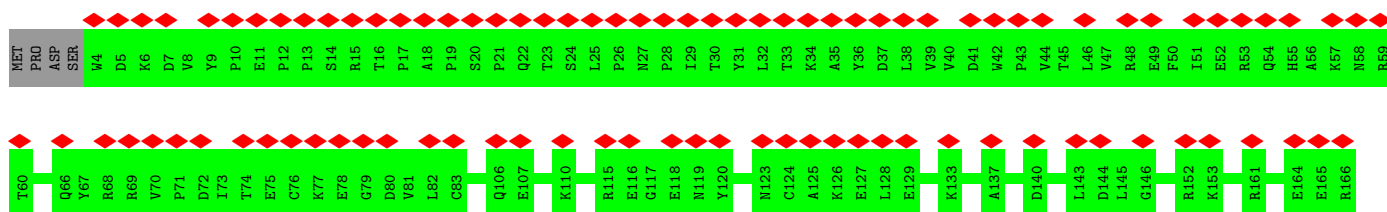
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

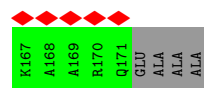


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

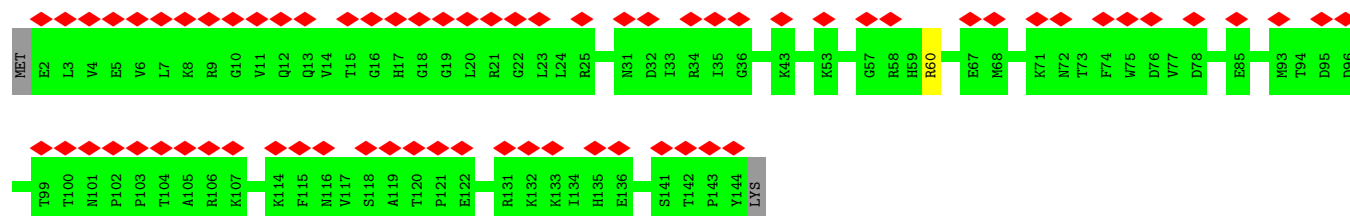


- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

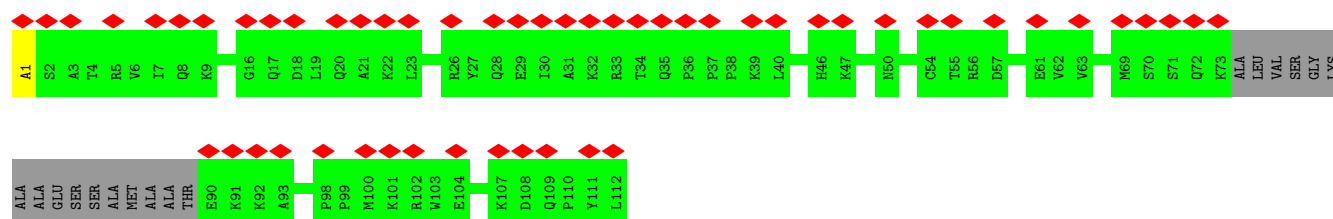
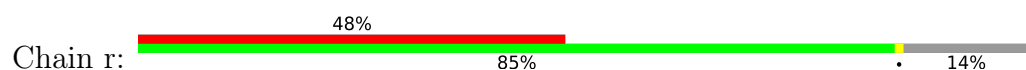




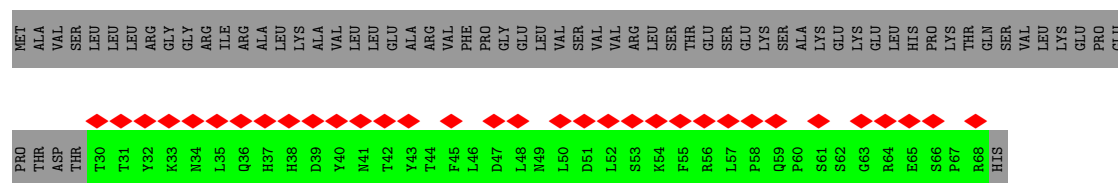
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25629	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 ($e^-/\text{\AA}^2$)	50.015	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.182	Depositor
Minimum map value	-0.046	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0268	Depositor
Map size (Å)	474.30002, 474.30002, 474.30002	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.054, 1.054, 1.054	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, SF4, ATP, EHZ, CDL, PC1, 2MR, FES, ZN, FME, AYA, 3PE, NDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/771	0.52	2/1054 (0.2%)
2	B	0.43	0/1272	0.48	0/1722
3	C	0.38	0/1771	0.47	0/2412
4	D	0.37	0/3440	0.45	0/4656
5	E	0.31	0/1679	0.45	0/2288
6	F	0.31	0/3376	0.46	0/4561
7	G	0.34	0/5368	0.47	0/7273
8	H	0.33	0/2504	0.43	0/3420
9	I	0.41	0/1438	0.48	0/1946
10	J	0.32	0/1297	0.44	0/1764
11	K	0.31	0/738	0.43	0/1002
12	L	0.31	0/4913	0.45	0/6686
13	M	0.31	0/3709	0.46	0/5052
14	N	0.33	0/2748	0.44	0/3741
15	O	0.32	0/2666	0.44	0/3615
16	P	0.32	0/2329	0.47	0/3145
17	Q	0.32	0/1038	0.47	0/1401
18	R	0.34	0/751	0.46	0/1011
19	S	0.27	0/670	0.47	0/904
20	T	0.28	0/593	0.44	0/799
20	U	0.29	0/718	0.41	0/970
21	V	0.31	0/937	0.42	0/1270
22	W	0.31	0/993	0.45	0/1335
23	X	0.30	0/1434	0.44	0/1937
24	Y	0.29	0/1061	0.45	0/1439
25	Z	0.32	0/1183	0.44	0/1597
26	a	0.34	0/569	0.43	0/766
27	b	0.29	0/666	0.41	0/914
28	c	0.30	0/392	0.40	0/533
29	d	0.34	0/1017	0.44	0/1373
30	e	0.30	0/892	0.45	0/1187
31	f	0.28	0/443	0.44	0/596

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.33	0/887	0.42	0/1209
33	h	0.33	0/1188	0.42	0/1610
34	i	0.30	0/828	0.45	0/1125
35	j	0.27	0/561	0.41	0/768
36	k	0.28	0/646	0.43	0/873
37	l	0.31	0/1367	0.41	0/1866
38	m	0.31	0/1073	0.45	0/1455
39	n	0.30	0/1581	0.41	0/2140
40	o	0.27	0/1009	0.42	0/1355
41	p	0.33	0/1457	0.42	0/1969
42	q	0.35	0/1234	0.45	0/1681
43	r	0.31	0/786	0.43	0/1062
44	s	0.27	0/338	0.45	0/458
All	All	0.33	0/66331	0.45	2/89940 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	LEU	CB-CG-CD2	5.81	120.88	111.00
1	A	49	LEU	CB-CG-CD1	5.60	120.51	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	89/115 (77%)	83 (93%)	6 (7%)	0	100	100
2	B	153/224 (68%)	136 (89%)	17 (11%)	0	100	100
3	C	205/263 (78%)	181 (88%)	24 (12%)	0	100	100
4	D	410/463 (89%)	379 (92%)	30 (7%)	1 (0%)	44	74
5	E	208/248 (84%)	180 (86%)	28 (14%)	0	100	100
6	F	426/464 (92%)	385 (90%)	41 (10%)	0	100	100
7	G	684/727 (94%)	617 (90%)	67 (10%)	0	100	100
8	H	299/318 (94%)	267 (89%)	32 (11%)	0	100	100
9	I	176/212 (83%)	157 (89%)	19 (11%)	0	100	100
10	J	169/172 (98%)	154 (91%)	15 (9%)	0	100	100
11	K	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
12	L	604/607 (100%)	544 (90%)	60 (10%)	0	100	100
13	M	457/459 (100%)	411 (90%)	46 (10%)	0	100	100
14	N	342/345 (99%)	316 (92%)	26 (8%)	0	100	100
15	O	317/355 (89%)	283 (89%)	34 (11%)	0	100	100
16	P	280/377 (74%)	244 (87%)	36 (13%)	0	100	100
17	Q	123/175 (70%)	111 (90%)	12 (10%)	0	100	100
18	R	92/116 (79%)	84 (91%)	8 (9%)	0	100	100
19	S	80/99 (81%)	76 (95%)	4 (5%)	0	100	100
20	T	70/156 (45%)	62 (89%)	8 (11%)	0	100	100
20	U	86/156 (55%)	75 (87%)	11 (13%)	0	100	100
21	V	110/116 (95%)	99 (90%)	11 (10%)	0	100	100
22	W	112/131 (86%)	103 (92%)	9 (8%)	0	100	100
23	X	169/172 (98%)	153 (90%)	15 (9%)	1 (1%)	22	57
24	Y	138/143 (96%)	129 (94%)	9 (6%)	0	100	100
25	Z	137/144 (95%)	126 (92%)	11 (8%)	0	100	100
26	a	66/68 (97%)	62 (94%)	4 (6%)	0	100	100
27	b	80/84 (95%)	69 (86%)	11 (14%)	0	100	100
28	c	44/76 (58%)	41 (93%)	3 (7%)	0	100	100
29	d	117/120 (98%)	109 (93%)	8 (7%)	0	100	100
30	e	102/106 (96%)	87 (85%)	15 (15%)	0	100	100
31	f	49/57 (86%)	41 (84%)	8 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	g	100/151 (66%)	88 (88%)	12 (12%)	0	100	100
33	h	135/189 (71%)	121 (90%)	14 (10%)	0	100	100
34	i	91/128 (71%)	71 (78%)	20 (22%)	0	100	100
35	j	60/105 (57%)	55 (92%)	5 (8%)	0	100	100
36	k	75/104 (72%)	69 (92%)	6 (8%)	0	100	100
37	l	154/186 (83%)	132 (86%)	22 (14%)	0	100	100
38	m	123/129 (95%)	114 (93%)	9 (7%)	0	100	100
39	n	174/179 (97%)	162 (93%)	12 (7%)	0	100	100
40	o	112/137 (82%)	95 (85%)	17 (15%)	0	100	100
41	p	166/176 (94%)	151 (91%)	15 (9%)	0	100	100
42	q	141/145 (97%)	122 (86%)	19 (14%)	0	100	100
43	r	92/112 (82%)	80 (87%)	12 (13%)	0	100	100
44	s	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
All	All	7950/9211 (86%)	7148 (90%)	800 (10%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	X	168	PHE
4	D	86	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/103 (82%)	84 (100%)	0	100	100
2	B	131/185 (71%)	131 (100%)	0	100	100
3	C	189/227 (83%)	188 (100%)	1 (0%)	86	90
4	D	361/394 (92%)	361 (100%)	0	100	100
5	E	183/206 (89%)	183 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	343/370 (93%)	343 (100%)	0	100	100
7	G	578/610 (95%)	575 (100%)	3 (0%)	86	90
8	H	267/279 (96%)	267 (100%)	0	100	100
9	I	145/178 (82%)	145 (100%)	0	100	100
10	J	131/137 (96%)	131 (100%)	0	100	100
11	K	87/87 (100%)	87 (100%)	0	100	100
12	L	548/549 (100%)	548 (100%)	0	100	100
13	M	414/414 (100%)	413 (100%)	1 (0%)	92	94
14	N	306/307 (100%)	306 (100%)	0	100	100
15	O	283/309 (92%)	283 (100%)	0	100	100
16	P	249/325 (77%)	247 (99%)	2 (1%)	79	85
17	Q	112/153 (73%)	112 (100%)	0	100	100
18	R	79/96 (82%)	78 (99%)	1 (1%)	65	76
19	S	73/80 (91%)	73 (100%)	0	100	100
20	T	67/135 (50%)	66 (98%)	1 (2%)	60	75
20	U	81/135 (60%)	81 (100%)	0	100	100
21	V	100/102 (98%)	100 (100%)	0	100	100
22	W	108/114 (95%)	107 (99%)	1 (1%)	75	83
23	X	153/154 (99%)	153 (100%)	0	100	100
24	Y	105/107 (98%)	105 (100%)	0	100	100
25	Z	120/123 (98%)	120 (100%)	0	100	100
26	a	58/58 (100%)	58 (100%)	0	100	100
27	b	72/73 (99%)	72 (100%)	0	100	100
28	c	40/67 (60%)	40 (100%)	0	100	100
29	d	106/107 (99%)	106 (100%)	0	100	100
30	e	92/94 (98%)	91 (99%)	1 (1%)	70	79
31	f	47/53 (89%)	47 (100%)	0	100	100
32	g	93/129 (72%)	93 (100%)	0	100	100
33	h	122/162 (75%)	122 (100%)	0	100	100
34	i	90/120 (75%)	89 (99%)	1 (1%)	70	79
35	j	58/87 (67%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	k	60/78 (77%)	59 (98%)	1 (2%)	56	72
37	l	141/161 (88%)	141 (100%)	0	100	100
38	m	111/114 (97%)	111 (100%)	0	100	100
39	n	161/164 (98%)	160 (99%)	1 (1%)	84	88
40	o	106/121 (88%)	106 (100%)	0	100	100
41	p	153/158 (97%)	153 (100%)	0	100	100
42	q	129/131 (98%)	128 (99%)	1 (1%)	79	85
43	r	86/95 (90%)	86 (100%)	0	100	100
44	s	38/95 (40%)	38 (100%)	0	100	100
All	All	7060/7946 (89%)	7045 (100%)	15 (0%)	91	94

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	195	ARG
7	G	495	ARG
7	G	515	ARG
7	G	679	ARG
13	M	340	ARG
16	P	174	ARG
16	P	177	ARG
18	R	80	LYS
20	T	12	LYS
22	W	59	LYS
30	e	100	ARG
34	i	120	ARG
36	k	25	ARG
39	n	174	ARG
42	q	60	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
2	B	172	GLN
3	C	41	GLN
3	C	88	ASN
3	C	144	ASN

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Mol	Chain	Res	Type
4	D	3	GLN
4	D	347	HIS
4	D	421	GLN
5	E	27	ASN
5	E	55	GLN
5	E	91	ASN
5	E	101	GLN
5	E	155	GLN
6	F	96	ASN
6	F	144	ASN
6	F	356	HIS
6	F	437	HIS
7	G	179	ASN
7	G	313	ASN
7	G	401	HIS
7	G	421	HIS
7	G	546	GLN
8	H	235	ASN
8	H	258	ASN
8	H	304	HIS
10	J	3	ASN
11	K	92	ASN
12	L	328	HIS
12	L	354	GLN
12	L	505	ASN
12	L	534	HIS
12	L	572	ASN
12	L	594	ASN
13	M	51	ASN
13	M	81	GLN
13	M	138	ASN
13	M	170	HIS
13	M	338	HIS
13	M	374	ASN
13	M	422	HIS
14	N	87	GLN
14	N	172	GLN
14	N	174	GLN
15	O	19	HIS
15	O	50	HIS
15	O	57	GLN
15	O	120	GLN

