



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 27, 2017 – 06:44 PM EST

PDB ID : 5XTH
EMDB ID: : EMD-6775
Title : Cryo-EM structure of human respiratory supercomplex I1III2IV1
Authors : Gu, J.; Wu, M.; Yang, M.
Deposited on : unknown
Resolution : 3.90 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

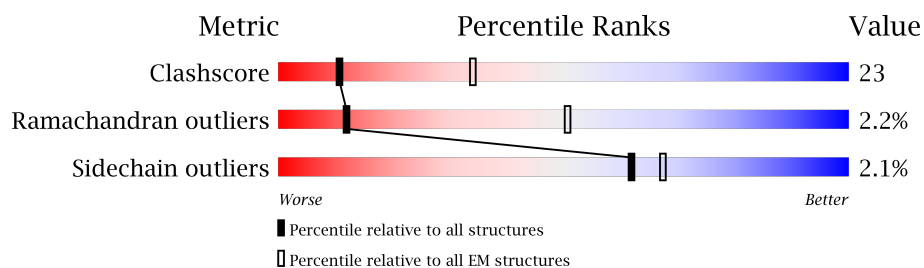
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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.






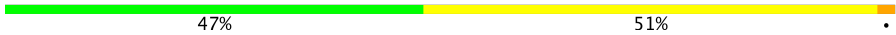

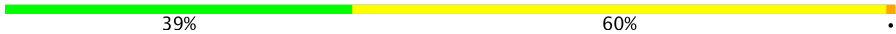







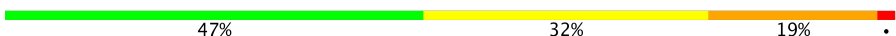

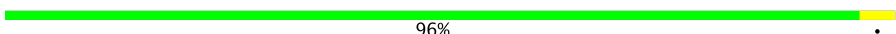

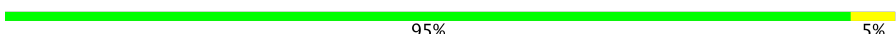
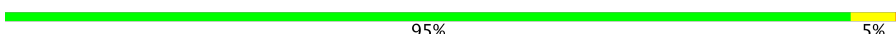
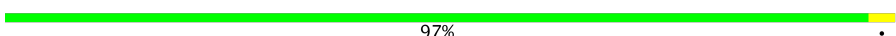
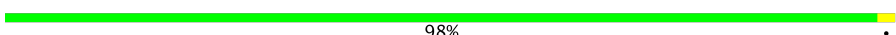
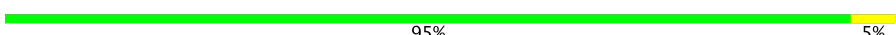
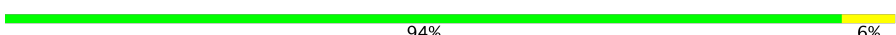
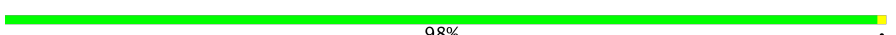

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	431	48% 51% .
2	B	176	49% 51% .
3	C	156	56% 42% .
4	E	113	49% 49% .
5	F	83	51% 49%
6	G	85	47% 51% .
6	X	85	58% 40% .
7	H	112	53% 46% .
8	I	110	46% 36% . 14%




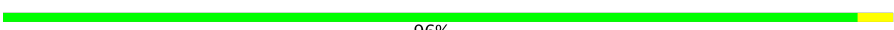
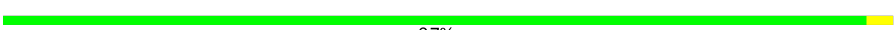





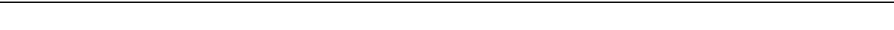

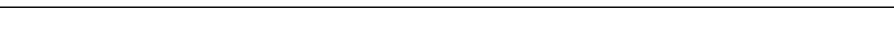
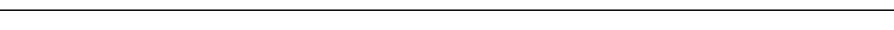











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Mol	Chain	Length	Quality of chain
9	J	337	
10	K	33	
11	L	118	
12	M	687	
13	N	143	
14	O	212	
15	P	208	
16	Q	430	
17	S	70	
18	T	95	
19	U	83	
20	V	140	
21	W	138	
22	Y	59	
23	Z	80	
24	a	138	
25	b	124	
26	c	153	
27	d	171	
28	e	97	
29	f	47	
30	g	119	
31	h	104	
32	i	347	
33	j	115	






















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Mol	Chain	Length	Quality of chain
34	k	97	 93% 6% .
35	l	603	 94% 5% .
36	m	174	 94% 6% .
37	n	56	 96% .
38	o	128	 97% .
39	p	172	 98% .
40	r	459	 98% .
41	s	318	 97% .
42	u	169	 97% .
43	v	122	 86% 5% 9%
44	w	320	 97% .
45	x	514	 92% 8%
46	y	227	 90% 10%
47	z	261	 90% 10%
48	0	144	 74% 23% .
49	1	109	 81% 17% .
50	2	98	 66% 28% 6%
51	3	84	 61% 32% 6% .
52	4	75	 69% 24% 7%
53	5	73	 79% 18% .
54	6	56	 70% 21% 5% .
55	7	49	 76% 24%
56	8	47	 81% 19%
57	9	43	 74% 23% .
58	AA	81	 65% 27% 7%

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Mol	Chain	Length	Quality of chain
58	AN	81	
59	AB	57	
59	AO	57	
60	AC	196	
60	AP	196	
61	AD	62	
61	AQ	62	
62	AE	74	
62	AR	74	
63	AF	106	
63	AS	106	
64	AG	51	
64	AT	51	
65	AH	241	
65	AU	241	
66	AJ	378	
66	AV	378	
67	AK	419	
67	AW	419	
68	AL	446	
68	AY	446	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
69	SF4	A	501	-	-	X	-
69	SF4	B	302	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
69	SF4	M	801	-	-	X	-
70	FMN	A	502	-	-	X	-
73	NDP	J	401	-	-	X	-
74	FES	AC	301	-	-	X	-
74	FES	AP	301	-	-	X	-
74	FES	O	301	-	-	X	-
75	CDL	AG	101	-	-	X	-
75	CDL	AL	502	-	-	X	-
76	PEE	AH	401	-	-	X	-
76	PEE	AL	503	-	-	X	-
76	PEE	AU	401	-	-	X	-
76	PEE	AV	403	-	-	X	-
76	PEE	AY	502	-	-	X	-
79	HEA	x	603	X	-	-	-
79	HEA	x	604	X	-	-	-

2 Entry composition

There are 82 unique types of molecules in this entry. The entry contains 115642 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

4.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 45 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	x	514	Total	C	N	O	S	0	0
			4025	2690	623	677	35		

- Molecule 46 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	y	227	Total	C	N	O	S	0	0
			1822	1184	281	339	18		

- Molecule 47 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	z	261	Total	C	N	O	S	0	0
			2124	1420	338	353	13		

- Molecule 48 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	0	144	Total	C	N	O	S	0	0
			1195	777	196	218	4		

- Molecule 49 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	109	Total	C	N	O	S	0	0
			878	558	150	168	2		

- Molecule 50 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	98	Total	C	N	O	S	0	0
			748	464	134	145	5		

- Molecule 51 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	84	Total	C	N	O	S	0	0
			672	431	129	111	1		

- Molecule 52 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	75	Total	C	N	O	S	0	0
			628	395	114	114	5		

- Molecule 53 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	5	73	Total	C	N	O	S	0	0
			598	388	107	99	4		

- Molecule 54 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	6	56	Total	C	N	O	S	0	0
			441	285	73	80	3		

- Molecule 55 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	7	49	Total	C	N	O	S	0	0
			384	250	65	67	2		

- Molecule 56 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	8	47	Total	C	N	O	S	0	0
			386	257	65	62	2		

- Molecule 57 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	9	43	Total	C	N	O	0	0
			335	223	53	59		

- Molecule 58 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AA	81	Total	C	N	O	S	0	0
			694	450	126	117	1		
58	AN	81	Total	C	N	O	S	0	0
			687	444	126	116	1		

- Molecule 59 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AB	57	Total	C	N	O	S	0	0
			413	261	75	76	1		
59	AO	57	Total	C	N	O	S	0	0
			409	259	74	75	1		

- Molecule 60 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AC	196	Total	C	N	O	S	0	0
			1521	960	264	290	7		
60	AP	196	Total	C	N	O	S	0	0
			1521	960	264	290	7		

- Molecule 61 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AD	62	Total	C	N	O	S	0	0
			509	332	87	89	1		
61	AQ	62	Total	C	N	O	S	0	0
			509	332	87	89	1		

- Molecule 62 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AE	74	Total	C	N	O	S	0	0
			580	351	108	116	5		
62	AR	74	Total	C	N	O	S	0	0
			580	351	108	116	5		

- Molecule 63 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AF	106	Total	C	N	O	S	0	0
			921	589	162	168	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
63	AS	106	Total	C	N	O	S	0	0
			921	589	162	168	2		

- Molecule 64 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AG	51	Total	C	N	O		0	0
			425	287	72	66			
64	AT	51	Total	C	N	O		0	0
			425	287	72	66			

- Molecule 65 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AH	241	Total	C	N	O	S	0	0
			1924	1231	329	349	15		
65	AU	241	Total	C	N	O	S	0	0
			1924	1231	329	349	15		

- Molecule 66 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AJ	378	Total	C	N	O	S	0	0
			3009	2017	467	509	16		
66	AV	378	Total	C	N	O	S	0	0
			3009	2017	467	509	16		

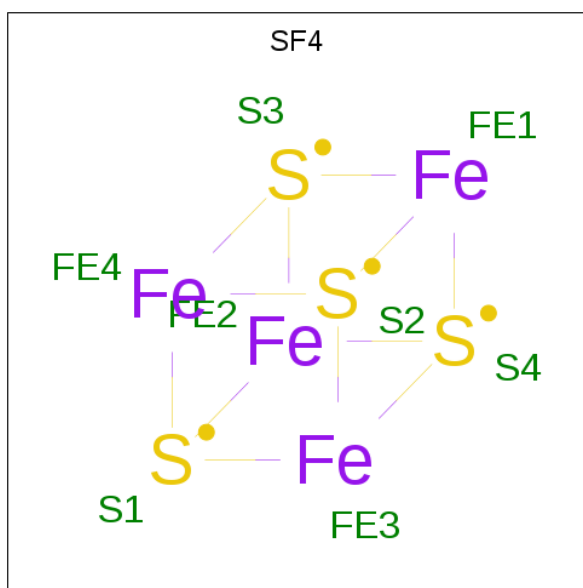
- Molecule 67 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AK	419	Total	C	N	O	S	0	0
			3159	1986	553	610	10		
67	AW	419	Total	C	N	O	S	0	0
			3162	1989	553	610	10		

- Molecule 68 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

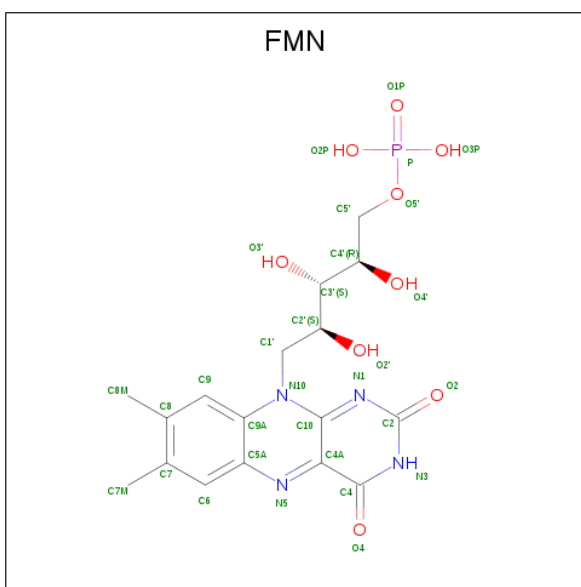
Mol	Chain	Residues	Atoms					AltConf	Trace
68	AL	446	Total	C	N	O	S	0	0
			3453	2169	603	661	20		
68	AY	446	Total	C	N	O	S	0	0
			3453	2169	603	661	20		

- Molecule 69 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



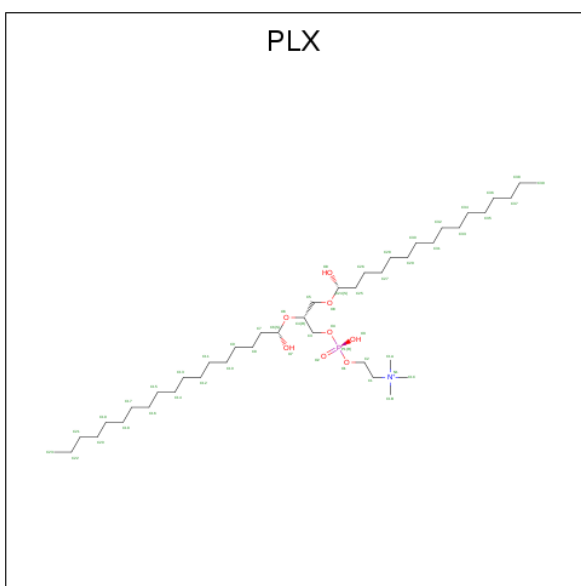
Mol	Chain	Residues	Atoms			AltConf
69	A	1	Total	Fe	S	0
			8	4	4	
69	B	1	Total	Fe	S	0
			16	8	8	
69	B	1	Total	Fe	S	0
			16	8	8	
69	C	1	Total	Fe	S	0
			8	4	4	
69	M	1	Total	Fe	S	0
			16	8	8	
69	M	1	Total	Fe	S	0
			16	8	8	

- Molecule 70 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).



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

- Molecule 71 is (9R,11S)-9-([[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (three-letter code: PLX) (formula: C₄₂H₈₉NO₈P).



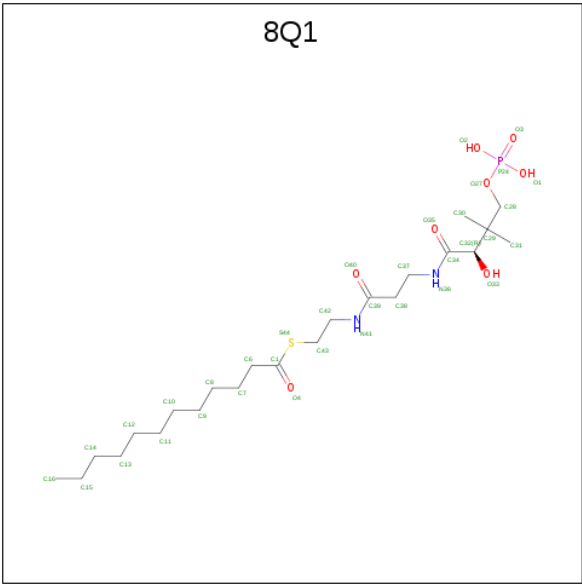
Mol	Chain	Residues	Atoms					AltConf
71	B	1	Total 52	C 42	N 1	O 8	P 1	0
71	U	1	Total 52	C 42	N 1	O 8	P 1	0

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

- Molecule 72 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: C₂₃H₄₅N₂O₈PS).



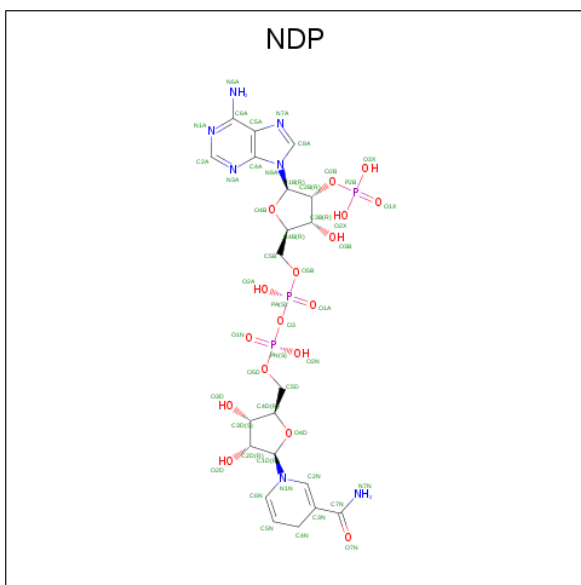
Mol	Chain	Residues	Atoms						AltConf
72	E	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

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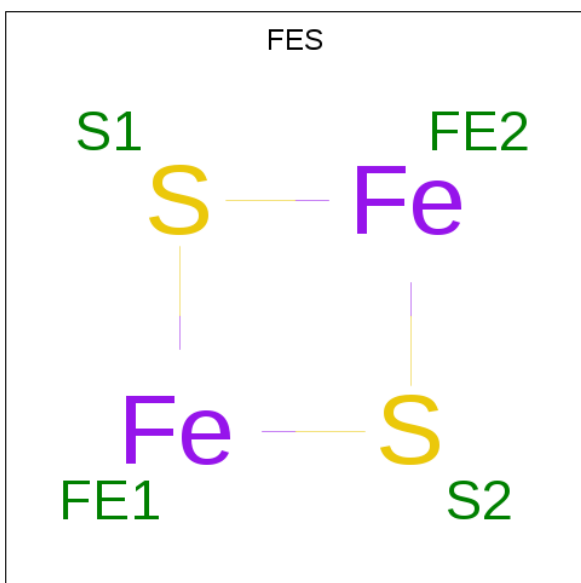
Mol	Chain	Residues	Atoms						AltConf
72	p	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 73 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



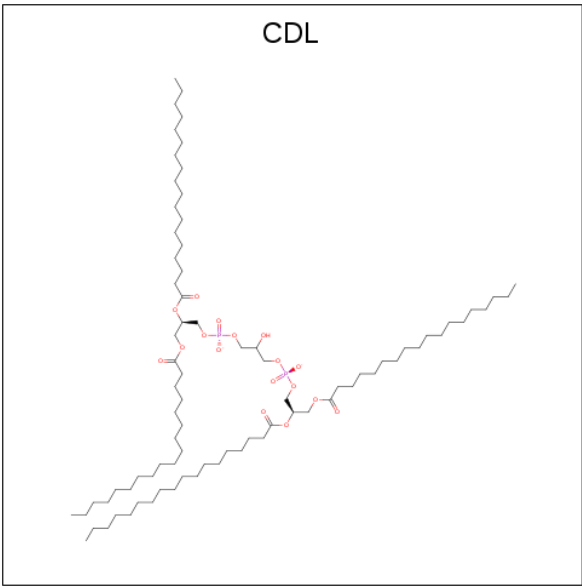
Mol	Chain	Residues	Atoms					AltConf
73	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 74 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
74	M	1	Total	Fe	S	0
			4	2	2	
74	O	1	Total	Fe	S	0
			4	2	2	
74	AC	1	Total	Fe	S	0
			4	2	2	
74	AP	1	Total	Fe	S	0
			4	2	2	

- Molecule 75 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



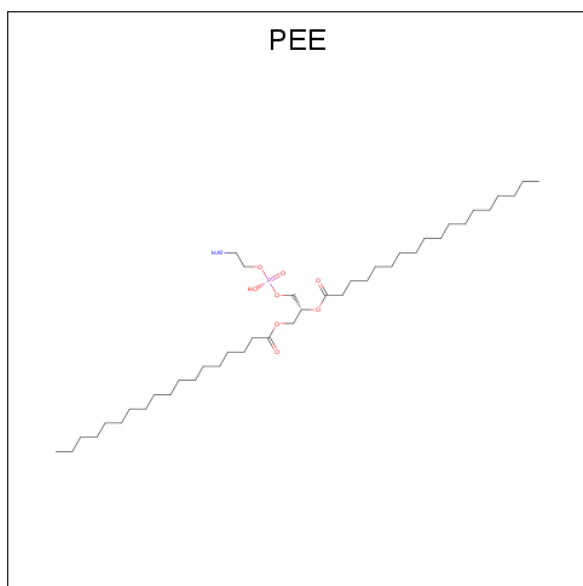
Mol	Chain	Residues	Atoms				AltConf
75	V	1	Total	C	O	P	0
			63	44	17	2	
75	i	1	Total	C	O	P	0
			64	45	17	2	
75	l	1	Total	C	O	P	0
			128	90	34	4	
75	l	1	Total	C	O	P	0
			128	90	34	4	
75	n	1	Total	C	O	P	0
			64	45	17	2	
75	AA	1	Total	C	O	P	0
			64	45	17	2	
75	AG	1	Total	C	O	P	0
			64	45	17	2	
75	AH	1	Total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

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Mol	Chain	Residues	Atoms				AltConf
75	AJ	1	Total	C	O	P	0
			128	90	34	4	
75	AJ	1	Total	C	O	P	0
			128	90	34	4	
75	AL	1	Total	C	O	P	0
			64	45	17	2	
75	AN	1	Total	C	O	P	0
			64	45	17	2	
75	AU	1	Total	C	O	P	0
			64	45	17	2	
75	AY	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 76 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
76	V	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	W	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	l	1	Total	C	N	O	P	0
			100	80	2	16	2	
76	l	1	Total	C	N	O	P	0
			100	80	2	16	2	
76	AH	1	Total	C	N	O	P	0
			49	39	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
76	AJ	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	AL	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	AU	1	Total	C	N	O	P	0
			41	31	1	8	1	
76	AV	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	AY	1	Total	C	N	O	P	0
			49	39	1	8	1	

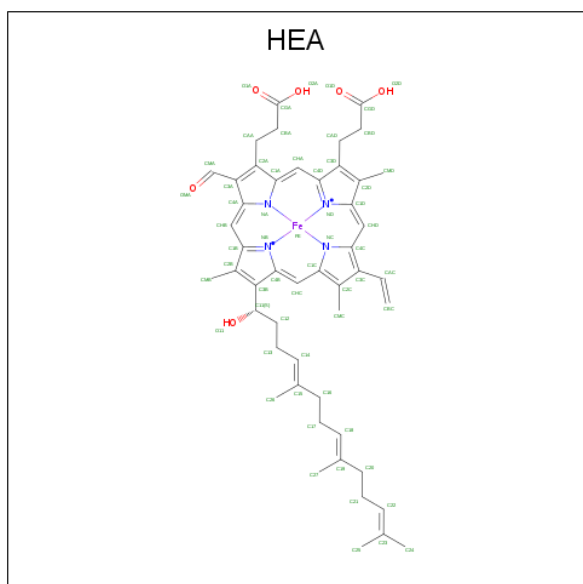
- Molecule 77 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
77	x	1	Total	Cu	0
			1	1	
77	y	2	Total	Cu	0
			2	2	

- Molecule 78 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
78	x	1	Total	Mg	0
			1	1	

- Molecule 79 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).

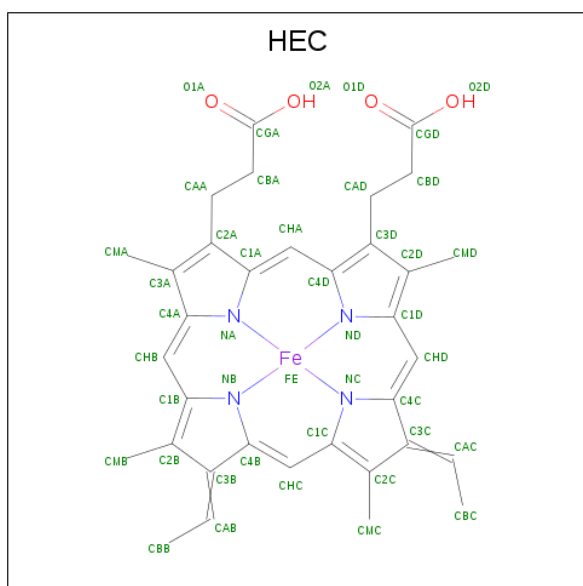


Mol	Chain	Residues	Atoms					AltConf
79	x	1	Total 120	C 98	Fe 2	N 8	O 12	0
79	x	1	Total 120	C 98	Fe 2	N 8	O 12	0

- Molecule 80 is ZINC ION (three-letter code: ZN) (formula: Zn).