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Mol	Chain	Res	Type
15	O	141	GLN
16	P	2	HIS
16	P	36	ASN
16	P	131	HIS
16	P	134	HIS
16	P	240	HIS
18	R	3	GLN
18	R	68	HIS
20	U	33	ASN
20	U	74	GLN
23	X	34	GLN
23	X	101	GLN
23	X	102	GLN
23	X	108	GLN
23	X	142	HIS
24	Y	18	GLN
25	Z	23	ASN
25	Z	75	GLN
25	Z	89	ASN
25	Z	134	ASN
26	a	68	ASN
27	b	51	ASN
30	e	76	HIS
30	e	97	HIS
33	h	44	ASN
33	h	135	HIS
37	l	2	HIS
37	l	65	HIS
37	l	71	ASN
37	l	77	HIS
37	l	103	HIS
38	m	74	ASN
38	m	125	ASN
40	o	84	HIS
41	p	90	GLN
41	p	119	ASN
41	p	158	GLN
42	q	12	GLN
42	q	123	GLN
43	r	109	GLN
44	s	34	ASN
44	s	38	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 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	$\# Z > 2$
8	FME	H	1	8	8,9,10	0.93	0	7,9,11	1.13	1 (14%)
13	FME	M	1	13	8,9,10	0.95	0	7,9,11	0.67	0
43	AYA	r	1	43	6,7,8	1.29	1 (16%)	5,8,10	1.26	1 (20%)
1	FME	A	1	1	8,9,10	0.89	0	7,9,11	1.46	1 (14%)
12	FME	L	1	12	8,9,10	0.95	0	7,9,11	0.93	0
10	FME	J	1	10	8,9,10	0.92	0	7,9,11	0.85	0
4	2MR	D	85	4	10,12,13	2.46	2 (20%)	5,13,15	1.72	2 (40%)
11	FME	K	1	11	8,9,10	0.94	0	7,9,11	1.35	1 (14%)
14	FME	N	1	14	8,9,10	0.89	0	7,9,11	1.22	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
8	FME	H	1	8	-	2/7/9/11	-
13	FME	M	1	13	-	1/7/9/11	-
43	AYA	r	1	43	-	1/4/6/8	-
1	FME	A	1	1	-	4/7/9/11	-
12	FME	L	1	12	-	3/7/9/11	-
10	FME	J	1	10	-	1/7/9/11	-
4	2MR	D	85	4	-	3/10/13/15	-
11	FME	K	1	11	-	3/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	N	1	14	-	4/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NE	5.31	1.45	1.34
4	D	85	2MR	CZ-NH2	4.94	1.44	1.33
43	r	1	AYA	CA-N	-2.54	1.43	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	C-CA-N	3.12	115.36	109.73
11	K	1	FME	C-CA-N	2.90	114.97	109.73
4	D	85	2MR	CD-NE-CZ	2.87	128.79	123.41
43	r	1	AYA	CB-CA-N	2.50	112.39	109.61
4	D	85	2MR	NE-CZ-NH2	-2.46	117.23	119.48
8	H	1	FME	C-CA-N	2.38	114.04	109.73
14	N	1	FME	CA-N-CN	2.09	126.04	122.82

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O-C-CA-CB
8	H	1	FME	CB-CA-N-CN
8	H	1	FME	CA-CB-CG-SD
11	K	1	FME	N-CA-CB-CG
12	L	1	FME	O-C-CA-CB
12	L	1	FME	CA-CB-CG-SD
13	M	1	FME	O-C-CA-CB
14	N	1	FME	CB-CA-N-CN
14	N	1	FME	C-CA-CB-CG
14	N	1	FME	O-C-CA-CB
4	D	85	2MR	NE-CD-CG-CB
12	L	1	FME	CB-CG-SD-CE
1	A	1	FME	N-CA-CB-CG
14	N	1	FME	N-CA-CB-CG
1	A	1	FME	CB-CG-SD-CE
10	J	1	FME	CB-CG-SD-CE
43	r	1	AYA	C-CA-N-CT

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Mol	Chain	Res	Type	Atoms
11	K	1	FME	CB-CG-SD-CE
11	K	1	FME	C-CA-CB-CG
4	D	85	2MR	CA-CB-CG-CD
1	A	1	FME	CB-CA-N-CN
4	D	85	2MR	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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	$\# Z > 2$
47	FES	G	803	7	0,4,4	-	-	-		
45	SF4	B	201	2	0,12,12	-	-	-		
47	FES	E	301	5	0,4,4	-	-	-		
50	CDL	d	201	-	49,49,99	1.22	7 (14%)	55,61,111	1.35	5 (9%)
54	EHZ	U	201	20	29,36,37	1.72	5 (17%)	35,44,47	1.55	6 (17%)
50	CDL	L	702	-	53,53,99	1.18	8 (15%)	59,65,111	1.13	4 (6%)
45	SF4	I	201	9	0,12,12	-	-	-		
45	SF4	I	202	9	0,12,12	-	-	-		
49	3PE	H	401	-	41,41,50	0.95	4 (9%)	44,46,55	1.26	4 (9%)
45	SF4	G	801	7	0,12,12	-	-	-		
45	SF4	G	802	7	0,12,12	-	-	-		
51	ATP	O	401	-	26,33,33	0.92	1 (3%)	31,52,52	1.73	5 (16%)
52	NDP	P	501	-	45,52,52	2.23	5 (11%)	53,80,80	1.76	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PC1	B	202	-	25,25,53	1.36	4 (16%)	31,33,61	1.10	2 (6%)
49	3PE	J	401	-	37,37,50	0.99	4 (10%)	40,42,55	1.11	2 (5%)
45	SF4	F	502	6	0,12,12	-	-	-	-	-
49	3PE	L	701	-	44,44,50	0.90	4 (9%)	47,49,55	1.12	2 (4%)
48	FMN	F	501	-	33,33,33	1.09	2 (6%)	48,50,50	1.25	9 (18%)
49	3PE	M	501	-	37,37,50	0.99	4 (10%)	40,42,55	1.10	2 (5%)
54	EHZ	T	201	20	29,36,37	1.69	5 (17%)	35,44,47	1.53	4 (11%)

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
47	FES	G	803	7	-	-	0/1/1/1
45	SF4	B	201	2	-	-	0/6/5/5
47	FES	E	301	5	-	-	0/1/1/1
50	CDL	d	201	-	-	22/59/59/110	-
54	EHZ	U	201	20	-	24/42/44/45	-
50	CDL	L	702	-	-	25/64/64/110	-
45	SF4	I	201	9	-	-	0/6/5/5
45	SF4	I	202	9	-	-	0/6/5/5
49	3PE	H	401	-	-	13/45/45/54	-
45	SF4	G	801	7	-	-	0/6/5/5
45	SF4	G	802	7	-	-	0/6/5/5
51	ATP	O	401	-	-	5/18/38/38	0/3/3/3
52	NDP	P	501	-	-	9/30/77/77	0/5/5/5
46	PC1	B	202	-	-	15/29/29/57	-
49	3PE	J	401	-	-	18/41/41/54	-
45	SF4	F	502	6	-	-	0/6/5/5
49	3PE	L	701	-	-	25/48/48/54	-
48	FMN	F	501	-	-	10/18/18/18	0/3/3/3
49	3PE	M	501	-	-	23/41/41/54	-
54	EHZ	T	201	20	-	15/42/44/45	-

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	P	501	NDP	P2B-O2B	12.32	1.82	1.59
54	U	201	EHZ	C15-N2	5.60	1.45	1.33
54	T	201	EHZ	C15-N2	5.51	1.45	1.33
54	U	201	EHZ	C12-N1	5.38	1.45	1.33
54	T	201	EHZ	C12-N1	5.28	1.45	1.33
52	P	501	NDP	PN-O5D	4.09	1.75	1.59
48	F	501	FMN	C4A-N5	3.70	1.37	1.30
52	P	501	NDP	O2B-C2B	-3.14	1.32	1.44
50	d	201	CDL	OA6-CA4	-2.65	1.40	1.46
50	L	702	CDL	OB6-CB4	-2.63	1.40	1.46
50	L	702	CDL	OA6-CA4	-2.61	1.40	1.46
49	J	401	3PE	O21-C2	-2.57	1.40	1.46
49	M	501	3PE	O21-C2	-2.55	1.40	1.46
48	F	501	FMN	C10-N1	2.55	1.38	1.33
50	L	702	CDL	OB8-CB7	2.52	1.40	1.33
46	B	202	PC1	O21-C2	-2.51	1.40	1.46
50	d	201	CDL	OA8-CA7	2.50	1.40	1.33
50	d	201	CDL	OB8-CB7	2.49	1.40	1.33
50	L	702	CDL	OA8-CA7	2.46	1.40	1.33
54	U	201	EHZ	C9-S1	2.45	1.82	1.76
49	H	401	3PE	O31-C31	2.40	1.40	1.33
49	H	401	3PE	O21-C2	-2.39	1.40	1.46
49	M	501	3PE	O31-C31	2.35	1.40	1.33
54	T	201	EHZ	C9-S1	2.34	1.81	1.76
51	O	401	ATP	C5-C4	2.31	1.47	1.40
54	U	201	EHZ	O4-C15	-2.30	1.18	1.23
50	d	201	CDL	OB6-CB5	2.29	1.40	1.34
54	T	201	EHZ	O4-C15	-2.28	1.18	1.23
46	B	202	PC1	O31-C31	2.27	1.40	1.33
49	L	701	3PE	O31-C31	2.27	1.40	1.33
46	B	202	PC1	O31-C3	-2.26	1.40	1.45
49	L	701	3PE	O21-C21	2.25	1.40	1.34
49	J	401	3PE	O31-C31	2.25	1.39	1.33
49	J	401	3PE	O31-C3	-2.24	1.40	1.45
50	d	201	CDL	OB6-CB4	-2.24	1.41	1.46
49	L	701	3PE	O31-C3	-2.21	1.40	1.45
54	U	201	EHZ	O3-C12	-2.20	1.18	1.23
50	d	201	CDL	OA6-CA5	2.20	1.40	1.35
54	T	201	EHZ	O3-C12	-2.19	1.18	1.23
52	P	501	NDP	O5D-C5D	-2.17	1.36	1.44
49	H	401	3PE	O21-C21	2.17	1.40	1.34
49	M	501	3PE	O31-C3	-2.16	1.40	1.45
46	B	202	PC1	O21-C21	2.15	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	P	501	NDP	C7N-N7N	2.15	1.39	1.33
50	L	702	CDL	OA6-CA5	2.14	1.40	1.34
50	d	201	CDL	OB8-CB6	-2.14	1.40	1.45
49	L	701	3PE	O21-C2	-2.11	1.41	1.46
50	L	702	CDL	OB6-CB5	2.11	1.40	1.34
49	J	401	3PE	O21-C21	2.09	1.40	1.34
50	L	702	CDL	OA8-CA6	-2.09	1.40	1.45
49	M	501	3PE	O21-C21	2.06	1.40	1.34
49	H	401	3PE	O31-C3	-2.05	1.40	1.45
50	L	702	CDL	OB8-CB6	-2.04	1.40	1.45

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	P	501	NDP	PN-O3-PA	-7.51	107.07	132.83
54	T	201	EHZ	C8-C9-S1	5.46	120.39	113.63
54	U	201	EHZ	C8-C9-S1	5.36	120.26	113.63
50	d	201	CDL	OA6-CA5-C11	4.75	119.83	111.09
49	L	701	3PE	O21-C21-C22	4.64	121.51	111.50
51	O	401	ATP	PA-O3A-PB	-4.55	117.21	132.83
50	d	201	CDL	OB6-CB5-C51	4.30	120.78	111.50
51	O	401	ATP	PB-O3B-PG	-4.00	119.11	132.83
49	J	401	3PE	O21-C21-C22	3.98	120.07	111.50
50	L	702	CDL	OB6-CB5-C51	3.81	119.72	111.50
49	M	501	3PE	O21-C21-C22	3.77	119.62	111.50
46	B	202	PC1	O21-C21-C22	3.70	119.47	111.50
49	H	401	3PE	O21-C21-C22	3.64	119.34	111.50
51	O	401	ATP	N3-C2-N1	-3.61	123.03	128.68
50	L	702	CDL	OA6-CA5-C11	3.33	120.08	110.80
51	O	401	ATP	C3'-C2'-C1'	3.28	105.92	100.98
48	F	501	FMN	C4-N3-C2	-3.21	119.71	125.64
52	P	501	NDP	O2B-P2B-O1X	-3.18	97.13	109.39
52	P	501	NDP	PA-O5B-C5B	-3.16	103.15	121.68
49	H	401	3PE	O31-C31-C32	3.13	121.72	111.91
50	d	201	CDL	OB8-CB7-C71	3.00	121.33	111.91
52	P	501	NDP	PN-O5D-C5D	-2.78	105.38	121.68
49	M	501	3PE	O31-C31-C32	2.70	120.37	111.91
48	F	501	FMN	C4A-C4-N3	2.68	120.00	113.19
54	U	201	EHZ	C18-C17-C16	2.66	113.43	108.82
49	H	401	3PE	C2-O21-C21	-2.65	111.26	117.79
48	F	501	FMN	O4-C4-C4A	-2.64	119.60	126.60
50	d	201	CDL	OA8-CA7-C31	2.64	120.19	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	H	401	3PE	C24-C23-C22	-2.53	104.10	113.19
50	L	702	CDL	OA8-CA7-C31	2.51	119.80	111.91
52	P	501	NDP	O3X-P2B-O2X	2.51	117.24	107.64
50	d	201	CDL	CA4-OA6-CA5	-2.50	113.23	117.90
54	T	201	EHZ	O2-C9-S1	-2.49	119.39	122.61
46	B	202	PC1	O31-C31-C32	2.48	119.68	111.91
50	L	702	CDL	OB8-CB7-C71	2.47	119.67	111.91
54	U	201	EHZ	C10-S1-C9	2.47	109.57	101.87
51	O	401	ATP	C4-C5-N7	-2.46	106.84	109.40
54	U	201	EHZ	C16-C15-N2	2.45	121.46	116.58
48	F	501	FMN	C4A-C10-N1	-2.43	119.10	124.73
49	J	401	3PE	O31-C31-C32	2.42	119.51	111.91
49	L	701	3PE	O31-C31-C32	2.37	119.36	111.91
52	P	501	NDP	C2A-N1A-C6A	-2.36	114.72	118.75
48	F	501	FMN	C4A-C10-N10	2.32	119.88	116.48
54	U	201	EHZ	O2-C9-S1	-2.24	119.71	122.61
48	F	501	FMN	C9A-C5A-N5	-2.18	120.06	122.43
52	P	501	NDP	O2N-PN-O1N	2.17	122.96	112.24
48	F	501	FMN	C5A-C9A-N10	2.16	120.18	117.95
52	P	501	NDP	O4B-C4B-C3B	2.12	109.32	105.11
48	F	501	FMN	C4-C4A-C10	2.12	120.35	116.79
48	F	501	FMN	C10-C4A-N5	-2.08	120.44	124.86
54	T	201	EHZ	C13-C12-N1	2.05	119.87	116.42
54	U	201	EHZ	C7-C8-C9	-2.03	109.27	113.89
54	T	201	EHZ	C10-S1-C9	2.00	108.10	101.87

There are no chirality outliers.