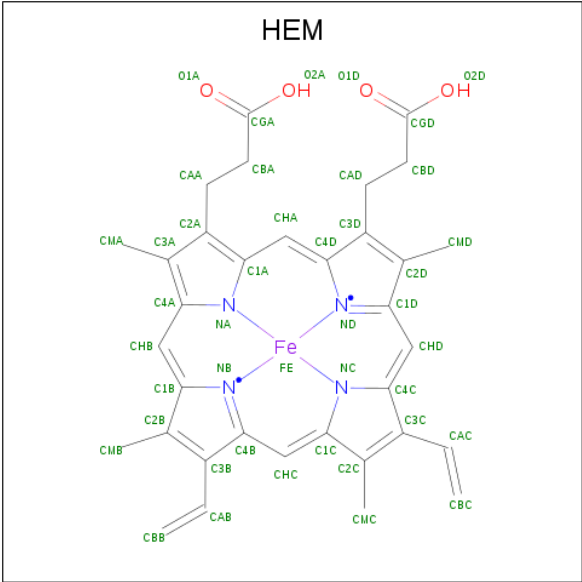
Mol	Chain	Residues	Atoms	AltConf
80	2	1	Total Zn 1 1	0

- Molecule 81 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms					AltConf
81	AH	1	Total 43	C 34	Fe 1	N 4	O 4	0
81	AU	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 82 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

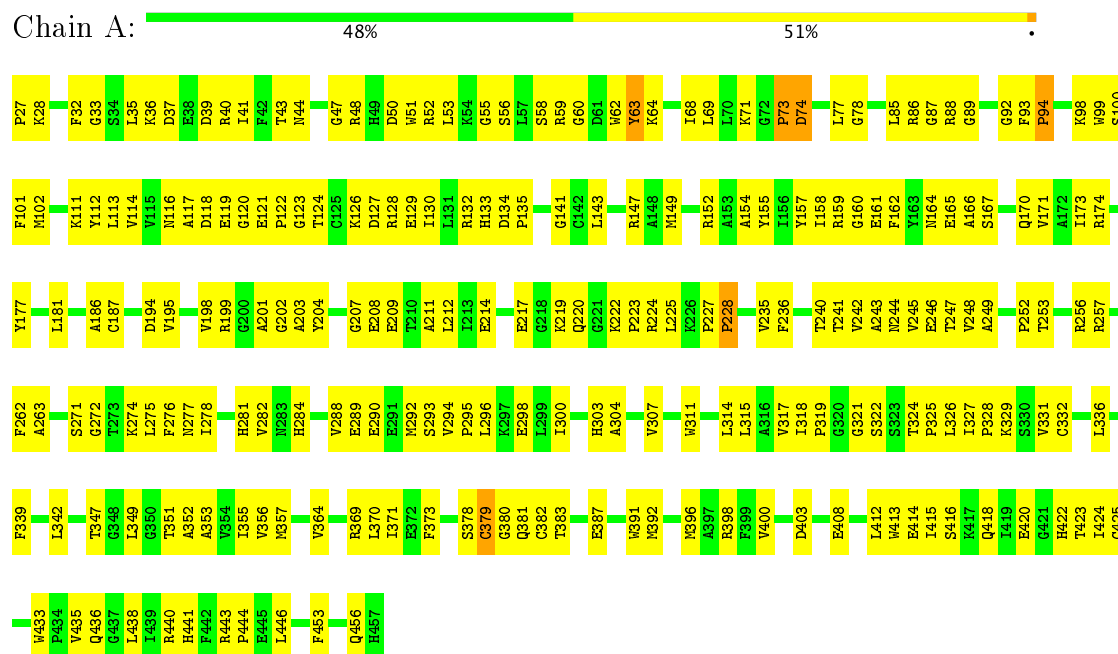


Mol	Chain	Residues	Atoms					AltConf
82	AJ	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
82	AJ	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
82	AV	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
82	AV	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

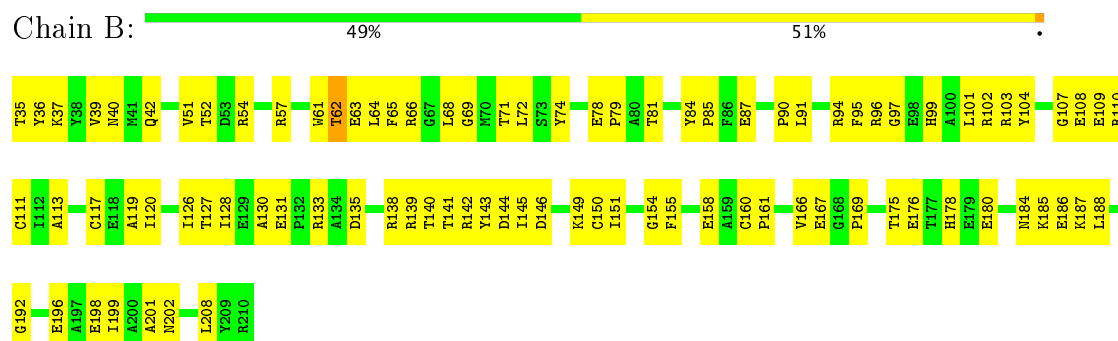
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

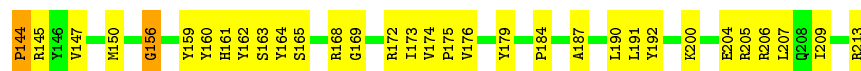


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



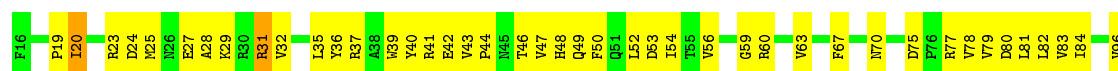
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial





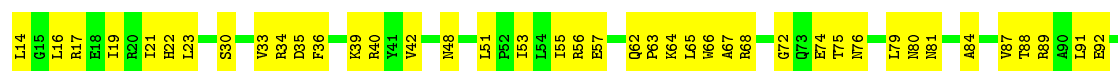
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain E: 49%



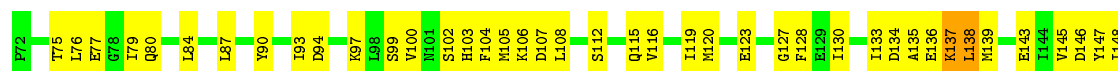
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain F: 51%



- Molecule 6: Acyl carrier protein, mitochondrial

Chain G: 47%



- Molecule 6: Acyl carrier protein, mitochondrial

Chain X: 58%

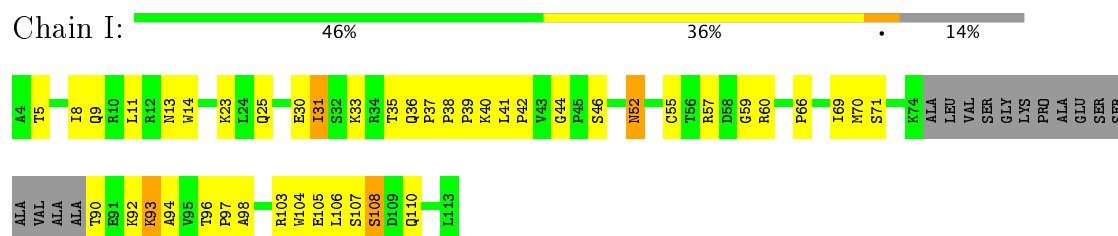


- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

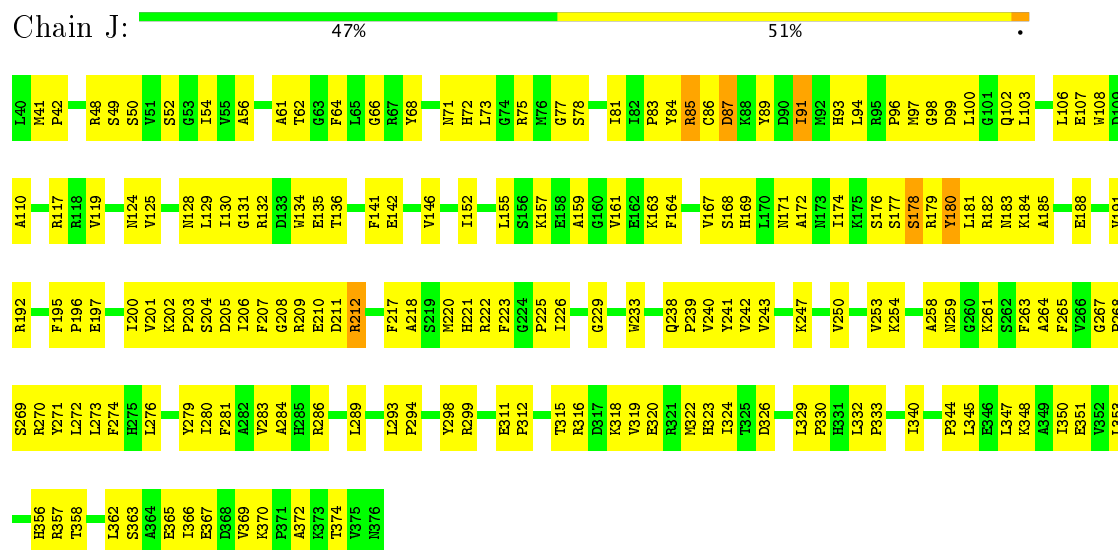
Chain H: 53%



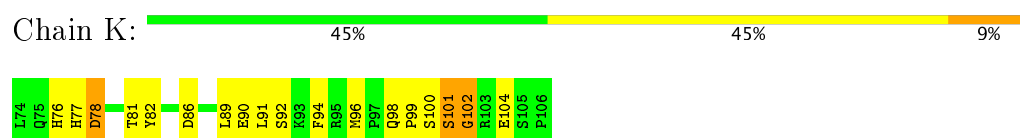
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



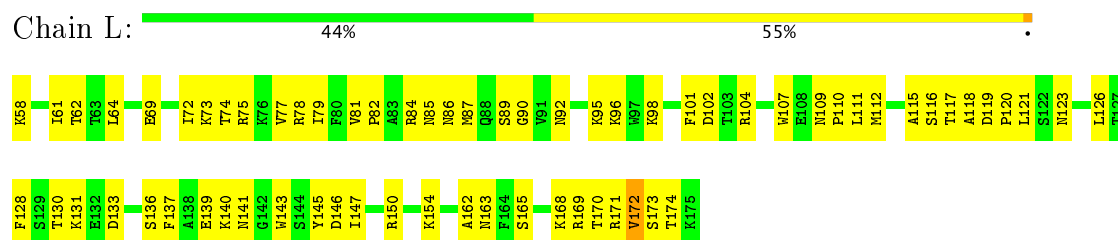
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



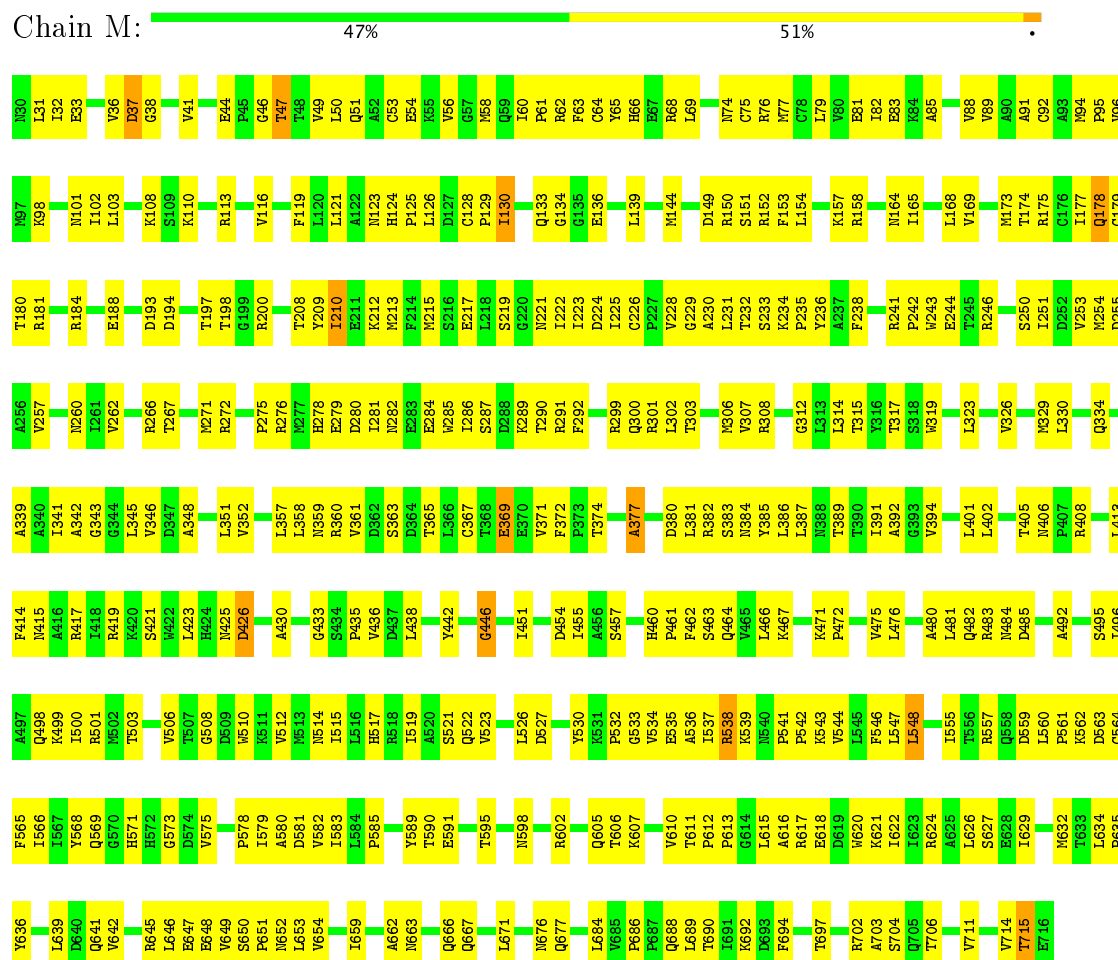
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