All (204) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	B	202	PC1	C1-O11-P-O12
46	B	202	PC1	C1-O11-P-O14
46	B	202	PC1	O13-C11-C12-N
48	F	501	FMN	N10-C1'-C2'-O2'
48	F	501	FMN	N10-C1'-C2'-C3'
48	F	501	FMN	C2'-C3'-C4'-O4'
48	F	501	FMN	C2'-C3'-C4'-C5'
48	F	501	FMN	O3'-C3'-C4'-O4'
49	H	401	3PE	C1-O11-P-O12
49	H	401	3PE	C1-O11-P-O13
49	H	401	3PE	C1-O11-P-O14
49	H	401	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
49	J	401	3PE	O11-C1-C2-O21
49	J	401	3PE	O22-C21-O21-C2
49	L	701	3PE	C1-O11-P-O12
49	L	701	3PE	C11-O13-P-O12
49	L	701	3PE	C11-O13-P-O14
49	L	701	3PE	O13-C11-C12-N
49	L	701	3PE	O22-C21-O21-C2
49	M	501	3PE	C1-O11-P-O12
49	M	501	3PE	C1-O11-P-O14
49	M	501	3PE	O13-C11-C12-N
49	M	501	3PE	C22-C21-O21-C2
50	L	702	CDL	C51-CB5-OB6-CB4
50	d	201	CDL	O1-C1-CB2-OB2
50	d	201	CDL	OB7-CB5-OB6-CB4
50	d	201	CDL	C71-CB7-OB8-CB6
51	O	401	ATP	PB-O3B-PG-O3G
51	O	401	ATP	C5'-O5'-PA-O1A
51	O	401	ATP	C5'-O5'-PA-O2A
52	P	501	NDP	C5D-O5D-PN-O1N
54	T	201	EHZ	C11-C10-S1-C9
54	T	201	EHZ	N2-C15-C16-C17
54	T	201	EHZ	N2-C15-C16-O5
54	T	201	EHZ	O4-C15-C16-C17
54	T	201	EHZ	O2-C9-S1-C10
54	T	201	EHZ	C8-C9-S1-C10
54	U	201	EHZ	O1-C7-C8-C9
54	U	201	EHZ	C7-C8-C9-S1
54	U	201	EHZ	N2-C15-C16-C17
54	U	201	EHZ	N2-C15-C16-O5
54	U	201	EHZ	O4-C15-C16-C17
54	U	201	EHZ	O4-C15-C16-O5
54	U	201	EHZ	C15-C16-C17-C18
54	U	201	EHZ	C15-C16-C17-C19
54	U	201	EHZ	C15-C16-C17-C20
54	U	201	EHZ	O5-C16-C17-C18
54	U	201	EHZ	O5-C16-C17-C19
54	U	201	EHZ	O5-C16-C17-C20
54	U	201	EHZ	O2-C9-S1-C10
54	U	201	EHZ	C8-C9-S1-C10
50	d	201	CDL	C11-CA5-OA6-CA4
46	B	202	PC1	O32-C31-O31-C3
50	d	201	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
49	J	401	3PE	O32-C31-O31-C3
50	d	201	CDL	OA7-CA5-OA6-CA4
49	H	401	3PE	O22-C21-O21-C2
49	M	501	3PE	O22-C21-O21-C2
50	L	702	CDL	OB7-CB5-OB6-CB4
46	B	202	PC1	C32-C31-O31-C3
49	J	401	3PE	C22-C21-O21-C2
49	L	701	3PE	C22-C21-O21-C2
50	d	201	CDL	C51-CB5-OB6-CB4
49	J	401	3PE	C32-C31-O31-C3
49	M	501	3PE	C32-C31-O31-C3
49	M	501	3PE	O32-C31-O31-C3
52	P	501	NDP	O4D-C1D-N1N-C6N
50	L	702	CDL	O1-C1-CB2-OB2
48	F	501	FMN	O3'-C3'-C4'-C5'
54	T	201	EHZ	C13-C14-N2-C15
50	L	702	CDL	CA2-C1-CB2-OB2
49	J	401	3PE	C31-C32-C33-C34
49	M	501	3PE	C21-C22-C23-C24
46	B	202	PC1	C11-O13-P-O11
46	B	202	PC1	C1-O11-P-O13
49	J	401	3PE	C11-O13-P-O11
49	L	701	3PE	C1-O11-P-O13
49	L	701	3PE	C11-O13-P-O11
49	M	501	3PE	C1-O11-P-O13
50	L	702	CDL	CA2-OA2-PA1-OA5
50	d	201	CDL	CA2-C1-CB2-OB2
50	L	702	CDL	C11-CA5-OA6-CA4
50	L	702	CDL	C74-C75-C76-C77
49	L	701	3PE	C3-C2-O21-C21
50	L	702	CDL	OA7-CA5-OA6-CA4
49	M	501	3PE	C35-C36-C37-C38
49	L	701	3PE	C2A-C2B-C2C-C2D
49	L	701	3PE	C22-C23-C24-C25
49	L	701	3PE	C35-C36-C37-C38
54	T	201	EHZ	C3-C4-C5-C6
49	J	401	3PE	C23-C24-C25-C26
50	L	702	CDL	C52-C53-C54-C55
54	U	201	EHZ	S1-C10-C11-N1
49	M	501	3PE	C3E-C3F-C3G-C3H
50	L	702	CDL	C71-C72-C73-C74
50	d	201	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
49	L	701	3PE	C33-C34-C35-C36
54	U	201	EHZ	C2-C3-C4-C5
54	T	201	EHZ	C1-C21-C22-C23
54	U	201	EHZ	C13-C14-N2-C15
50	d	201	CDL	OA5-CA3-CA4-OA6
54	U	201	EHZ	C21-C22-C23-C24
49	M	501	3PE	C3A-C3B-C3C-C3D
49	J	401	3PE	C22-C23-C24-C25
48	F	501	FMN	O2'-C2'-C3'-C4'
49	M	501	3PE	C39-C3A-C3B-C3C
49	L	701	3PE	C1-C2-C3-O31
49	H	401	3PE	C33-C34-C35-C36
49	J	401	3PE	C34-C35-C36-C37
50	L	702	CDL	C76-C77-C78-C79
54	T	201	EHZ	O4-C15-C16-O5
49	L	701	3PE	C21-C22-C23-C24
50	d	201	CDL	OB6-CB4-CB6-OB8
50	d	201	CDL	C56-C57-C58-C59
54	U	201	EHZ	C5-C6-C7-C8
49	J	401	3PE	O11-C1-C2-C3
49	M	501	3PE	O11-C1-C2-C3
50	d	201	CDL	OA5-CA3-CA4-CA6
49	H	401	3PE	C3B-C3C-C3D-C3E
49	M	501	3PE	C3C-C3D-C3E-C3F
46	B	202	PC1	C2-C1-O11-P
50	L	702	CDL	C51-C52-C53-C54
49	M	501	3PE	C32-C33-C34-C35
50	d	201	CDL	CB3-CB4-CB6-OB8
54	U	201	EHZ	C7-C8-C9-O2
49	M	501	3PE	C36-C37-C38-C39
54	U	201	EHZ	C5-C6-C7-O1
49	M	501	3PE	C33-C34-C35-C36
49	L	701	3PE	C28-C29-C2A-C2B
49	L	701	3PE	C34-C35-C36-C37
50	L	702	CDL	C72-C73-C74-C75
49	J	401	3PE	C3-C2-O21-C21
54	T	201	EHZ	C12-C13-C14-N2
50	L	702	CDL	C1-CA2-OA2-PA1
50	L	702	CDL	CA4-CA3-OA5-PA1
49	M	501	3PE	O11-C1-C2-O21
49	H	401	3PE	C35-C36-C37-C38
54	T	201	EHZ	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
49	H	401	3PE	C28-C29-C2A-C2B
52	P	501	NDP	C5D-O5D-PN-O3
52	P	501	NDP	PN-O3-PA-O2A
50	d	201	CDL	C52-C53-C54-C55
50	L	702	CDL	C31-CA7-OA8-CA6
46	B	202	PC1	C11-O13-P-O12
46	B	202	PC1	C11-O13-P-O14
49	J	401	3PE	C11-O13-P-O12
49	J	401	3PE	C11-O13-P-O14
49	L	701	3PE	C1-O11-P-O14
50	L	702	CDL	CA2-OA2-PA1-OA4
52	P	501	NDP	C5D-O5D-PN-O2N
54	U	201	EHZ	C6-C7-C8-C9
49	J	401	3PE	O13-C11-C12-N
48	F	501	FMN	C1'-C2'-C3'-O3'
54	U	201	EHZ	C1-C2-C3-C4
50	L	702	CDL	OA9-CA7-OA8-CA6
54	U	201	EHZ	C21-C1-C2-C3
49	H	401	3PE	C3A-C3B-C3C-C3D
50	d	201	CDL	CB3-CB4-OB6-CB5
49	L	701	3PE	C37-C38-C39-C3A
49	M	501	3PE	C2-C1-O11-P
49	M	501	3PE	C3F-C3G-C3H-C3I
49	L	701	3PE	O21-C2-C3-O31
50	L	702	CDL	CA3-OA5-PA1-OA2
50	L	702	CDL	CB2-OB2-PB2-OB5
50	d	201	CDL	CA3-OA5-PA1-OA2
50	d	201	CDL	CB3-OB5-PB2-OB2
49	L	701	3PE	C3A-C3B-C3C-C3D
50	d	201	CDL	C54-C55-C56-C57
54	T	201	EHZ	C1-C2-C3-C4
49	L	701	3PE	C26-C27-C28-C29
54	T	201	EHZ	S1-C10-C11-N1
49	H	401	3PE	C24-C25-C26-C27
49	M	501	3PE	C3D-C3E-C3F-C3G
52	P	501	NDP	C1B-C2B-O2B-P2B
49	L	701	3PE	C2B-C2C-C2D-C2E
46	B	202	PC1	O22-C21-O21-C2
54	T	201	EHZ	C2-C1-C21-C22
49	H	401	3PE	C36-C37-C38-C39
49	H	401	3PE	C2A-C2B-C2C-C2D
50	L	702	CDL	OB6-CB4-CB6-OB8

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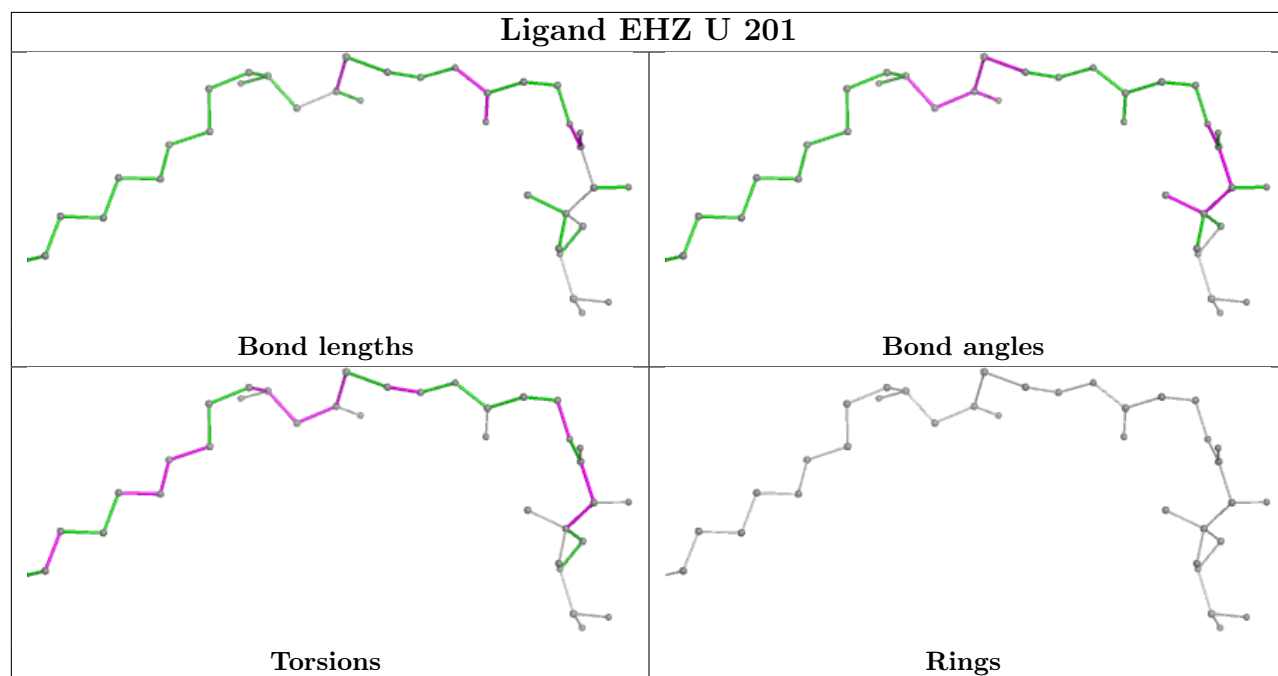
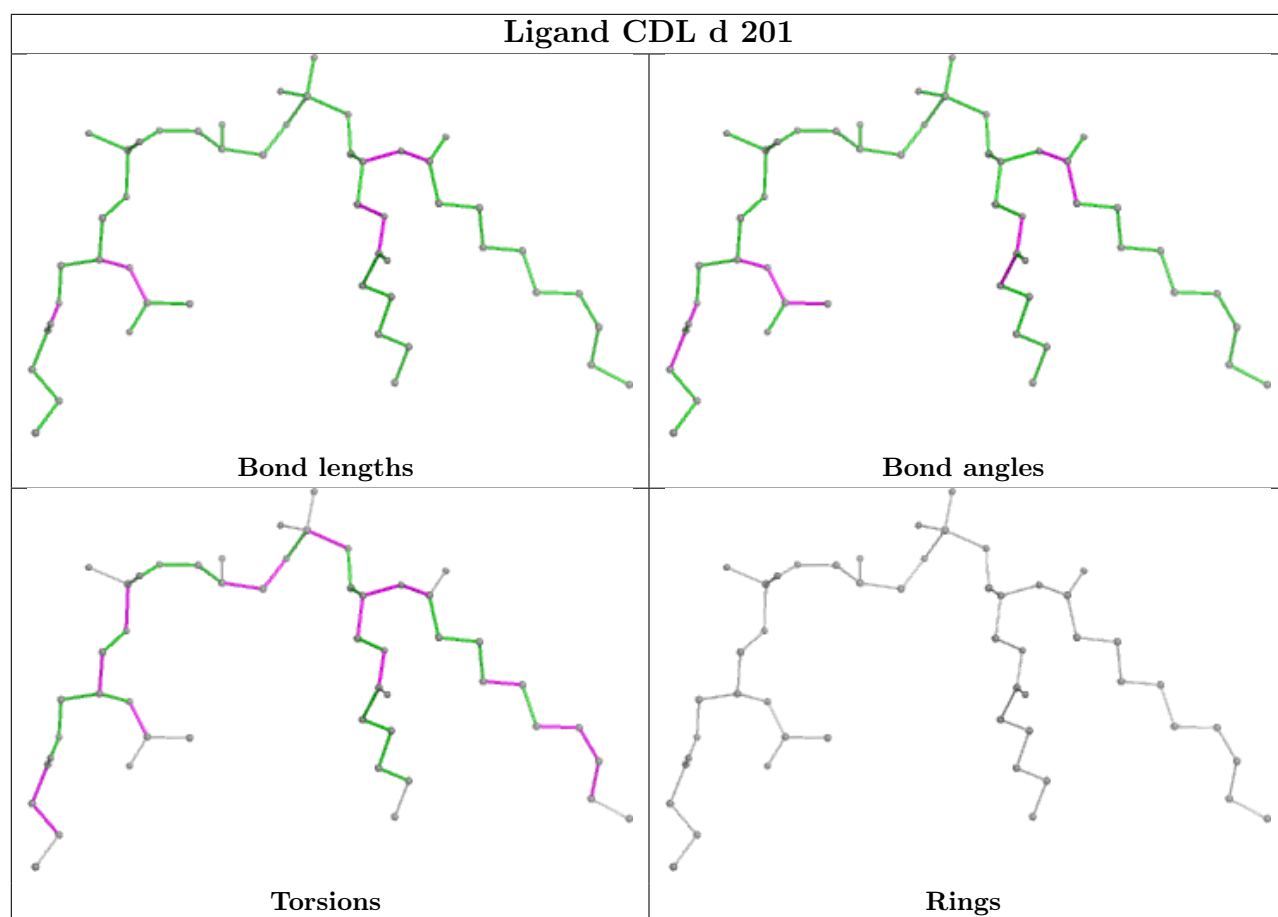
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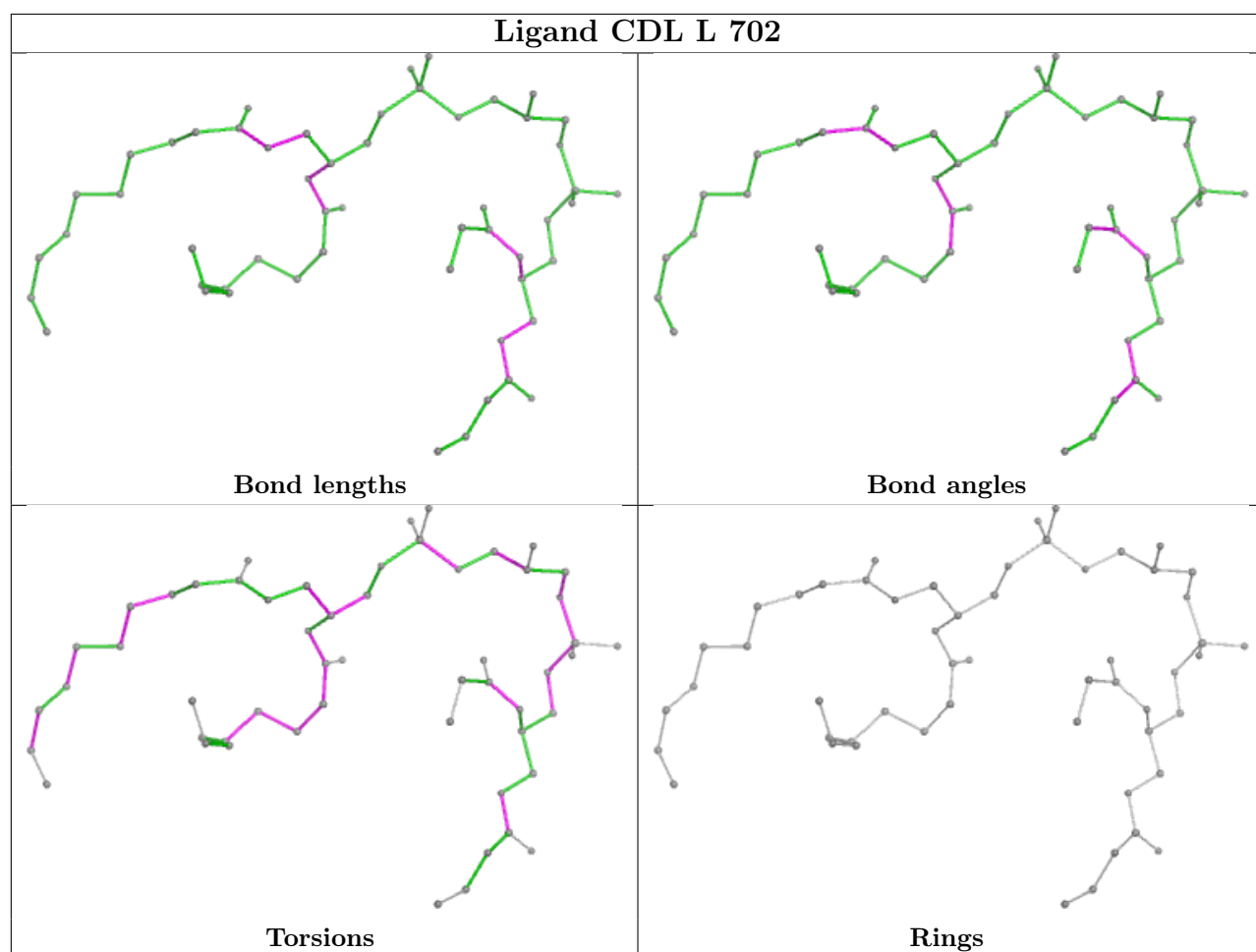
Mol	Chain	Res	Type	Atoms
50	d	201	CDL	C1-CB2-OB2-PB2
49	J	401	3PE	O31-C31-C32-C33
46	B	202	PC1	O21-C21-C22-C23
51	O	401	ATP	C5'-O5'-PA-O3A
52	P	501	NDP	O4D-C4D-C5D-O5D
52	P	501	NDP	PN-O3-PA-O1A
46	B	202	PC1	C22-C21-O21-C2
49	L	701	3PE	C24-C25-C26-C27
49	J	401	3PE	O32-C31-C32-C33
48	F	501	FMN	O2'-C2'-C3'-O3'
49	L	701	3PE	C36-C37-C38-C39
51	O	401	ATP	O4'-C4'-C5'-O5'
46	B	202	PC1	O22-C21-C22-C23
50	L	702	CDL	CB5-C51-C52-C53
46	B	202	PC1	C12-C11-O13-P
49	M	501	3PE	C12-C11-O13-P
50	d	201	CDL	C55-C56-C57-C58
52	P	501	NDP	C3B-C2B-O2B-P2B
50	L	702	CDL	OB5-CB3-CB4-OB6
49	J	401	3PE	C37-C38-C39-C3A
50	L	702	CDL	C52-C51-CB5-OB6
48	F	501	FMN	C2'-C1'-N10-C10
50	d	201	CDL	C32-C31-CA7-OA8
50	L	702	CDL	C52-C51-CB5-OB7

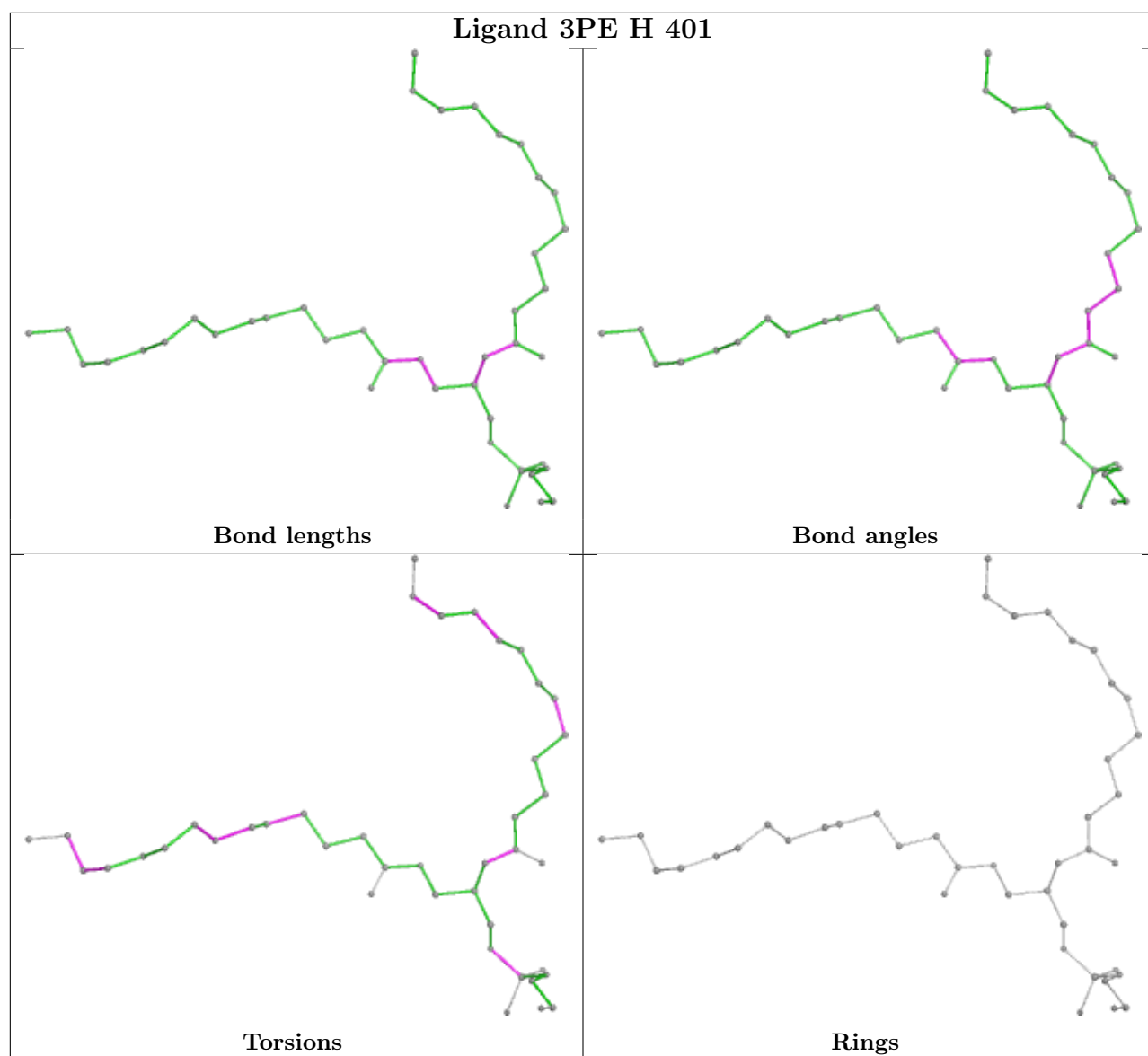
There are no ring outliers.

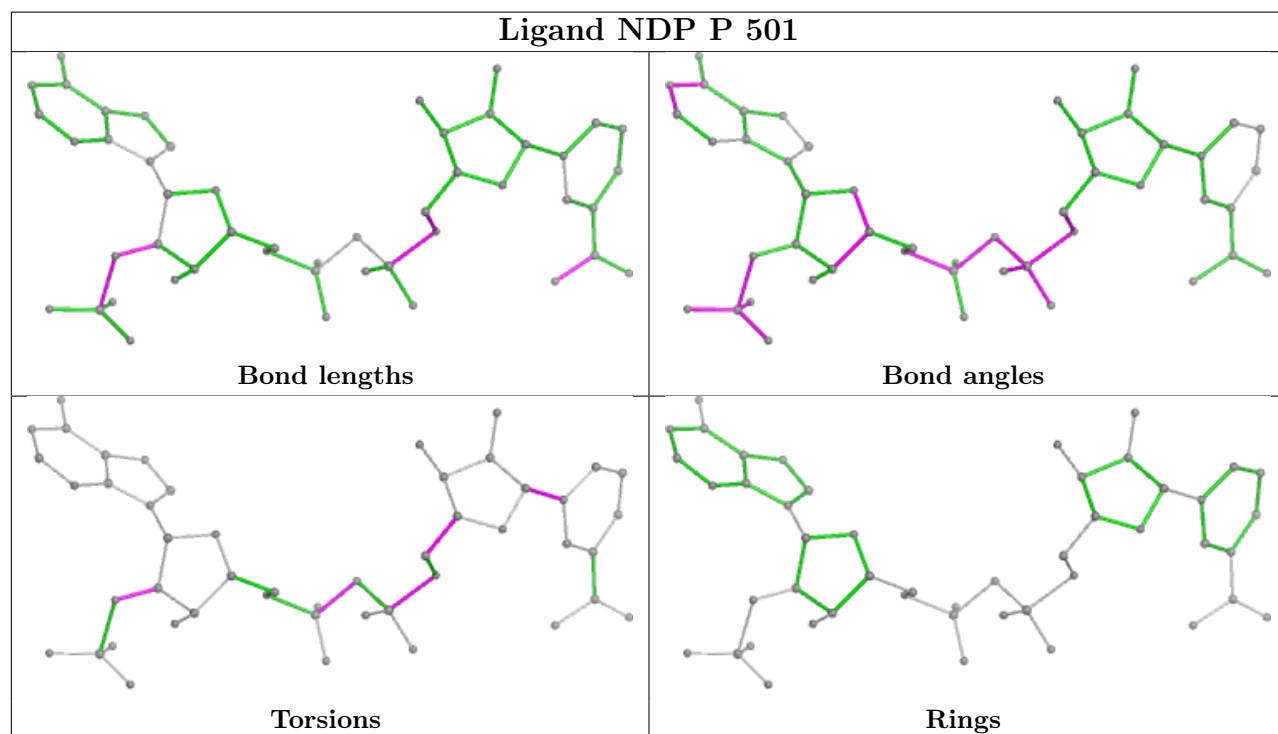
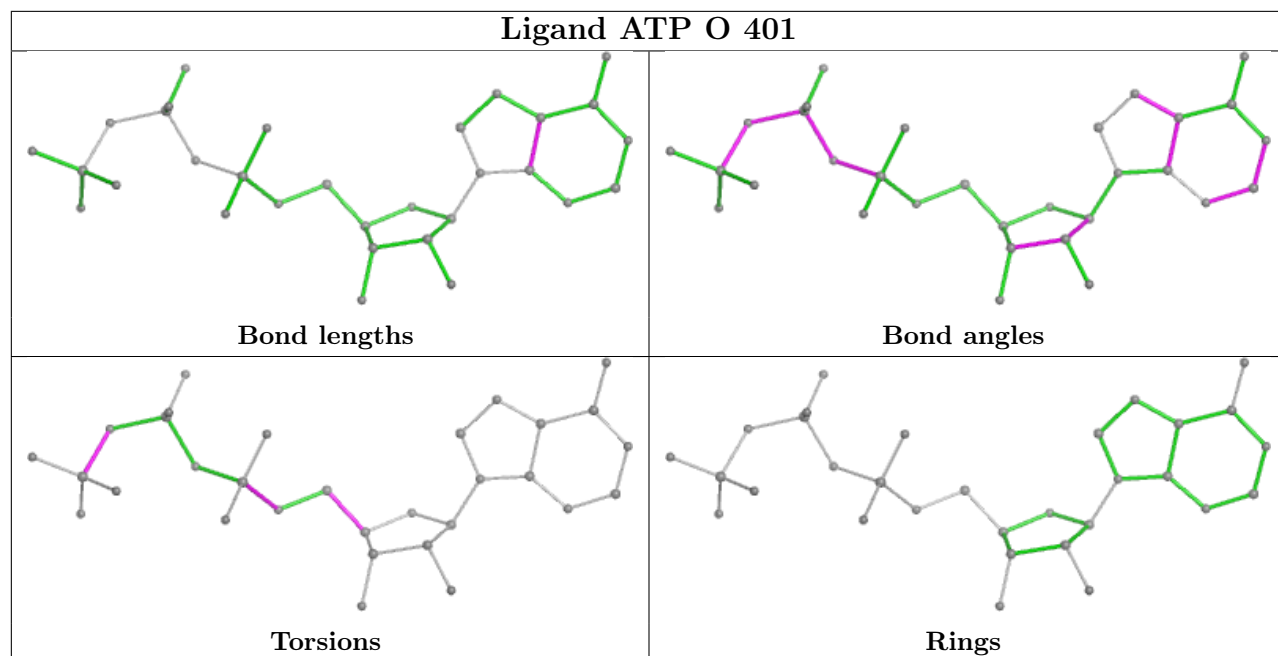
No monomer is involved in short contacts.

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.