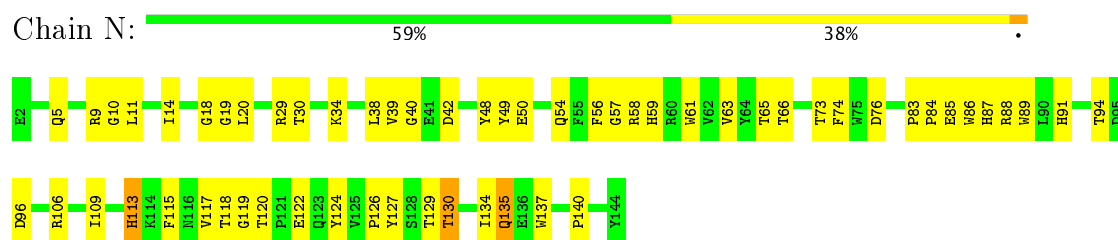
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



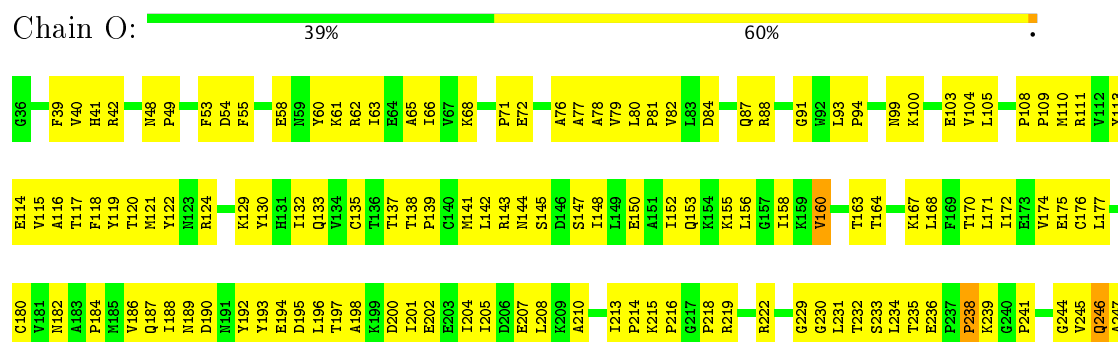
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



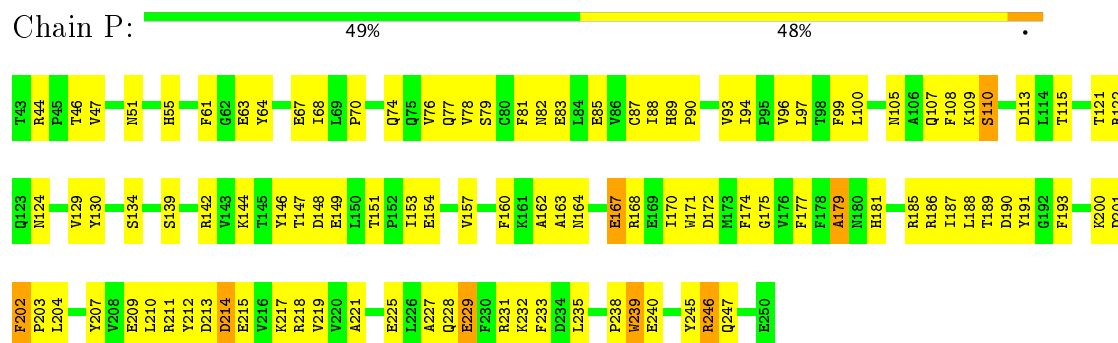
• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



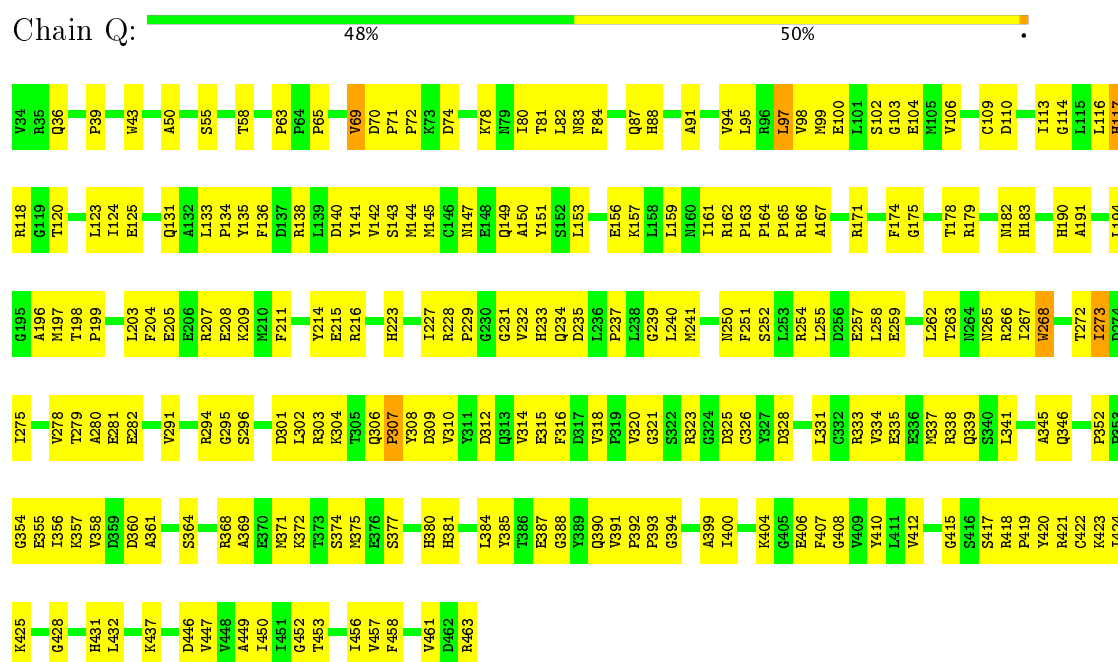
• Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



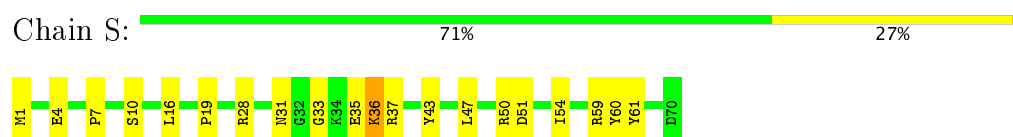
- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



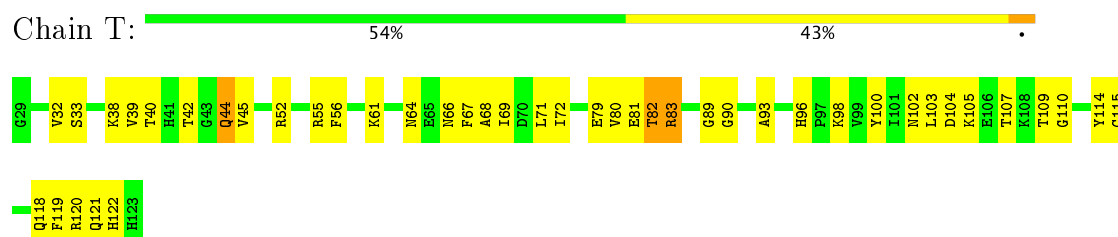
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



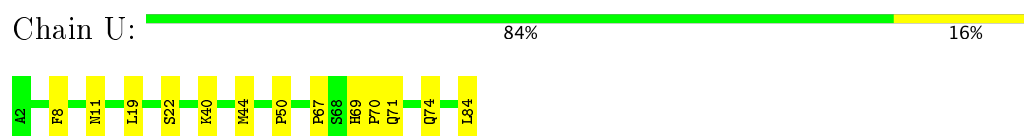
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



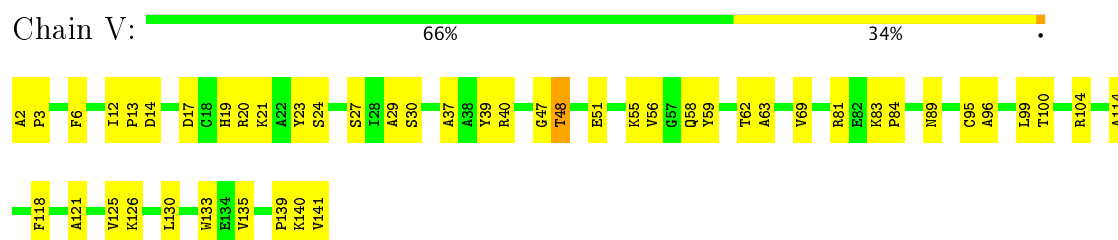
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



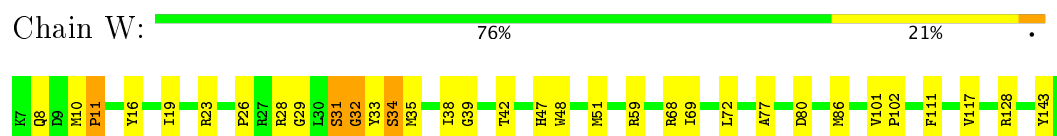
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



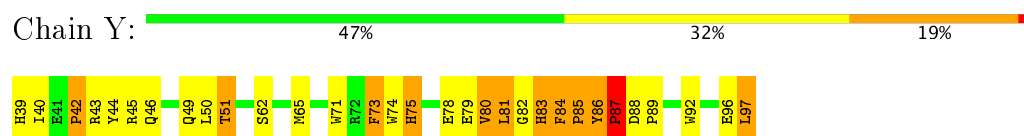
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



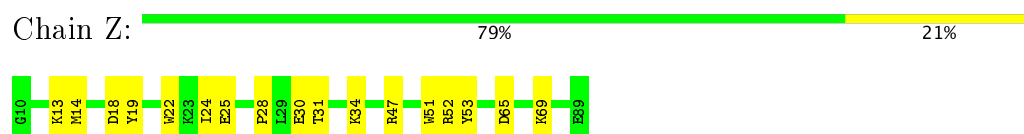
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



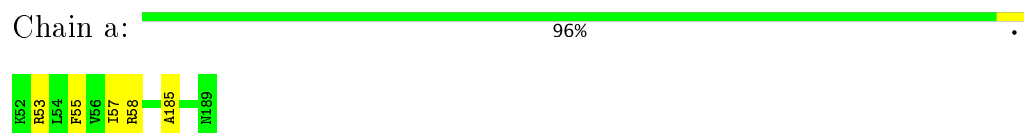
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



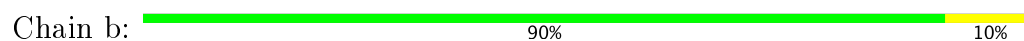
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



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



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





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

Chain c: 95% 5%



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

Chain d: 95% 5%



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

Chain e: 97% .



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

Chain f: 98% .



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

Chain g: 95% 5%



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

Chain h: 94% 6%



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain i: 98% .



- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j: 97%



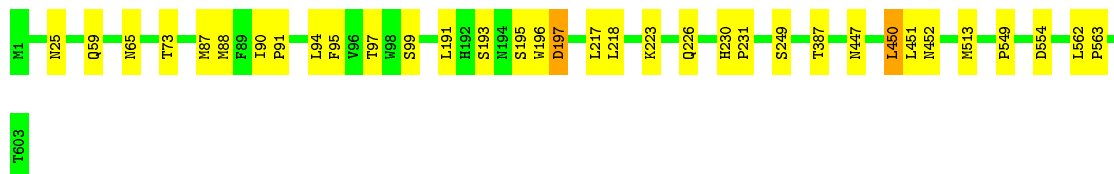
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain k: 93%



- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l: 94%



- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain m: 94%



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

Chain n: 96%



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

Chain o: 97%



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

Chain p: 98%



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r: 98%



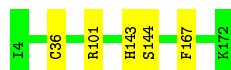
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s: 97%



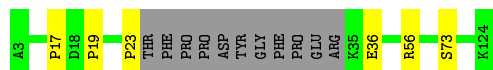
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u: 97%



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

Chain v: 86% 5% 9%



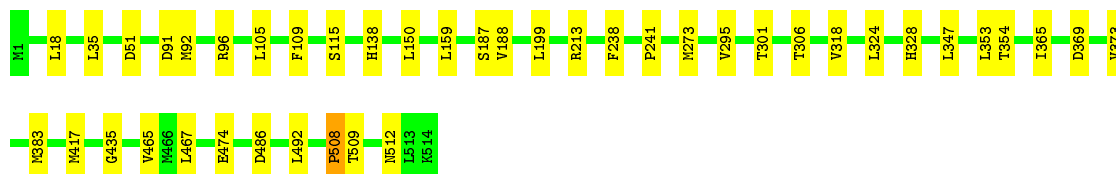
- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain w: 97%




- Molecule 45: Cytochrome c oxidase subunit 1

Chain x: 92% 8%




- Molecule 46: Cytochrome c oxidase subunit 2

Chain y:  90% 10%



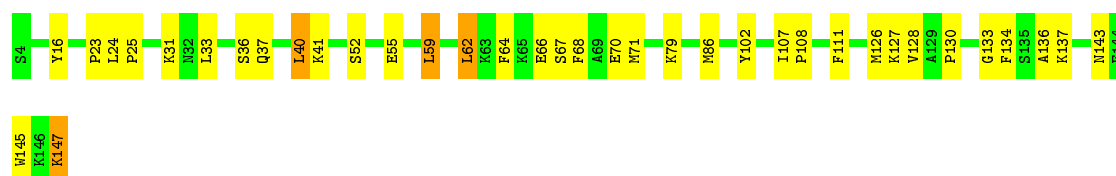
- Molecule 47: Cytochrome c oxidase subunit 3

Chain z:  90% 10%




- Molecule 48: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain 0:  74% 23% .