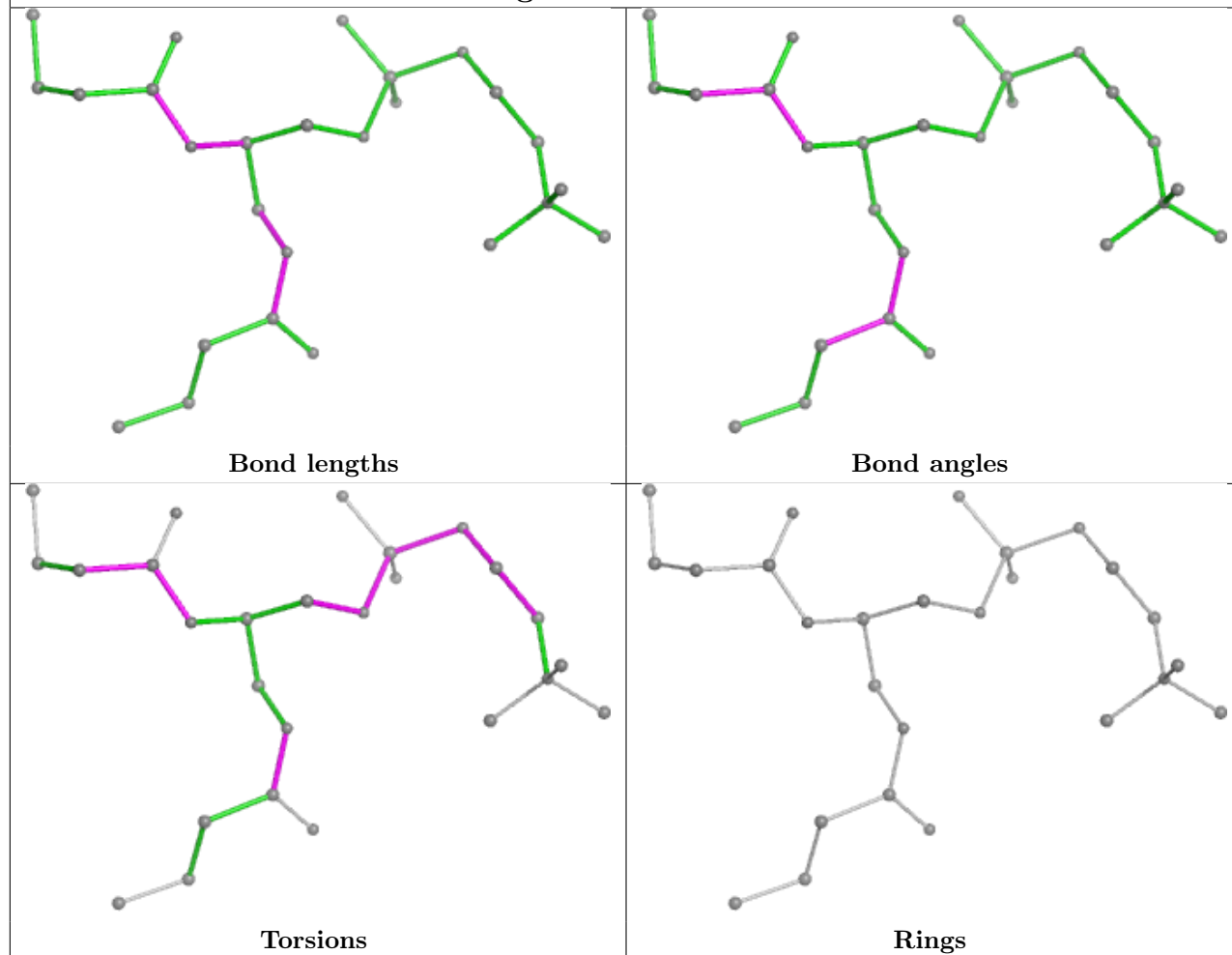




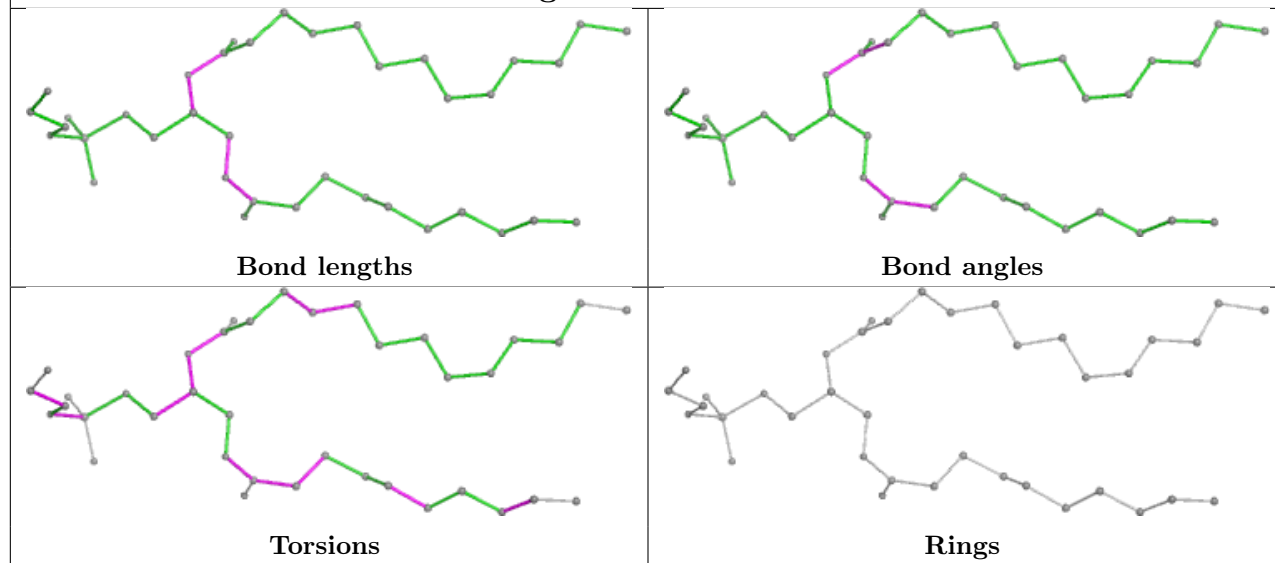


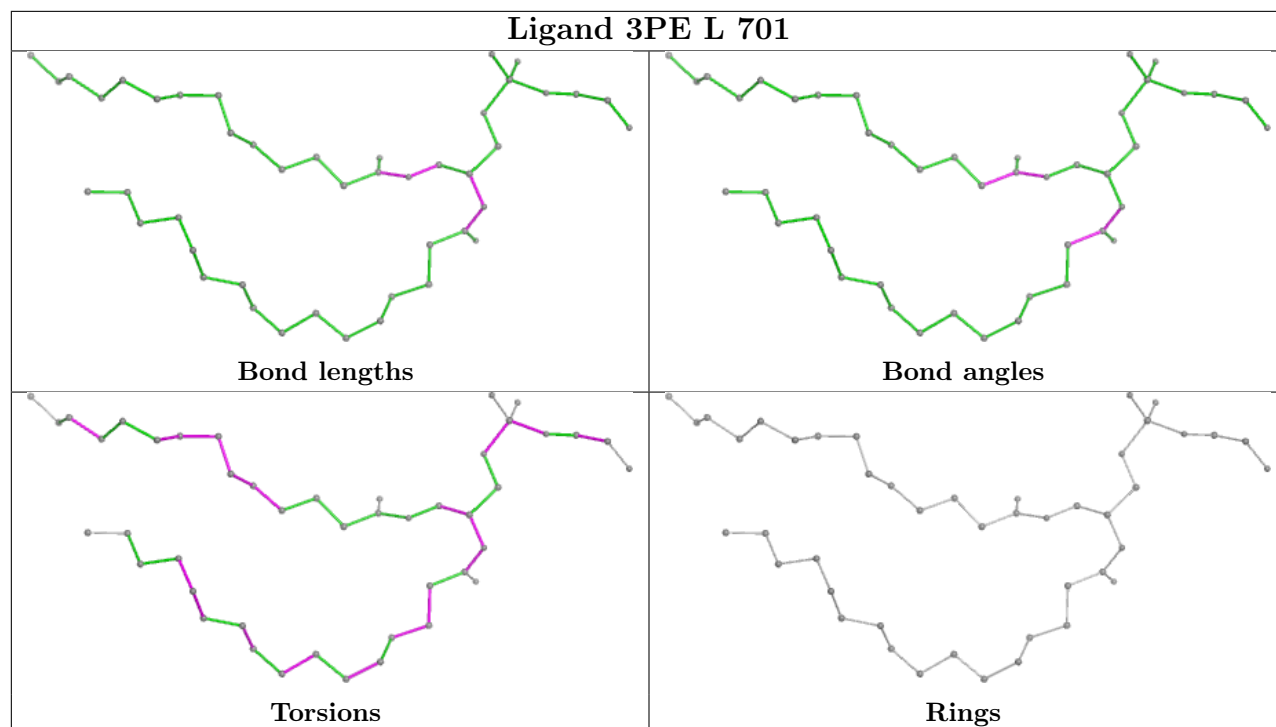


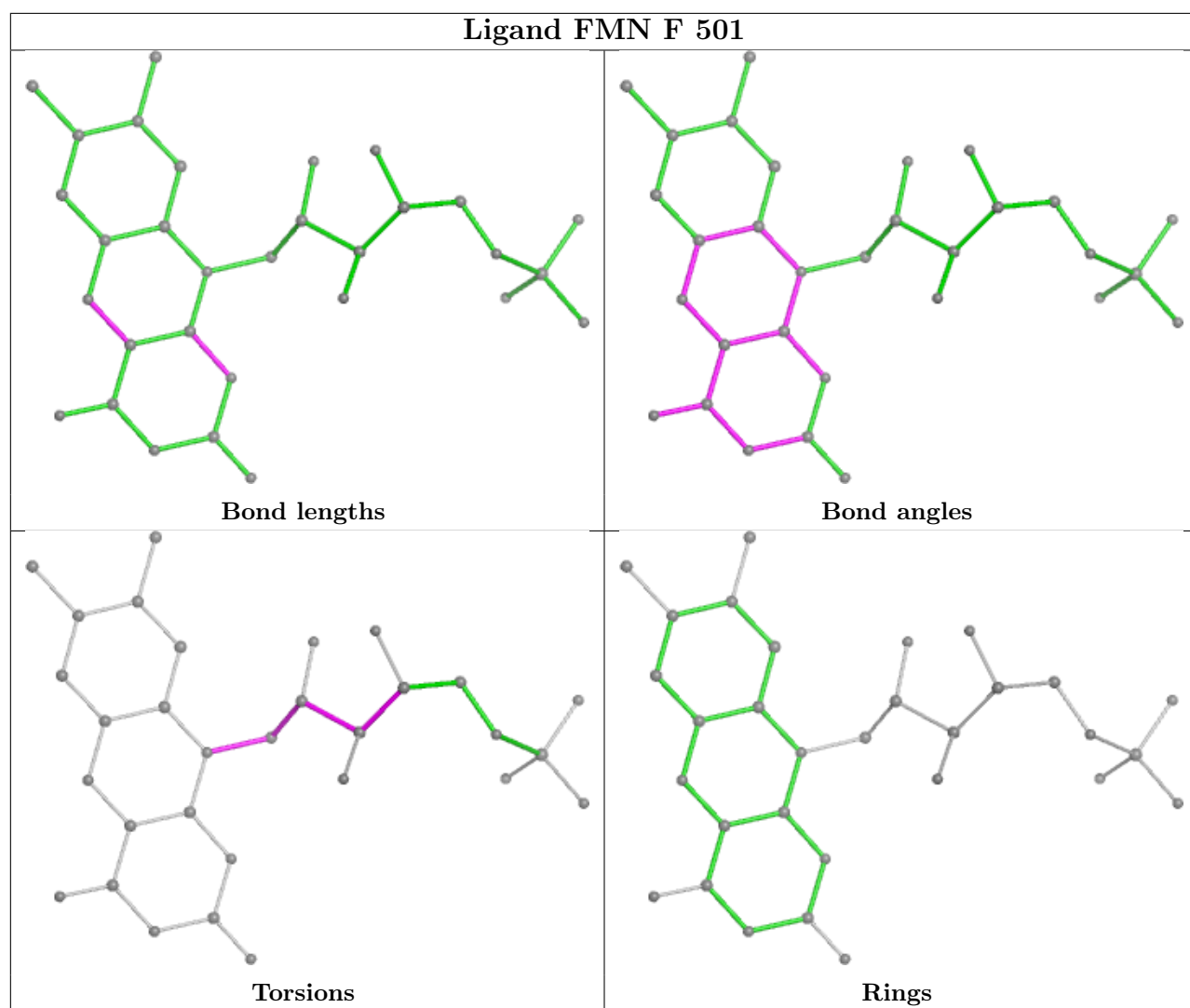
Ligand PC1 B 202

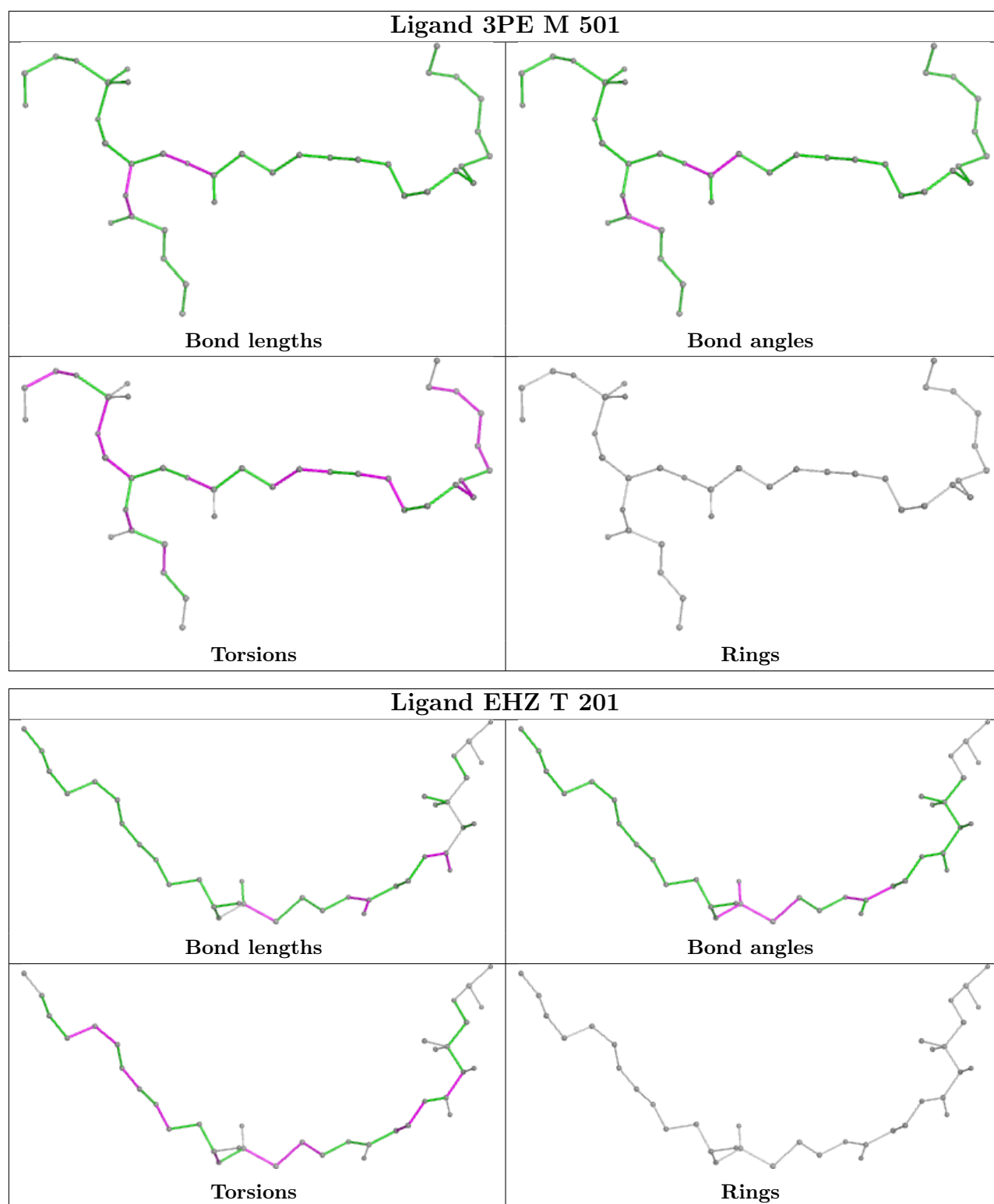


Ligand 3PE J 401









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

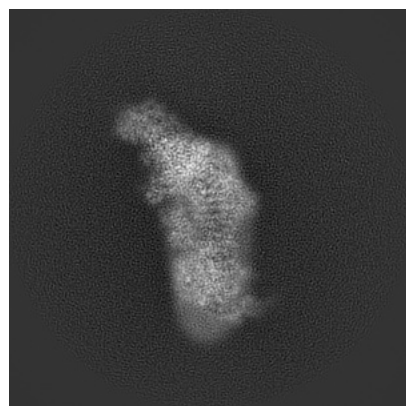
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11811. These allow visual inspection of the internal detail of the map and identification of artifacts.