- Molecule 49: Cytochrome c oxidase subunit 5A, mitochondrial

Chain 1:  81% 17% .



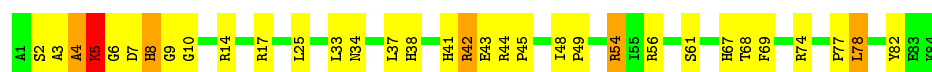
- Molecule 50: Cytochrome c oxidase subunit 5B, mitochondrial

Chain 2:  66% 28% 6%



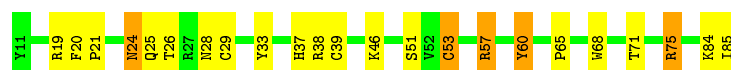
- Molecule 51: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain 3:  61% 32% 6% .




- Molecule 52: Cytochrome c oxidase subunit 6B1

Chain 4:  69% 24% 7%



- Molecule 53: Cytochrome c oxidase subunit 6C

Chain 5:  79% 18% .




- Molecule 54: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain 6:  70% 21% 5% .




- Molecule 55: Cytochrome c oxidase subunit 7B, mitochondrial

Chain 7:  76% 24%



- Molecule 56: Cytochrome c oxidase subunit 7C, mitochondrial

Chain 8:  81% 19%



- Molecule 57: Cytochrome c oxidase subunit 8B, mitochondrial

Chain 9:  74% 23% .




- Molecule 58: Cytochrome b-c1 complex subunit 8

Chain AA:  65% 27% 7%



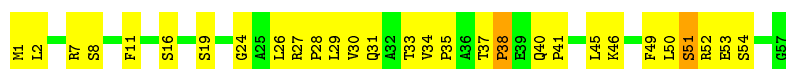
- Molecule 58: Cytochrome b-c1 complex subunit 8

Chain AN:  75% 23% .



- Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AB:  49% 47%



- Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial



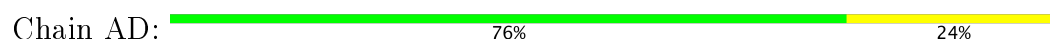
- Molecule 60: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 60: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 61: Cytochrome b-c1 complex subunit 9




- Molecule 61: Cytochrome b-c1 complex subunit 9



- Molecule 62: Cytochrome b-c1 complex subunit 6, mitochondrial



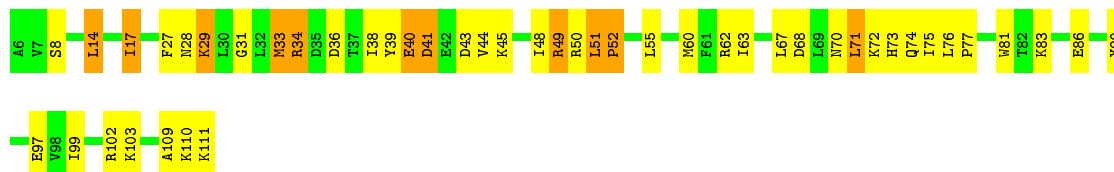
- Molecule 62: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain AR:  74% 24% .



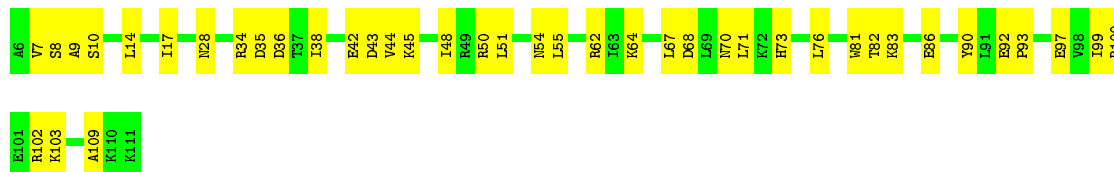
- Molecule 63: Cytochrome b-c1 complex subunit 7

Chain AF:  56% 34% 10%




- Molecule 63: Cytochrome b-c1 complex subunit 7

Chain AS:  61% 39%



- Molecule 64: Cytochrome b-c1 complex subunit 10

Chain AG:  73% 27%




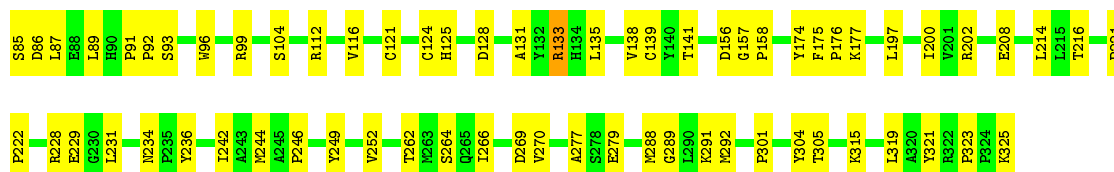
- Molecule 64: Cytochrome b-c1 complex subunit 10

Chain AT:  65% 31% .



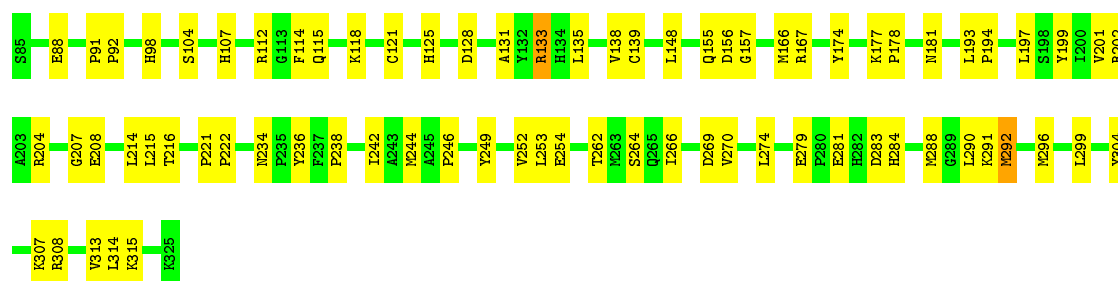
- Molecule 65: Cytochrome c1, heme protein, mitochondrial

Chain AH:  73% 27%



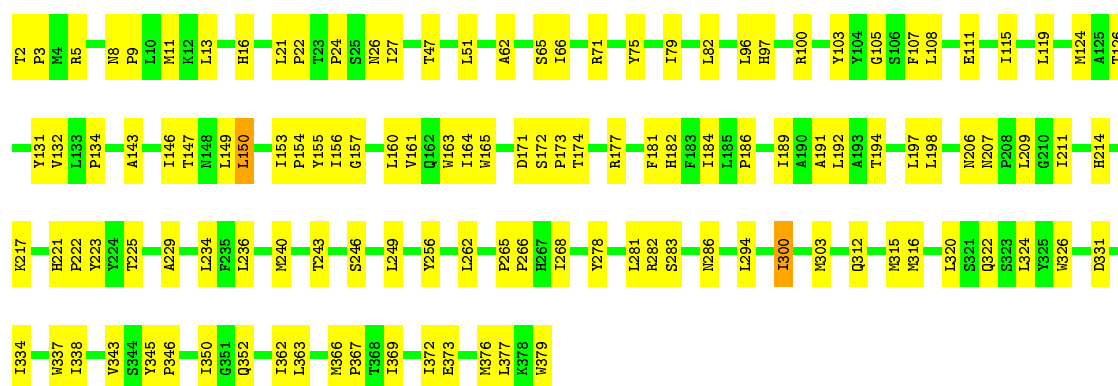
- Molecule 65: Cytochrome c1, heme protein, mitochondrial

Chain AU:  69% 30% .



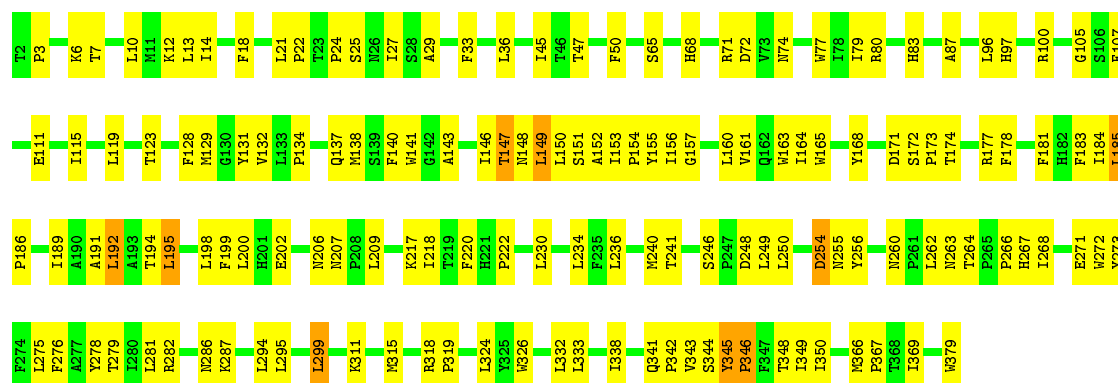
• Molecule 66: Cytochrome b

Chain AJ:  67% 32% .



• Molecule 66: Cytochrome b

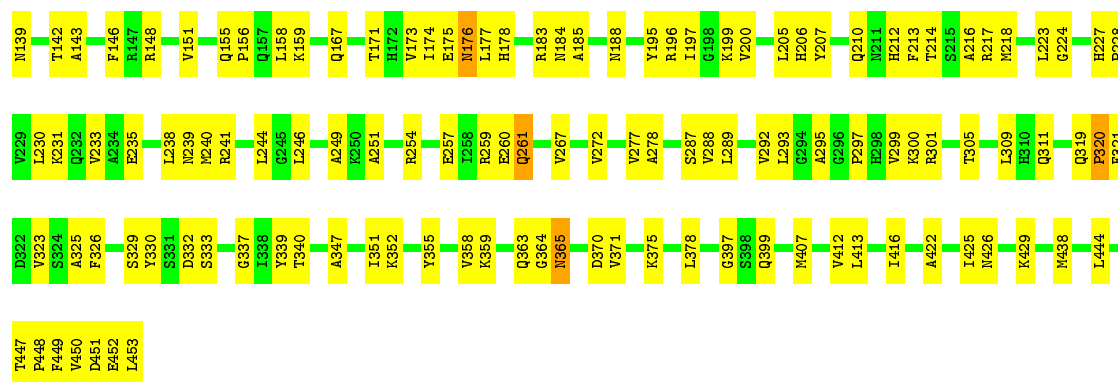
Chain AV:  61% 37% .



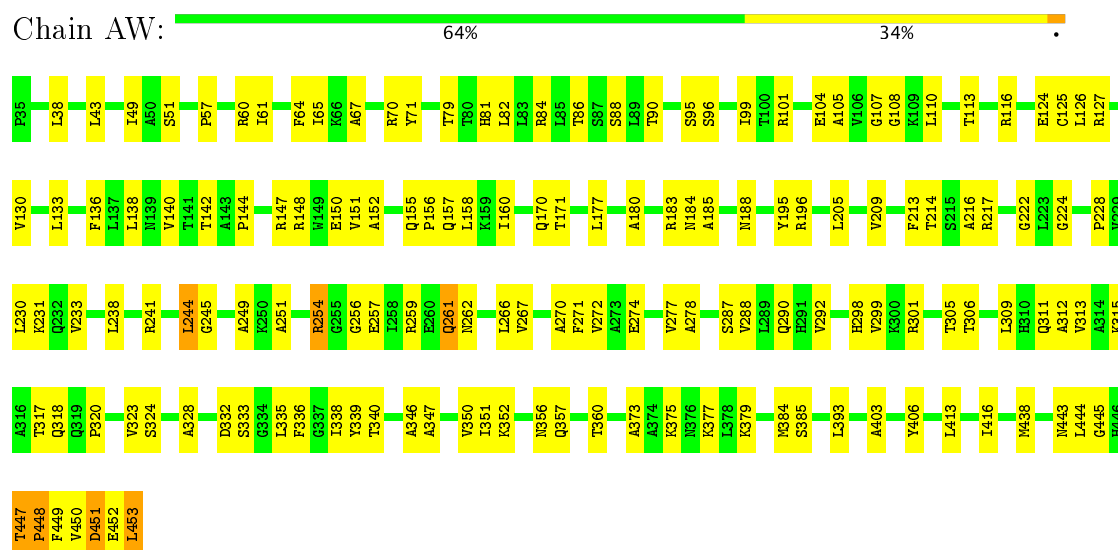
• Molecule 67: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain AK:  62% 37% .

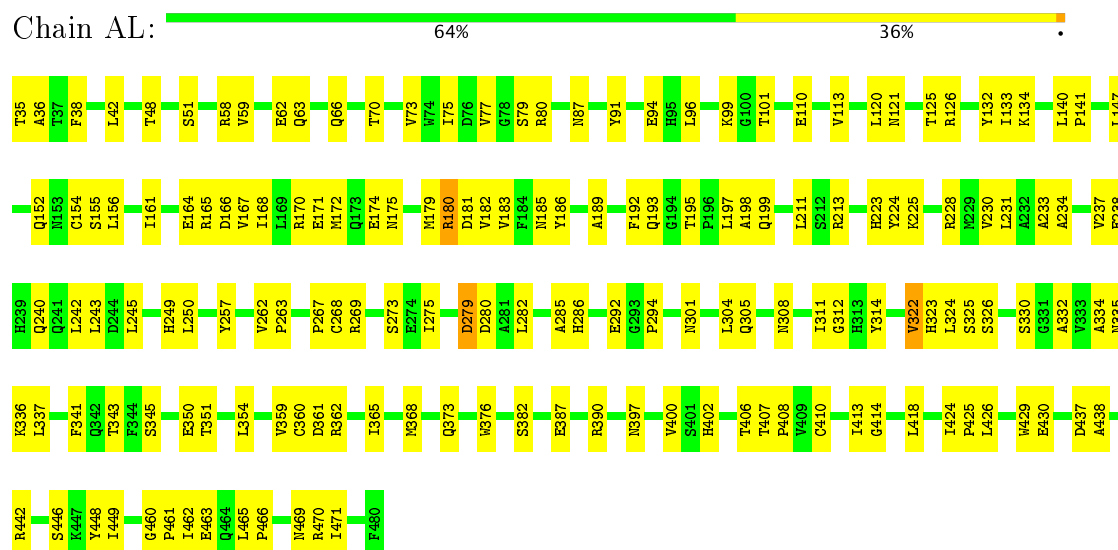




- Molecule 67: Cytochrome b-c1 complex subunit 2, mitochondrial



- Molecule 68: Cytochrome b-c1 complex subunit 1, mitochondrial

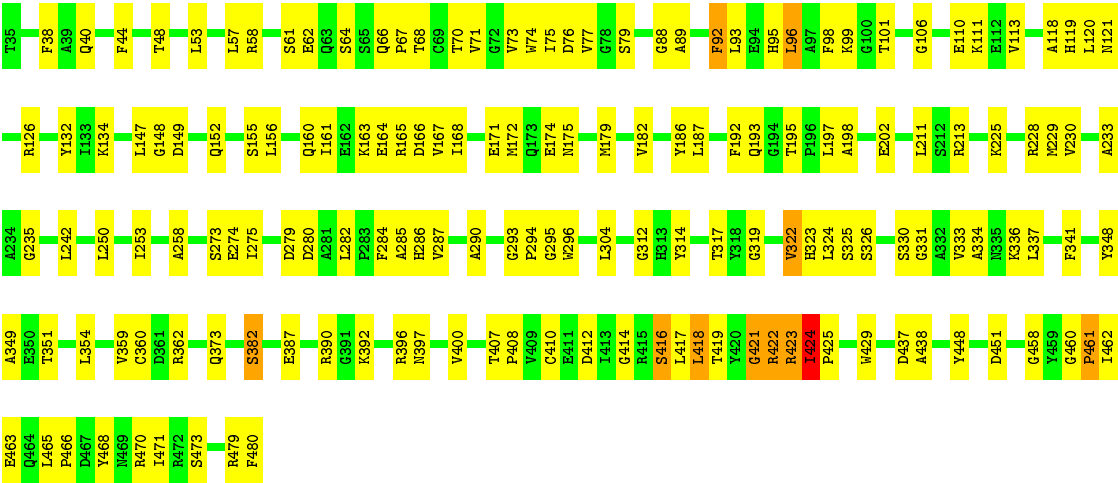


- Molecule 68: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain AY:

64%

33%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	167761	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, MG, CDL, SF4, HEM, ZN, PLX, FMN, FES, HEC, 8Q1, PEE, CU, HEA

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 > 2$	RMSZ	# $ Z > 2$
1	A	0.30	0/3398	0.49	0/4590
10	K	0.27	0/282	0.47	0/381
11	L	0.33	0/987	0.53	0/1331
12	M	0.32	0/5362	0.53	0/7266
13	N	0.37	0/1236	0.55	0/1681
14	O	0.29	0/1682	0.51	0/2289
15	P	0.38	0/1780	0.59	0/2424
16	Q	0.43	0/3552	0.59	1/4815 (0.0%)
17	S	0.60	0/583	0.64	0/785
18	T	0.32	0/755	0.47	0/1017
19	U	0.52	0/670	0.63	0/920
2	B	0.50	0/1452	0.57	0/1964
20	V	0.51	0/1065	0.61	0/1450
21	W	0.57	0/1166	0.68	1/1579 (0.1%)
22	Y	0.52	0/559	0.73	3/763 (0.4%)
23	Z	0.45	0/669	0.53	0/899
24	a	0.68	0/1209	0.65	0/1639
25	b	0.59	1/1095 (0.1%)	0.69	4/1480 (0.3%)
26	c	0.59	0/1287	0.58	0/1761
27	d	0.63	0/1445	0.65	1/1945 (0.1%)
28	e	0.61	0/835	0.62	0/1134
29	f	0.48	0/418	0.58	0/566
3	C	0.58	0/1280	0.57	0/1732
30	g	0.64	0/1035	0.63	0/1398
31	h	0.62	0/884	0.65	0/1182
32	i	0.67	0/2808	0.77	2/3843 (0.1%)
33	j	0.55	0/945	0.69	1/1292 (0.1%)
34	k	0.68	1/751 (0.1%)	0.79	1/1019 (0.1%)
35	l	0.61	2/4840 (0.0%)	0.70	3/6611 (0.0%)
36	m	0.68	0/1346	0.67	0/1832
37	n	0.49	0/484	0.62	0/652
38	o	0.54	0/1093	0.61	0/1479

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	p	0.59	0/1549	0.59	0/2098
4	E	0.34	0/993	0.53	0/1335
40	r	0.70	0/3723	0.76	2/5089 (0.0%)
41	s	0.62	0/2580	0.73	0/3539
42	u	0.57	0/1433	0.61	0/1937
43	v	0.49	0/934	0.67	3/1241 (0.2%)
44	w	0.44	0/2533	0.56	0/3440
45	x	0.60	0/4164	0.76	1/5688 (0.0%)
46	y	0.58	0/1868	0.80	0/2544
47	z	0.56	0/2211	0.69	0/3023
48	0	0.57	0/1229	0.65	1/1658 (0.1%)
49	1	0.50	0/898	0.66	0/1218
5	F	0.28	0/682	0.53	0/922
50	2	0.56	0/765	0.81	0/1038
51	3	0.55	0/699	0.73	1/950 (0.1%)
52	4	0.55	0/648	0.73	0/877
53	5	0.60	0/611	0.65	0/810
54	6	0.60	0/451	0.71	0/610
55	7	0.58	0/398	0.66	0/546
56	8	0.63	0/399	0.62	0/534
57	9	0.51	0/345	0.65	0/470
58	AA	0.31	0/715	0.48	0/964
58	AN	0.27	0/707	0.49	0/953
59	AB	0.23	0/421	0.60	1/574 (0.2%)
59	AO	0.25	0/417	0.61	1/569 (0.2%)
6	G	0.33	0/684	0.53	0/926
6	X	0.57	0/698	0.61	0/942
60	AC	0.24	0/1554	0.43	0/2104
60	AP	0.23	0/1554	0.42	0/2104
61	AD	0.26	0/521	0.42	0/699
61	AQ	0.27	0/521	0.43	0/699
62	AE	0.35	0/587	0.54	1/789 (0.1%)
62	AR	0.27	0/587	0.46	0/789
63	AF	0.42	1/942 (0.1%)	0.52	1/1263 (0.1%)
63	AS	0.27	0/942	0.44	0/1263
64	AG	0.27	0/442	0.48	0/608
64	AT	0.28	0/442	0.49	0/608
65	AH	0.26	0/1983	0.46	0/2691
65	AU	0.27	0/1983	0.45	0/2691
66	AJ	0.31	1/3108 (0.0%)	0.52	1/4254 (0.0%)
66	AV	0.34	2/3108 (0.1%)	0.54	2/4254 (0.0%)
67	AK	0.27	0/3217	0.49	0/4361
67	AW	0.29	1/3220 (0.0%)	0.48	1/4365 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
68	AL	0.27	0/3527	0.47	0/4788
68	AY	0.29	1/3527 (0.0%)	0.50	2/4788 (0.0%)
7	H	0.34	0/941	0.59	0/1275
8	I	0.29	0/788	0.54	0/1066
9	J	0.35	0/2785	0.52	0/3771
All	All	0.47	10/115987 (0.0%)	0.60	35/157444 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
44	w	0	1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	AW	448	PRO	N-CD	5.34	1.55	1.47
66	AJ	154	PRO	N-CD	5.22	1.55	1.47
66	AV	154	PRO	N-CD	5.22	1.55	1.47
34	k	2	PRO	N-CD	5.17	1.55	1.47
25	b	118	PRO	N-CD	5.17	1.55	1.47

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	i	323	THR	C-N-CD	-7.38	104.37	120.60
21	W	31	SER	N-CA-C	-7.00	92.09	111.00
22	Y	92	TRP	N-CA-C	-6.99	92.12	111.00
27	d	2	PRO	N-CA-CB	6.77	111.43	103.30
22	Y	87	PRO	CA-N-CD	-6.56	102.31	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	w	338	LYS	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3322	0	3289	209	0
2	B	1420	0	1371	104	0
3	C	1249	0	1253	67	0
4	E	968	0	982	62	0
5	F	670	0	679	36	0
6	G	672	0	650	31	0
6	X	686	0	676	23	0
7	H	922	0	950	58	0
8	I	769	0	788	45	0
9	J	2712	0	2757	236	0
10	K	274	0	257	24	0
11	L	964	0	962	65	0
12	M	5274	0	5312	326	0
13	N	1195	0	1155	48	0
14	O	1643	0	1646	113	0
15	P	1730	0	1685	116	0
16	Q	3460	0	3419	253	0
17	S	568	0	567	17	0
18	T	742	0	723	39	0
19	U	647	0	653	9	0
20	V	1038	0	1027	35	0
21	W	1135	0	1129	38	0
22	Y	533	0	475	45	0
23	Z	648	0	627	13	0
24	a	1174	0	1177	0	0
25	b	1059	0	1079	0	0
26	c	1236	0	1092	0	0
27	d	1418	0	1375	0	0
28	e	810	0	772	0	0
29	f	405	0	407	0	0
30	g	1004	0	1008	0	0
31	h	863	0	861	0	0
32	i	2735	0	2893	0	0
33	j	919	0	968	0	0
34	k	740	0	792	0	0
35	l	4717	0	4893	0	0
36	m	1313	0	1330	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	n	473	0	480	0	0
38	o	1066	0	1086	0	0
39	p	1495	0	1440	0	0
40	r	3629	0	3825	0	0
41	s	2509	0	2617	0	0
42	u	1394	0	1367	0	0
43	v	921	0	892	0	0
44	w	2474	0	2304	0	0
45	x	4025	0	4003	0	0
46	y	1822	0	1834	0	0
47	z	2124	0	2042	0	0
48	0	1195	0	1183	30	0
49	1	878	0	868	17	0
50	2	748	0	728	22	0
51	3	672	0	645	24	0
52	4	628	0	582	18	0
53	5	598	0	612	11	0
54	6	441	0	439	12	0
55	7	384	0	366	6	0
56	8	386	0	388	6	0
57	9	335	0	352	11	0
58	AA	694	0	683	46	0
58	AN	687	0	676	25	0
59	AB	413	0	438	25	0
59	AO	409	0	432	26	0
60	AC	1521	0	1505	54	0
60	AP	1521	0	1505	62	0
61	AD	509	0	511	15	0
61	AQ	509	0	511	24	0
62	AE	580	0	526	51	0
62	AR	580	0	526	34	0
63	AF	921	0	909	71	0
63	AS	921	0	910	30	0
64	AG	425	0	422	15	0
64	AT	425	0	422	31	0
65	AH	1924	0	1874	58	0
65	AU	1924	0	1874	82	0
66	AJ	3009	0	3065	107	0
66	AV	3009	0	3065	169	0
67	AK	3159	0	3130	152	0
67	AW	3162	0	3139	127	0
68	AL	3453	0	3370	140	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
68	AY	3453	0	3368	157	0
69	A	8	0	0	6	0
69	B	16	0	0	3	0
69	C	8	0	0	0	0
69	M	16	0	0	3	0
70	A	31	0	19	17	0
71	AL	52	0	88	3	0
71	AQ	52	0	88	7	0
71	AT	52	0	88	3	0
71	B	52	0	88	1	0
71	U	52	0	88	1	0
71	V	52	0	88	2	0
71	b	52	0	88	0	0
71	g	156	0	264	0	0
71	r	104	0	176	0	0
72	E	35	0	0	4	0
72	p	35	0	0	0	0
73	J	48	0	26	27	0
74	AC	4	0	0	3	0
74	AP	4	0	0	2	0
74	M	4	0	0	1	0
74	O	4	0	0	2	0
75	AA	64	0	72	1	0
75	AG	64	0	72	29	0
75	AH	64	0	72	6	0
75	AJ	128	0	144	23	0
75	AL	64	0	72	23	0
75	AN	64	0	72	8	0
75	AU	64	0	72	12	0
75	AY	64	0	72	4	0
75	V	63	0	68	8	0
75	i	64	0	72	0	0
75	l	128	0	144	0	0
75	n	64	0	72	0	0
76	AH	49	0	75	30	0
76	AJ	49	0	75	8	0
76	AL	49	0	75	38	0
76	AU	41	0	56	25	0
76	AV	49	0	75	21	0
76	AY	49	0	75	22	0
76	V	51	0	82	12	0
76	W	51	0	82	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
76	l	100	0	157	0	0
77	x	1	0	0	0	0
77	y	2	0	0	0	0
78	x	1	0	0	0	0
79	x	120	0	108	0	0
80	2	1	0	0	0	0
81	AH	43	0	32	5	0
81	AU	43	0	32	7	0
82	AJ	86	0	60	7	0
82	AV	86	0	60	13	0
All	All	115642	0	115742	3308	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