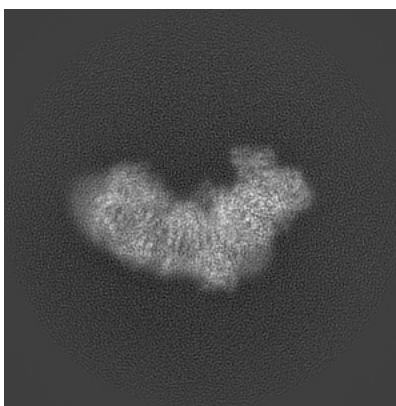
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

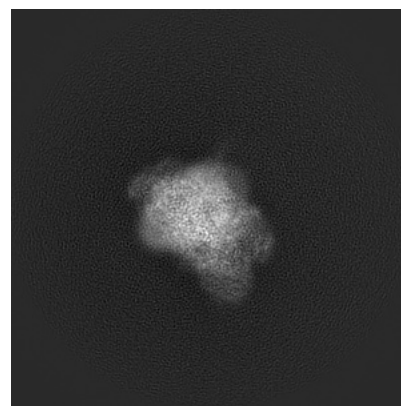
6.1.1 Primary map



X

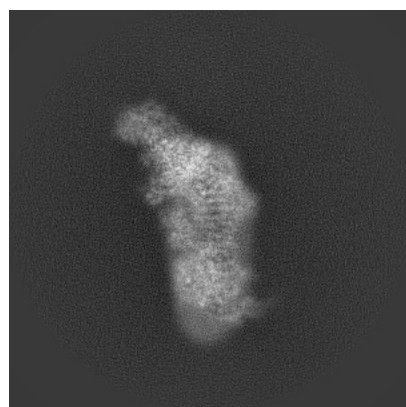


Y

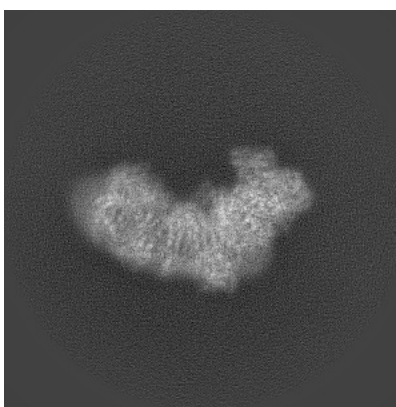


Z

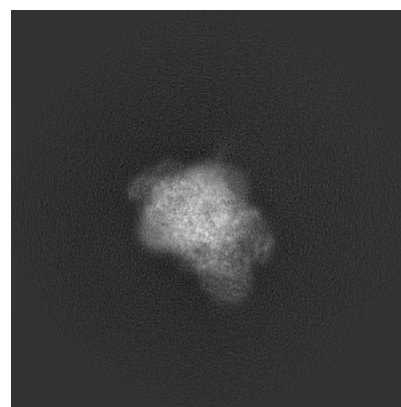
6.1.2 Raw map



X



Y

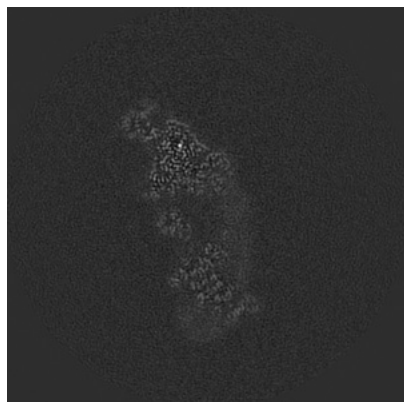


Z

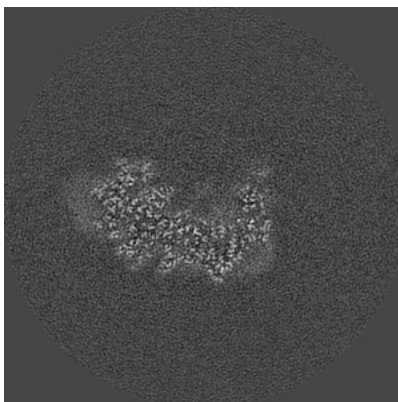
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

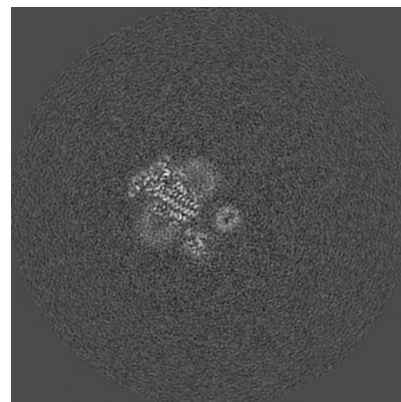
6.2.1 Primary map



X Index: 225

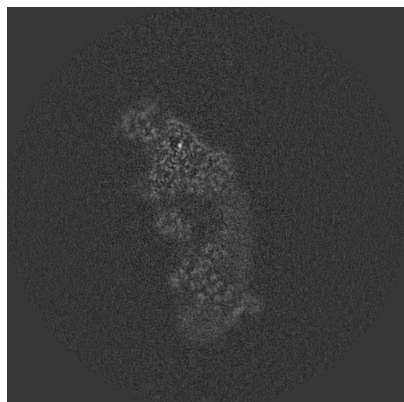


Y Index: 225

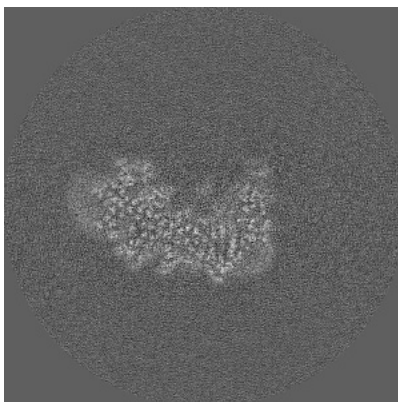


Z Index: 225

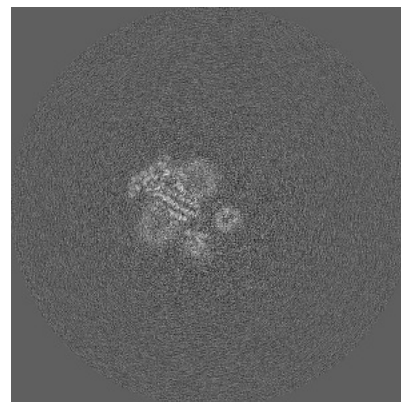
6.2.2 Raw map



X Index: 225



Y Index: 225

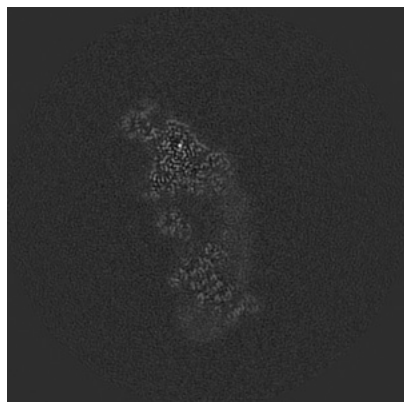


Z Index: 225

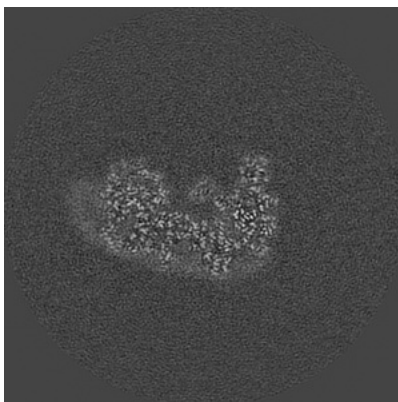
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

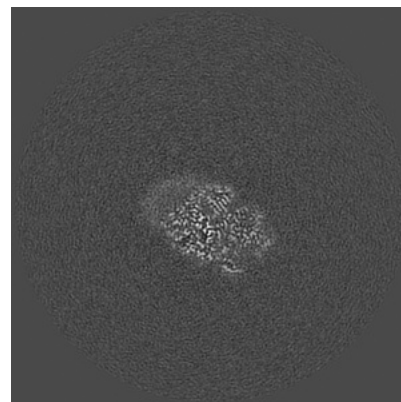
6.3.1 Primary map



X Index: 225

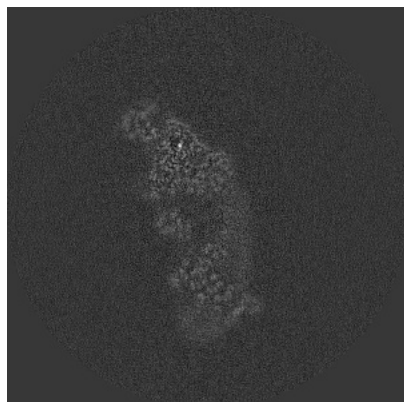


Y Index: 216

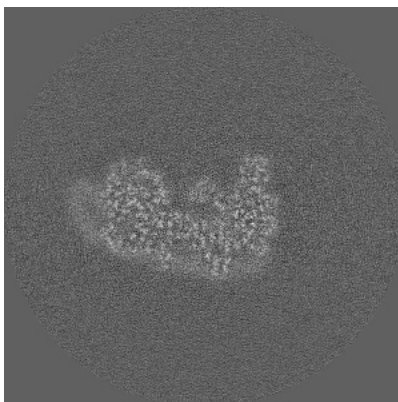


Z Index: 279

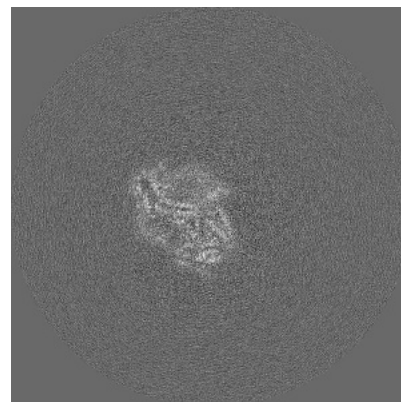
6.3.2 Raw map



X Index: 225



Y Index: 216

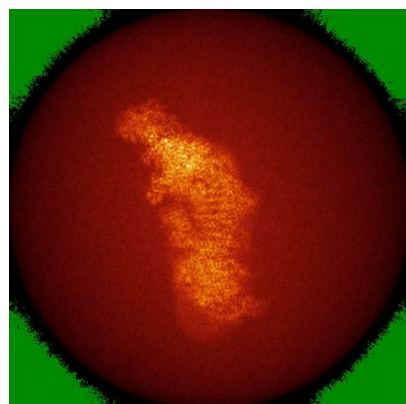


Z Index: 245

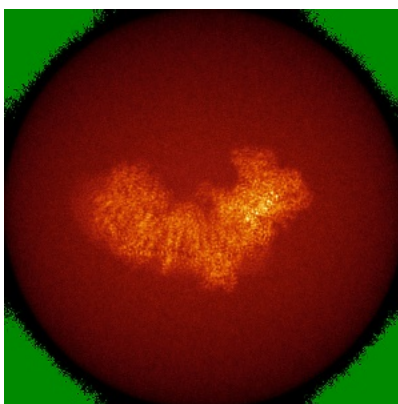
The images above show the largest variance slices of the map in three orthogonal directions.

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

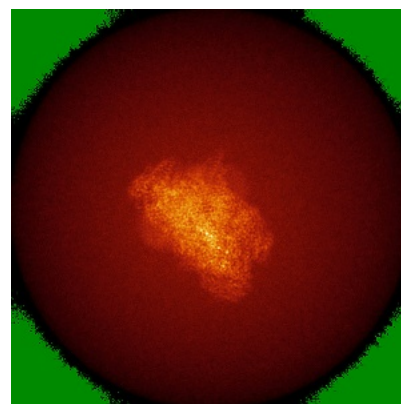
6.4.1 Primary map



X

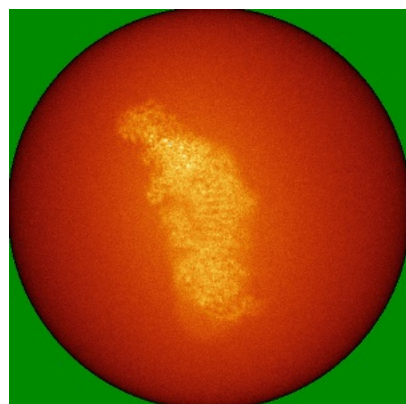


Y

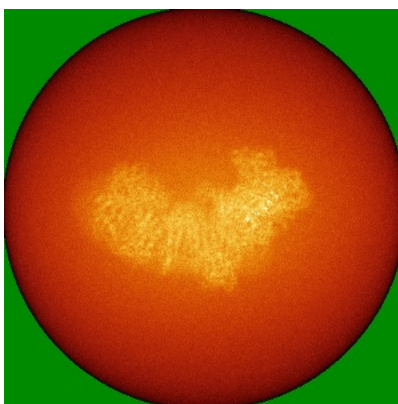


Z

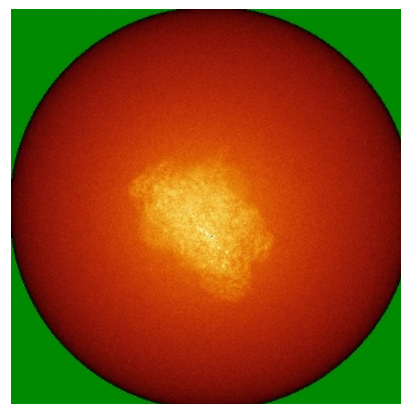
6.4.2 Raw map



X



Y

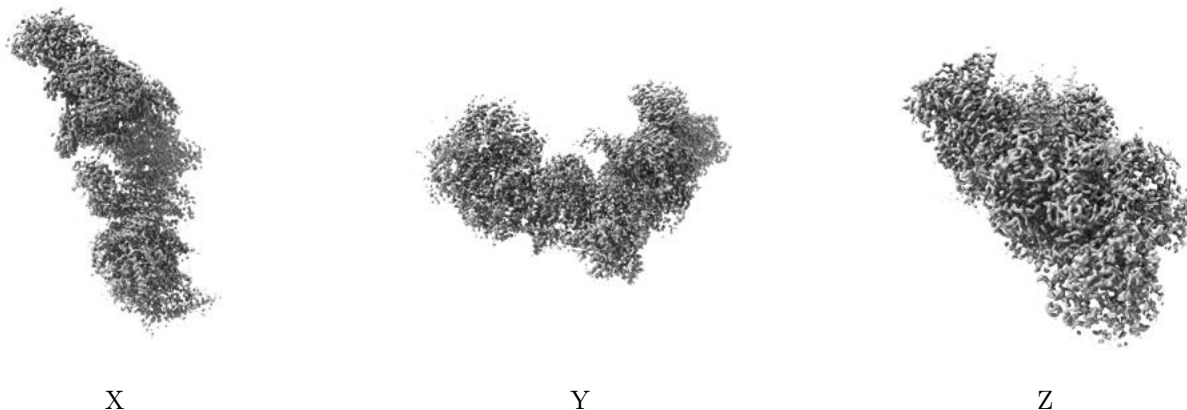


Z

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.