The worst 5 of 3308 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AY:296:TRP:CD1	68:AY:419:THR:CG2	1.74	1.60
63:AF:29:LYS:CD	63:AF:75:ILE:HD11	1.31	1.58
75:AJ:405:CDL:H112	76:AY:502:PEE:C45	1.18	1.56
63:AF:29:LYS:CG	63:AF:75:ILE:HD11	1.16	1.55
68:AY:296:TRP:CD1	68:AY:419:THR:HG23	0.99	1.52

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	429/431 (100%)	396 (92%)	24 (6%)	9 (2%)	8 48
2	B	174/176 (99%)	163 (94%)	10 (6%)	1 (1%)	28 70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	154/156 (99%)	136 (88%)	13 (8%)	5 (3%)	5	40
4	E	111/113 (98%)	101 (91%)	8 (7%)	2 (2%)	10	51
5	F	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
6	G	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	7	45
6	X	83/85 (98%)	73 (88%)	6 (7%)	4 (5%)	2	30
7	H	110/112 (98%)	100 (91%)	5 (4%)	5 (4%)	3	31
8	I	91/110 (83%)	79 (87%)	6 (7%)	6 (7%)	1	23
9	J	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	8	48
10	K	31/33 (94%)	27 (87%)	1 (3%)	3 (10%)	1	13
11	L	116/118 (98%)	104 (90%)	8 (7%)	4 (3%)	4	39
12	M	685/687 (100%)	608 (89%)	54 (8%)	23 (3%)	4	39
13	N	141/143 (99%)	119 (84%)	15 (11%)	7 (5%)	2	29
14	O	210/212 (99%)	188 (90%)	15 (7%)	7 (3%)	4	39
15	P	206/208 (99%)	173 (84%)	22 (11%)	11 (5%)	2	28
16	Q	428/430 (100%)	398 (93%)	23 (5%)	7 (2%)	11	53
17	S	68/70 (97%)	61 (90%)	5 (7%)	2 (3%)	5	42
18	T	93/95 (98%)	87 (94%)	2 (2%)	4 (4%)	3	32
19	U	81/83 (98%)	76 (94%)	4 (5%)	1 (1%)	15	58
20	V	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	8	47
21	W	136/138 (99%)	127 (93%)	4 (3%)	5 (4%)	4	36
22	Y	57/59 (97%)	50 (88%)	1 (2%)	6 (10%)	0	11
23	Z	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
24	a	136/138 (99%)	121 (89%)	12 (9%)	3 (2%)	8	47
25	b	122/124 (98%)	107 (88%)	10 (8%)	5 (4%)	3	33
26	c	151/153 (99%)	129 (85%)	15 (10%)	7 (5%)	3	30
27	d	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	28	70
28	e	95/97 (98%)	83 (87%)	9 (10%)	3 (3%)	5	40
29	f	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	8	47
30	g	117/119 (98%)	105 (90%)	6 (5%)	6 (5%)	2	28
31	h	102/104 (98%)	86 (84%)	10 (10%)	6 (6%)	2	25
32	i	345/347 (99%)	324 (94%)	15 (4%)	6 (2%)	11	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	j	113/115 (98%)	103 (91%)	7 (6%)	3 (3%)	6	43
34	k	95/97 (98%)	88 (93%)	4 (4%)	3 (3%)	5	40
35	l	601/603 (100%)	553 (92%)	38 (6%)	10 (2%)	11	52
36	m	172/174 (99%)	150 (87%)	12 (7%)	10 (6%)	2	26
37	n	54/56 (96%)	50 (93%)	2 (4%)	2 (4%)	4	36
38	o	126/128 (98%)	113 (90%)	9 (7%)	4 (3%)	5	40
39	p	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	10	51
40	r	457/459 (100%)	420 (92%)	28 (6%)	9 (2%)	9	49
41	s	316/318 (99%)	285 (90%)	22 (7%)	9 (3%)	6	43
42	u	167/169 (99%)	152 (91%)	10 (6%)	5 (3%)	5	41
43	v	107/122 (88%)	90 (84%)	14 (13%)	3 (3%)	6	43
44	w	318/320 (99%)	281 (88%)	28 (9%)	9 (3%)	6	43
45	x	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	22	65
46	y	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	14	57
47	z	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
48	0	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
49	1	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
50	2	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	3	32
51	3	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	2	25
52	4	73/75 (97%)	64 (88%)	8 (11%)	1 (1%)	13	55
53	5	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
54	6	54/56 (96%)	47 (87%)	5 (9%)	2 (4%)	4	36
55	7	47/49 (96%)	41 (87%)	6 (13%)	0	100	100
56	8	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
57	9	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
58	AA	79/81 (98%)	71 (90%)	6 (8%)	2 (2%)	6	44
58	AN	79/81 (98%)	74 (94%)	4 (5%)	1 (1%)	14	57
59	AB	55/57 (96%)	41 (74%)	11 (20%)	3 (6%)	2	27
59	AO	55/57 (96%)	43 (78%)	6 (11%)	6 (11%)	0	10
60	AC	194/196 (99%)	179 (92%)	10 (5%)	5 (3%)	6	44
60	AP	194/196 (99%)	178 (92%)	13 (7%)	3 (2%)	12	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	AD	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
61	AQ	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
62	AE	72/74 (97%)	65 (90%)	5 (7%)	2 (3%)	6	43
62	AR	72/74 (97%)	69 (96%)	2 (3%)	1 (1%)	13	55
63	AF	104/106 (98%)	100 (96%)	3 (3%)	1 (1%)	18	61
63	AS	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
64	AG	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
64	AT	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
65	AH	239/241 (99%)	225 (94%)	12 (5%)	2 (1%)	22	65
65	AU	239/241 (99%)	230 (96%)	7 (3%)	2 (1%)	22	65
66	AJ	376/378 (100%)	363 (96%)	10 (3%)	3 (1%)	22	65
66	AV	376/378 (100%)	359 (96%)	14 (4%)	3 (1%)	22	65
67	AK	417/419 (100%)	390 (94%)	22 (5%)	5 (1%)	15	58
67	AW	417/419 (100%)	397 (95%)	15 (4%)	5 (1%)	15	58
68	AL	444/446 (100%)	405 (91%)	33 (7%)	6 (1%)	13	55
68	AY	444/446 (100%)	413 (93%)	24 (5%)	7 (2%)	11	53
All	All	14029/14219 (99%)	12872 (92%)	849 (6%)	308 (2%)	12	47

5 of 308 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	TYR
1	A	73	PRO
1	A	379	CYS
2	B	62	THR
12	M	37	ASP

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	346/346 (100%)	346 (100%)	0	100	100
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	106/106 (100%)	105 (99%)	1 (1%)	82	92
5	F	74/74 (100%)	74 (100%)	0	100	100
6	G	74/79 (94%)	74 (100%)	0	100	100
6	X	78/79 (99%)	78 (100%)	0	100	100
7	H	100/100 (100%)	100 (100%)	0	100	100
8	I	87/96 (91%)	87 (100%)	0	100	100
9	J	292/292 (100%)	288 (99%)	4 (1%)	71	87
10	K	32/32 (100%)	32 (100%)	0	100	100
11	L	107/107 (100%)	107 (100%)	0	100	100
12	M	576/577 (100%)	574 (100%)	2 (0%)	94	97
13	N	129/129 (100%)	129 (100%)	0	100	100
14	O	181/181 (100%)	181 (100%)	0	100	100
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	371/371 (100%)	369 (100%)	2 (0%)	91	96
17	S	59/59 (100%)	59 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	72/72 (100%)	72 (100%)	0	100	100
20	V	102/102 (100%)	102 (100%)	0	100	100
21	W	119/119 (100%)	119 (100%)	0	100	100
22	Y	57/57 (100%)	49 (86%)	8 (14%)	4	27
23	Z	62/63 (98%)	62 (100%)	0	100	100
24	a	124/124 (100%)	122 (98%)	2 (2%)	68	86
25	b	118/118 (100%)	114 (97%)	4 (3%)	42	73
26	c	124/137 (90%)	124 (100%)	0	100	100
27	d	145/154 (94%)	137 (94%)	8 (6%)	25	62
28	e	90/90 (100%)	90 (100%)	0	100	100
29	f	43/43 (100%)	43 (100%)	0	100	100
30	g	105/105 (100%)	105 (100%)	0	100	100
31	h	90/90 (100%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	i	314/314 (100%)	314 (100%)	0	100	100
33	j	102/103 (99%)	102 (100%)	0	100	100
34	k	85/85 (100%)	82 (96%)	3 (4%)	41	72
35	l	531/532 (100%)	510 (96%)	21 (4%)	36	69
36	m	137/137 (100%)	137 (100%)	0	100	100
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	114/114 (100%)	114 (100%)	0	100	100
39	p	157/157 (100%)	156 (99%)	1 (1%)	89	95
40	r	416/416 (100%)	416 (100%)	0	100	100
41	s	278/278 (100%)	278 (100%)	0	100	100
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	89/111 (80%)	89 (100%)	0	100	100
44	w	249/288 (86%)	249 (100%)	0	100	100
45	x	427/427 (100%)	389 (91%)	38 (9%)	11	44
46	y	211/211 (100%)	191 (90%)	20 (10%)	10	41
47	z	226/226 (100%)	199 (88%)	27 (12%)	6	32
48	0	128/128 (100%)	120 (94%)	8 (6%)	21	57
49	1	95/95 (100%)	89 (94%)	6 (6%)	21	57
50	2	81/81 (100%)	76 (94%)	5 (6%)	21	58
51	3	68/68 (100%)	50 (74%)	18 (26%)	0	5
52	4	67/67 (100%)	58 (87%)	9 (13%)	4	28
53	5	58/58 (100%)	53 (91%)	5 (9%)	12	46
54	6	47/47 (100%)	40 (85%)	7 (15%)	3	24
55	7	39/39 (100%)	37 (95%)	2 (5%)	28	63
56	8	40/40 (100%)	38 (95%)	2 (5%)	28	64
57	9	37/37 (100%)	34 (92%)	3 (8%)	14	49
58	AA	74/74 (100%)	68 (92%)	6 (8%)	14	49
58	AN	73/74 (99%)	73 (100%)	0	100	100
59	AB	46/46 (100%)	46 (100%)	0	100	100
59	AO	45/46 (98%)	45 (100%)	0	100	100
60	AC	166/166 (100%)	166 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
60	AP	166/166 (100%)	166 (100%)	0	100	100
61	AD	52/52 (100%)	52 (100%)	0	100	100
61	AQ	52/52 (100%)	52 (100%)	0	100	100
62	AE	61/71 (86%)	59 (97%)	2 (3%)	43	73
62	AR	61/71 (86%)	59 (97%)	2 (3%)	43	73
63	AF	95/95 (100%)	84 (88%)	11 (12%)	6	33
63	AS	95/95 (100%)	95 (100%)	0	100	100
64	AG	42/42 (100%)	42 (100%)	0	100	100
64	AT	42/42 (100%)	40 (95%)	2 (5%)	30	65
65	AH	207/207 (100%)	207 (100%)	0	100	100
65	AU	207/207 (100%)	206 (100%)	1 (0%)	91	96
66	AJ	330/330 (100%)	327 (99%)	3 (1%)	82	92
66	AV	330/330 (100%)	322 (98%)	8 (2%)	54	79
67	AK	334/335 (100%)	331 (99%)	3 (1%)	82	92
67	AW	335/335 (100%)	332 (99%)	3 (1%)	82	92
68	AL	367/367 (100%)	367 (100%)	0	100	100
68	AY	367/367 (100%)	361 (98%)	6 (2%)	68	86
All	All	12164/12289 (99%)	11911 (98%)	253 (2%)	62	82