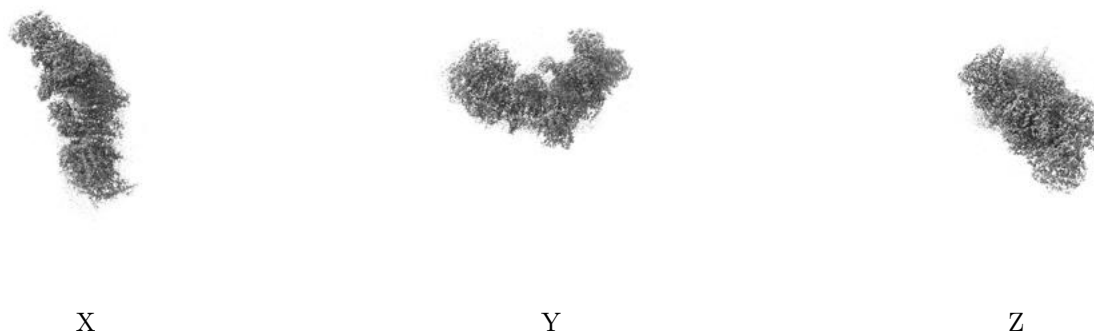
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0268. 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.

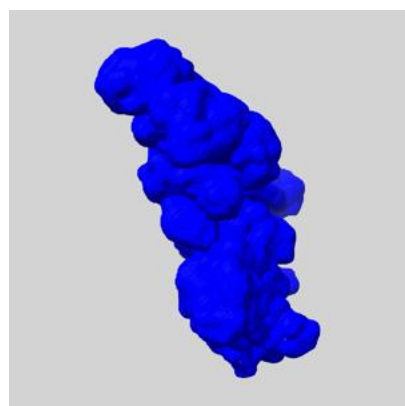
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

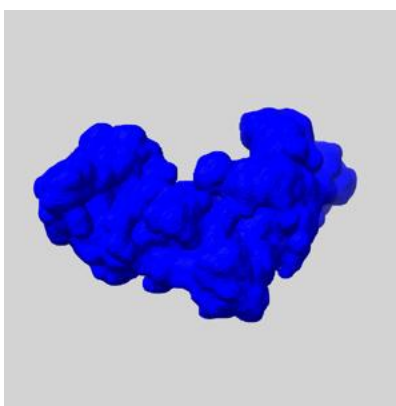
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

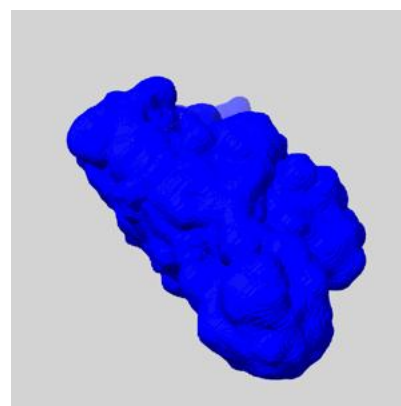
6.6.1 emd_11811_msk_1.map [i](#)



X



Y

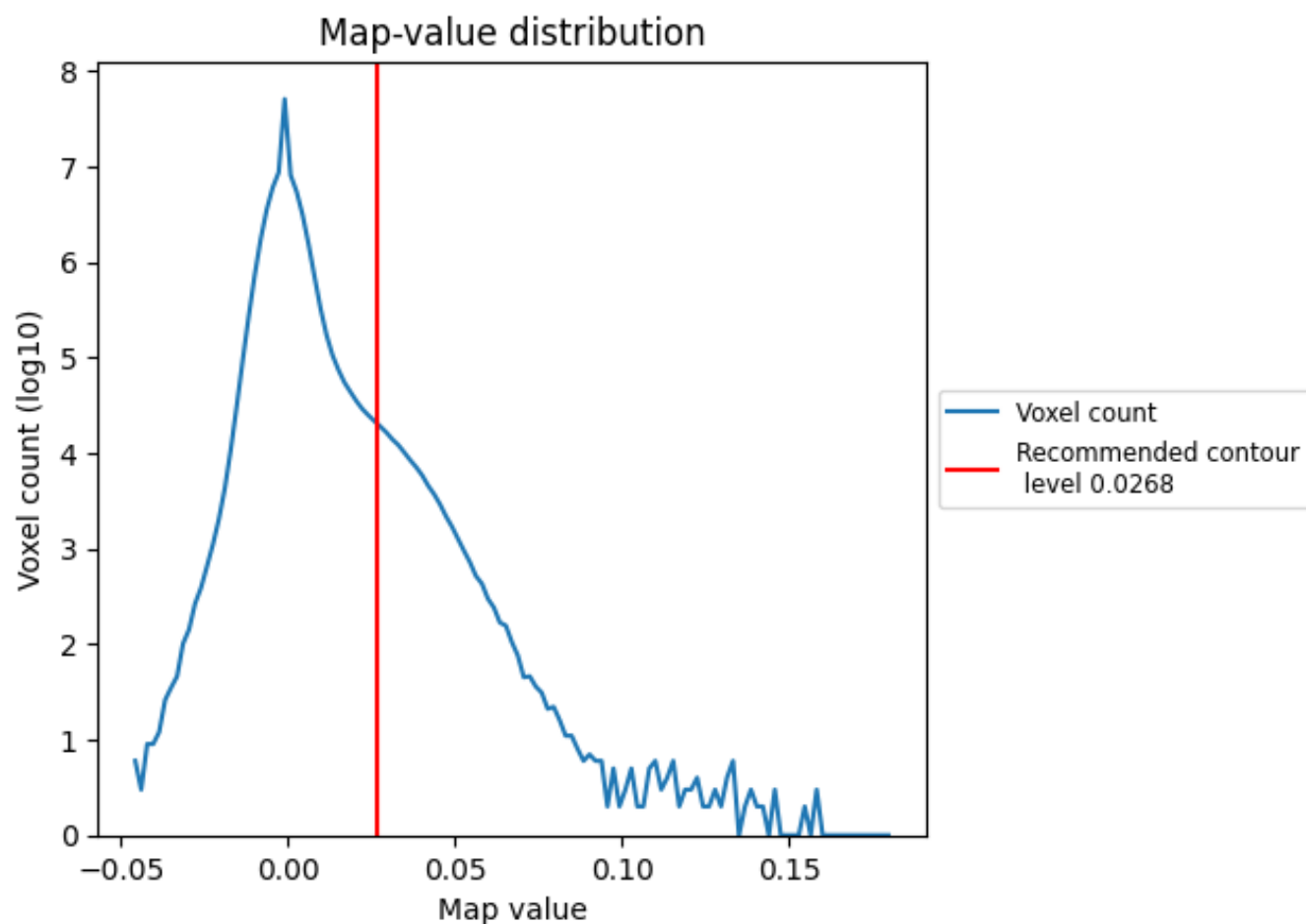


Z

7 Map analysis [i](#)

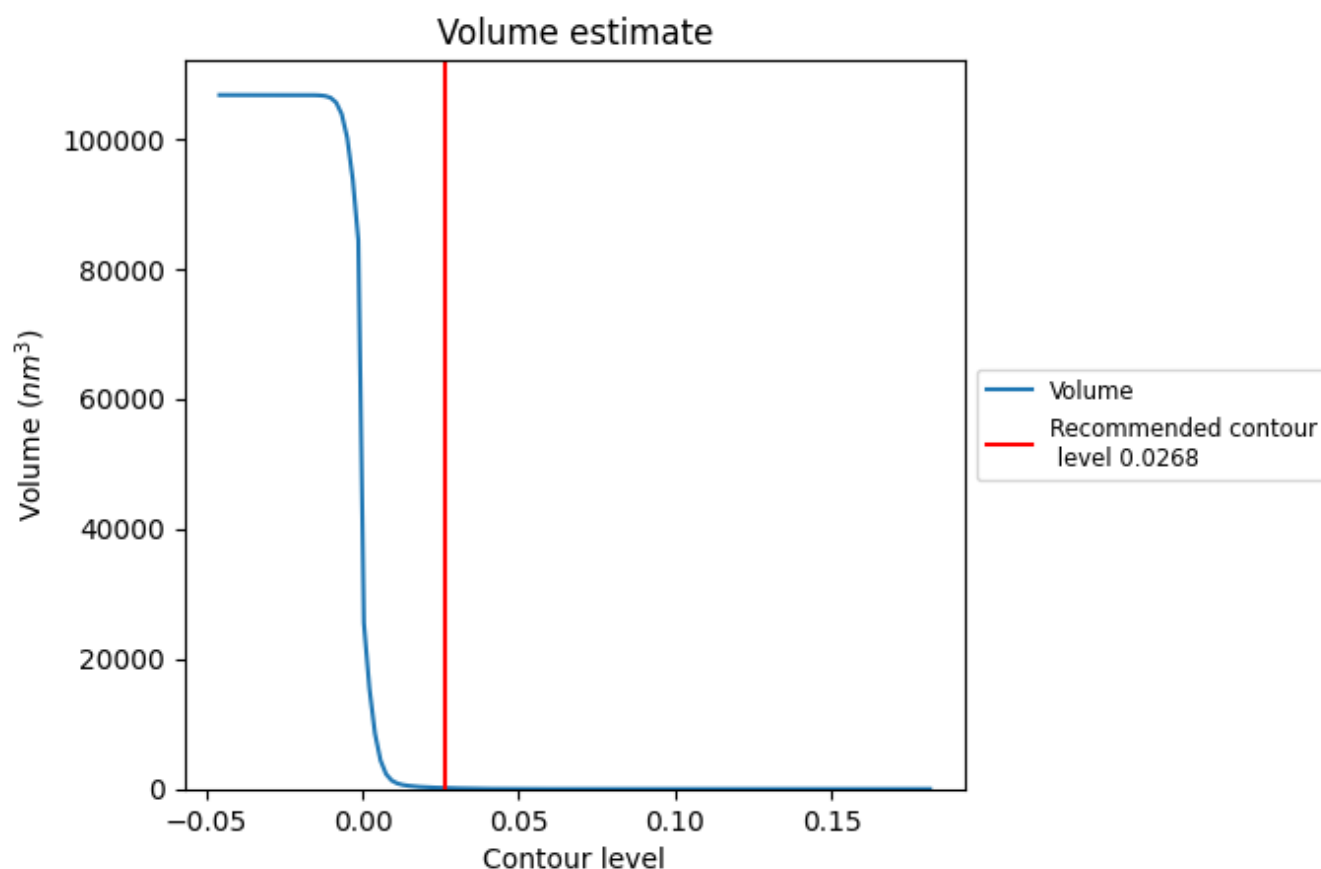
This section contains the results of statistical analysis of the map.

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.

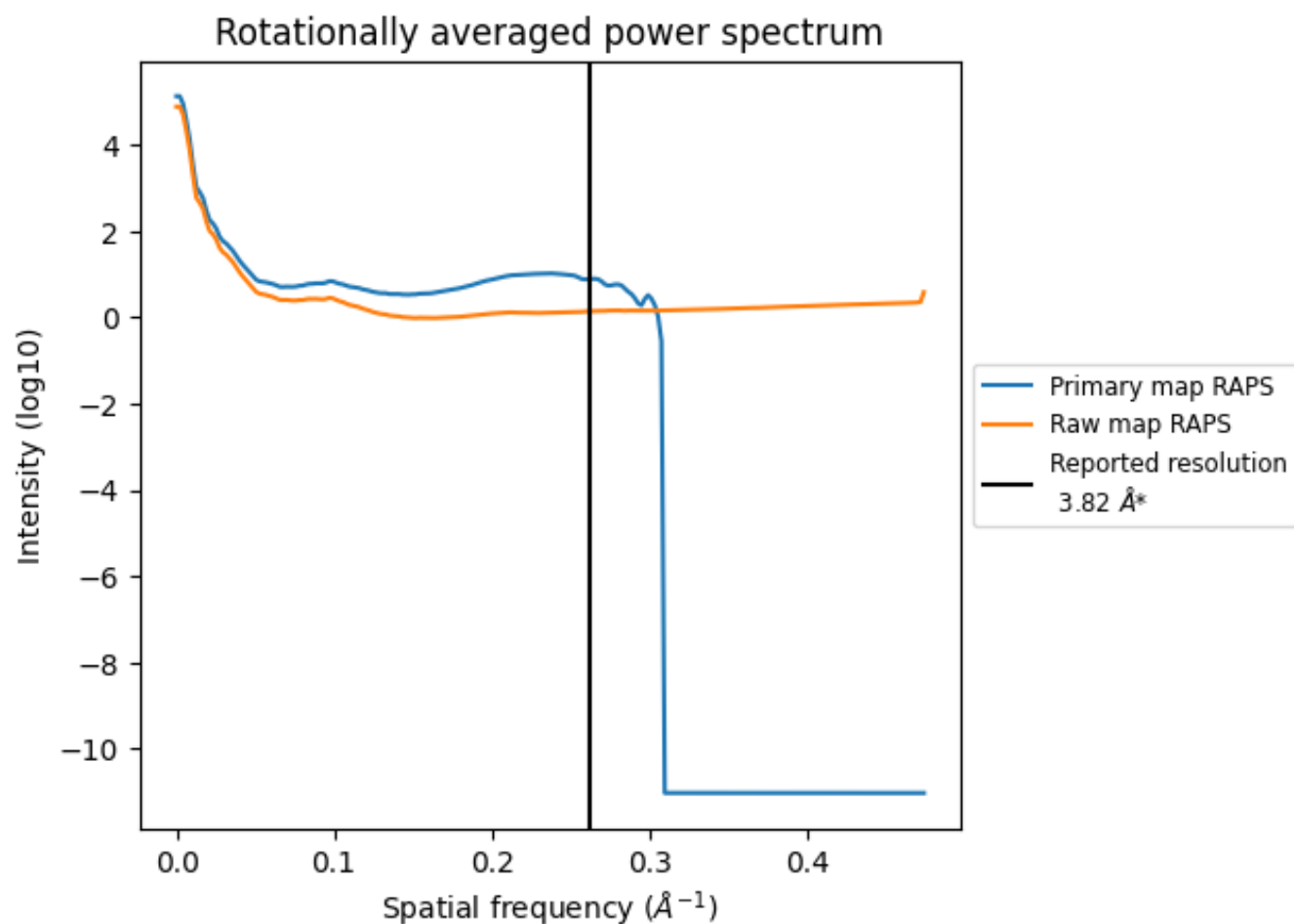
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 146 nm^3 ; this corresponds to an approximate mass of 132 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 ⓘ

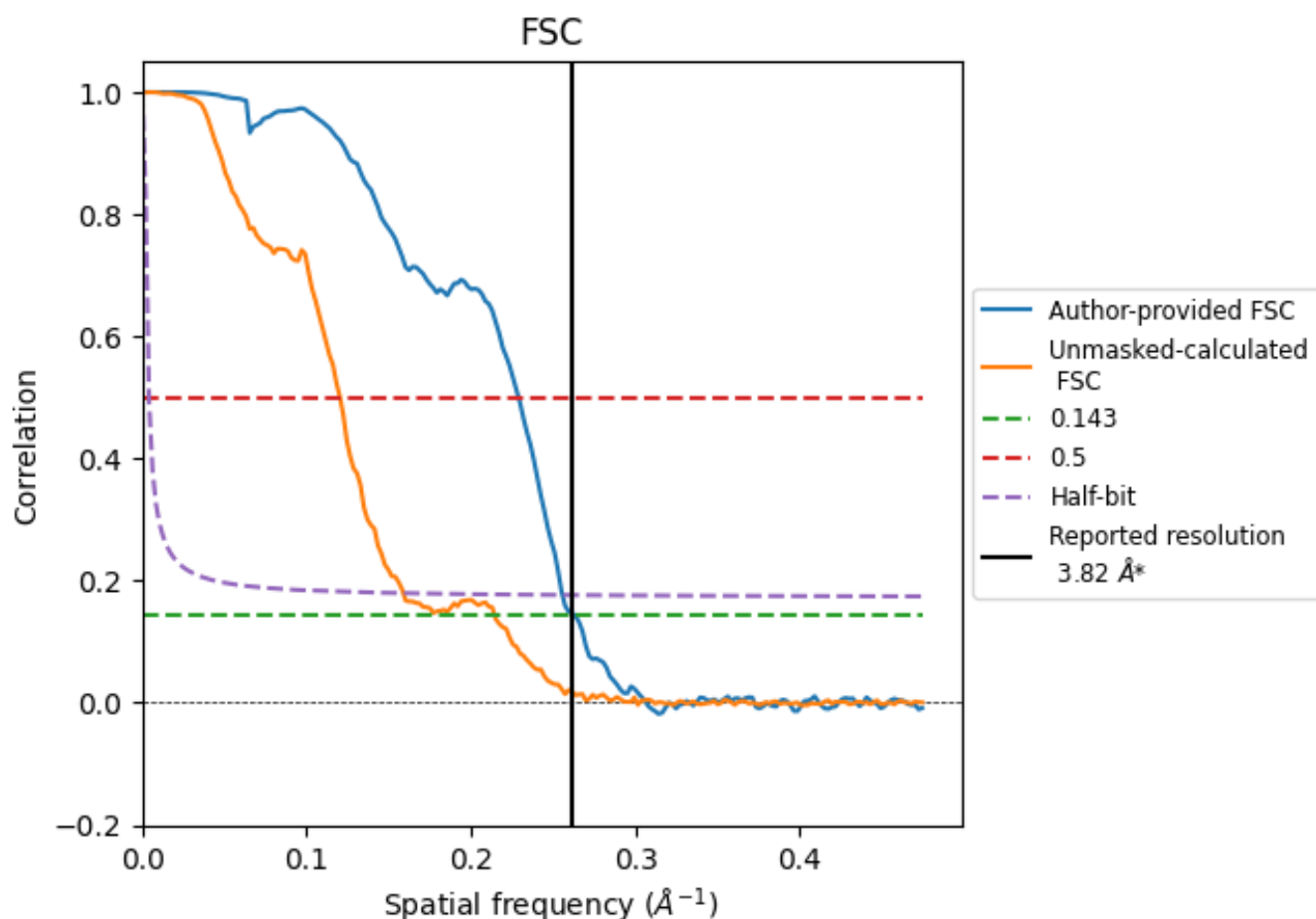


*Reported resolution corresponds to spatial frequency of 0.262 \AA^{-1}

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 0.262 \AA^{-1}

8.2 Resolution estimates [i](#)

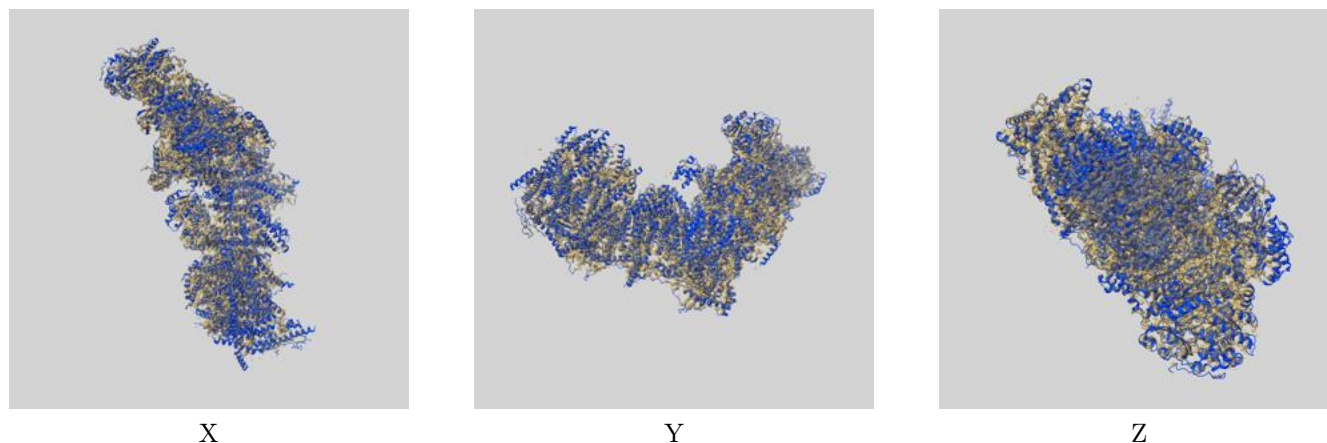
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.82	-	-
Author-provided FSC curve	3.80	4.37	3.91
Unmasked-calculated*	4.66	8.31	6.30

*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 4.66 differs from the reported value 3.82 by more than 10 %

9 Map-model fit [i](#)

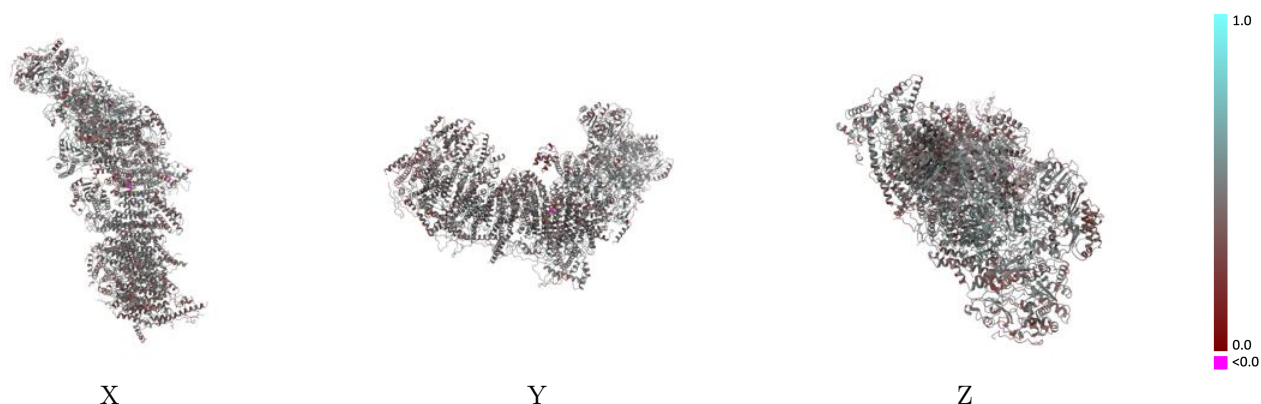
This section contains information regarding the fit between EMDB map EMD-11811 and PDB model 7AK6. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



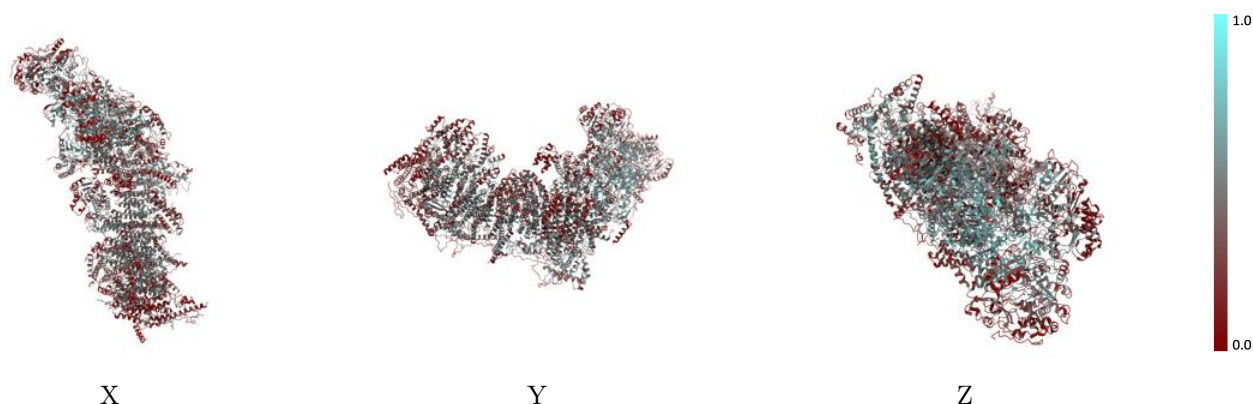
The images above show the 3D surface view of the map at the recommended contour level 0.0268 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



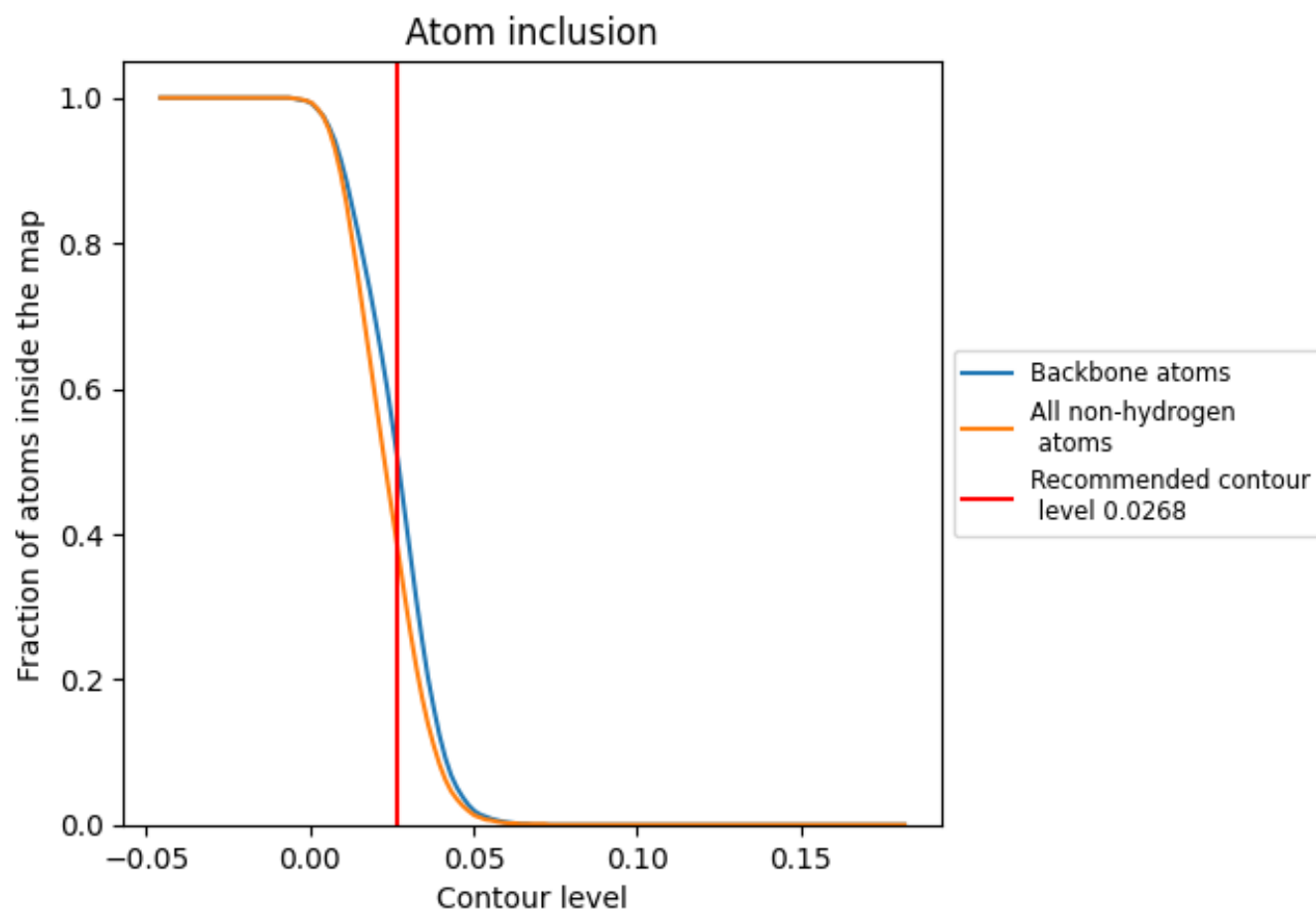
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0268).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 50% of all backbone atoms, 38% 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 (0.0268) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3810	 0.4470
A	 0.3090	 0.4300
B	 0.5680	 0.4850
C	 0.5340	 0.4930
D	 0.5190	 0.4770
E	 0.3040	 0.4230
F	 0.3490	 0.4430
G	 0.4310	 0.4570
H	 0.4020	 0.4510
I	 0.5890	 0.4930
J	 0.2760	 0.4190
K	 0.3850	 0.4600
L	 0.3490	 0.4400
M	 0.4610	 0.4670
N	 0.4800	 0.4640
O	 0.3610	 0.4480
P	 0.3410	 0.4350
Q	 0.4420	 0.4760
R	 0.4400	 0.4750
S	 0.1920	 0.3990
T	 0.0760	 0.3060
U	 0.1930	 0.3950
V	 0.3270	 0.4380
W	 0.3420	 0.4330
X	 0.3480	 0.4540
Y	 0.2180	 0.4140
Z	 0.4400	 0.4540
a	 0.4260	 0.4560
b	 0.3340	 0.4240
c	 0.2810	 0.4230
d	 0.3780	 0.4630
e	 0.3950	 0.4520
f	 0.2800	 0.4130
g	 0.3510	 0.4440
h	 0.4250	 0.4620



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Chain	Atom inclusion	Q-score
i	 0.2660	 0.4070
j	 0.1650	 0.3950
k	 0.1680	 0.4170
l	 0.3220	 0.4450
m	 0.2950	 0.4260
n	 0.3130	 0.4290
o	 0.2060	 0.3850
p	 0.3540	 0.4300
q	 0.4260	 0.4660
r	 0.3950	 0.4560
s	 0.2250	 0.4390