5 of 253 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	z	1	MET
48	0	31	LYS
64	AT	39	ARG
47	z	14	SER
47	z	131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 234 such sidechains are listed below:

Mol	Chain	Res	Type
35	l	348	HIS
42	u	77	HIS
66	AV	260	ASN
35	l	442	ASN

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Mol	Chain	Res	Type
39	p	75	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 63 ligands modelled in this entry, 5 are monoatomic - leaving 58 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$
69	SF4	A	501	1	0,12,12	0.00	-	0,24,24	0.00	-
70	FMN	A	502	-	31,33,33	1.47	5 (16%)	38,50,50	1.95	8 (21%)
75	CDL	AA	101	-	63,63,99	1.22	5 (7%)	65,75,111	1.13	5 (7%)
74	FES	AC	301	60	0,4,4	0.00	-	0,4,4	0.00	-
75	CDL	AG	101	-	63,63,99	1.13	4 (6%)	65,75,111	1.23	5 (7%)
76	PEE	AH	401	-	48,48,50	1.02	2 (4%)	50,53,55	0.89	2 (4%)
81	HEC	AH	402	65	28,50,50	2.31	3 (10%)	16,82,82	1.56	2 (12%)
75	CDL	AH	403	-	63,63,99	1.23	5 (7%)	65,75,111	1.09	5 (7%)
82	HEM	AJ	401	66	28,50,50	2.15	6 (21%)	17,82,82	1.52	3 (17%)
82	HEM	AJ	402	66	28,50,50	2.14	6 (21%)	17,82,82	1.42	4 (23%)
76	PEE	AJ	403	-	48,48,50	0.99	2 (4%)	50,53,55	0.93	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	CDL	AJ	404	-	63,63,99	1.22	5 (7%)	65,75,111	1.08	4 (6%)
75	CDL	AJ	405	-	63,63,99	1.11	4 (6%)	65,75,111	1.29	5 (7%)
71	PLX	AL	501	-	51,51,51	0.76	1 (1%)	54,59,59	0.64	1 (1%)
75	CDL	AL	502	-	63,63,99	1.23	5 (7%)	65,75,111	1.11	4 (6%)
76	PEE	AL	503	-	48,48,50	1.05	2 (4%)	50,53,55	0.84	2 (4%)
75	CDL	AN	101	-	63,63,99	1.22	5 (7%)	65,75,111	1.08	4 (6%)
74	FES	AP	301	60	0,4,4	0.00	-	0,4,4	0.00	-
71	PLX	AQ	101	-	51,51,51	0.76	1 (1%)	54,59,59	0.62	2 (3%)
71	PLX	AT	101	-	51,51,51	0.74	1 (1%)	54,59,59	0.61	1 (1%)
76	PEE	AU	401	-	40,40,50	1.10	2 (5%)	42,45,55	0.86	2 (4%)
81	HEC	AU	402	65	28,50,50	2.39	3 (10%)	16,82,82	1.61	3 (18%)
75	CDL	AU	403	-	63,63,99	1.22	6 (9%)	65,75,111	1.10	4 (6%)
82	HEM	AV	401	66	28,50,50	2.23	6 (21%)	17,82,82	1.59	3 (17%)
82	HEM	AV	402	66	28,50,50	2.15	6 (21%)	17,82,82	1.52	4 (23%)
76	PEE	AV	403	-	48,48,50	1.02	2 (4%)	50,53,55	0.98	2 (4%)
75	CDL	AY	501	-	63,63,99	1.22	5 (7%)	65,75,111	1.06	4 (6%)
76	PEE	AY	502	-	48,48,50	1.06	2 (4%)	50,53,55	0.90	2 (4%)
69	SF4	B	301	2	0,12,12	0.00	-	0,24,24	0.00	-
69	SF4	B	302	2	0,12,12	0.00	-	0,24,24	0.00	-
71	PLX	B	303	-	51,51,51	0.76	1 (1%)	54,59,59	0.69	1 (1%)
69	SF4	C	301	3	0,12,12	0.00	-	0,24,24	0.00	-
72	8Q1	E	201	-	32,34,34	1.64	6 (18%)	39,43,43	1.54	8 (20%)
73	NDP	J	401	-	43,52,52	0.99	2 (4%)	49,80,80	1.41	3 (6%)
69	SF4	M	801	12	0,12,12	0.00	-	0,24,24	0.00	-
69	SF4	M	802	12	0,12,12	0.00	-	0,24,24	0.00	-
74	FES	M	803	-	0,4,4	0.00	-	0,4,4	0.00	-
74	FES	O	301	14	0,4,4	0.00	-	0,4,4	0.00	-
71	PLX	U	101	-	51,51,51	0.73	1 (1%)	54,59,59	0.74	2 (3%)
75	CDL	V	201	-	61,61,99	1.24	5 (8%)	60,71,111	0.99	3 (5%)
76	PEE	V	202	-	50,50,50	0.87	4 (8%)	52,55,55	0.85	2 (3%)
71	PLX	V	203	-	51,51,51	0.77	1 (1%)	54,59,59	0.61	1 (1%)
76	PEE	W	201	-	50,50,50	0.86	4 (8%)	52,55,55	0.92	2 (3%)
71	PLX	b	201	-	51,51,51	0.60	0	54,59,59	0.64	0
71	PLX	g	201	-	51,51,51	0.81	1 (1%)	54,59,59	0.69	1 (1%)
71	PLX	g	202	-	51,51,51	0.74	1 (1%)	54,59,59	0.62	1 (1%)
71	PLX	g	203	-	51,51,51	0.77	1 (1%)	54,59,59	0.59	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	CDL	i	401	-	63,63,99	1.19	5 (7%)	65,75,111	1.10	5 (7%)
76	PEE	l	701	-	48,48,50	1.02	2 (4%)	50,53,55	0.89	2 (4%)
76	PEE	l	702	-	50,50,50	0.88	4 (8%)	52,55,55	0.93	2 (3%)
75	CDL	l	703	-	63,63,99	1.19	5 (7%)	65,75,111	1.12	4 (6%)
75	CDL	l	704	-	63,63,99	1.25	5 (7%)	65,75,111	1.06	4 (6%)
75	CDL	n	101	-	63,63,99	1.22	5 (7%)	65,75,111	1.12	4 (6%)
72	8Q1	p	201	-	32,34,34	1.67	5 (15%)	39,43,43	1.80	5 (12%)
71	PLX	r	501	-	51,51,51	0.74	1 (1%)	54,59,59	0.66	1 (1%)
71	PLX	r	502	-	51,51,51	0.67	0	54,59,59	0.67	1 (1%)
79	HEA	x	603	45	44,67,67	1.63	8 (18%)	37,103,103	1.87	9 (24%)
79	HEA	x	604	45	44,67,67	1.54	4 (9%)	37,103,103	1.37	8 (21%)

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
69	SF4	A	501	1	-	0/0/48/48	0/6/5/5
70	FMN	A	502	-	-	0/16/18/18	0/3/3/3
75	CDL	AA	101	-	-	0/74/74/110	0/0/0/0
74	FES	AC	301	60	-	0/0/4/4	0/1/1/1
75	CDL	AG	101	-	-	0/74/74/110	0/0/0/0
76	PEE	AH	401	-	-	0/52/52/54	0/0/0/0
81	HEC	AH	402	65	-	0/6/54/54	0/0/8/8
75	CDL	AH	403	-	-	1/74/74/110	0/0/0/0
82	HEM	AJ	401	66	-	0/6/54/54	0/0/8/8
82	HEM	AJ	402	66	-	0/6/54/54	0/0/8/8
76	PEE	AJ	403	-	-	0/52/52/54	0/0/0/0
75	CDL	AJ	404	-	-	0/74/74/110	0/0/0/0
75	CDL	AJ	405	-	-	0/74/74/110	0/0/0/0
71	PLX	AL	501	-	-	0/54/55/55	0/0/0/0
75	CDL	AL	502	-	-	0/74/74/110	0/0/0/0
76	PEE	AL	503	-	-	2/52/52/54	0/0/0/0
75	CDL	AN	101	-	-	0/74/74/110	0/0/0/0
74	FES	AP	301	60	-	0/0/4/4	0/1/1/1
71	PLX	AQ	101	-	-	0/54/55/55	0/0/0/0
71	PLX	AT	101	-	-	0/54/55/55	0/0/0/0
76	PEE	AU	401	-	-	0/44/44/54	0/0/0/0
81	HEC	AU	402	65	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	CDL	AU	403	-	-	0/74/74/110	0/0/0/0
82	HEM	AV	401	66	-	0/6/54/54	0/0/8/8
82	HEM	AV	402	66	-	0/6/54/54	0/0/8/8
76	PEE	AV	403	-	-	0/52/52/54	0/0/0/0
75	CDL	AY	501	-	-	0/74/74/110	0/0/0/0
76	PEE	AY	502	-	-	0/52/52/54	0/0/0/0
69	SF4	B	301	2	-	0/0/48/48	0/6/5/5
69	SF4	B	302	2	-	0/0/48/48	0/6/5/5
71	PLX	B	303	-	-	0/54/55/55	0/0/0/0
69	SF4	C	301	3	-	0/0/48/48	0/6/5/5
72	8Q1	E	201	-	-	2/41/41/41	0/0/0/0
73	NDP	J	401	-	-	0/30/77/77	0/5/5/5
69	SF4	M	801	12	-	0/0/48/48	0/6/5/5
69	SF4	M	802	12	-	0/0/48/48	0/6/5/5
74	FES	M	803	-	-	0/0/4/4	0/1/1/1
74	FES	O	301	14	-	0/0/4/4	0/1/1/1
71	PLX	U	101	-	-	0/54/55/55	0/0/0/0
75	CDL	V	201	-	-	0/69/69/110	0/0/0/0
76	PEE	V	202	-	-	0/54/54/54	0/0/0/0
71	PLX	V	203	-	-	0/54/55/55	0/0/0/0
76	PEE	W	201	-	-	0/54/54/54	0/0/0/0
71	PLX	b	201	-	-	0/54/55/55	0/0/0/0
71	PLX	g	201	-	-	0/54/55/55	0/0/0/0
71	PLX	g	202	-	-	0/54/55/55	0/0/0/0
71	PLX	g	203	-	-	0/54/55/55	0/0/0/0
75	CDL	i	401	-	-	0/74/74/110	0/0/0/0
76	PEE	l	701	-	-	0/52/52/54	0/0/0/0
76	PEE	l	702	-	-	0/54/54/54	0/0/0/0
75	CDL	l	703	-	-	0/74/74/110	0/0/0/0
75	CDL	l	704	-	-	0/74/74/110	0/0/0/0
75	CDL	n	101	-	-	2/74/74/110	0/0/0/0
72	8Q1	p	201	-	-	2/41/41/41	0/0/0/0
71	PLX	r	501	-	-	0/54/55/55	0/0/0/0
71	PLX	r	502	-	-	0/54/55/55	0/0/0/0
79	HEA	x	603	45	3/3/7/16	0/24/76/76	0/0/8/8
79	HEA	x	604	45	3/3/7/16	0/24/76/76	0/0/8/8

The worst 5 of 165 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	AU	402	HEC	C3C-C2C	-6.89	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	x	604	HEA	C3A-C2A	-6.82	1.31	1.40
81	AU	402	HEC	C3B-C2B	-6.62	1.33	1.40
81	AH	402	HEC	C3B-C2B	-6.48	1.33	1.40
81	AH	402	HEC	C3C-C2C	-6.47	1.33	1.40

The worst 5 of 153 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	J	401	NDP	N3A-C2A-N1A	-6.94	122.81	128.86
72	p	201	8Q1	O4-C1-C6	-4.87	119.68	123.95
79	x	603	HEA	C4B-C3B-C2B	-4.60	103.66	106.87
70	A	502	FMN	C4-C4A-C10	-3.93	116.78	119.96
79	x	603	HEA	CMB-C2B-C1B	-3.91	122.45	128.46

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
79	x	603	HEA	ND
79	x	603	HEA	NA
79	x	603	HEA	NB
79	x	604	HEA	ND
79	x	604	HEA	NA

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
72	E	201	8Q1	C29-C32-C34-N36
72	E	201	8Q1	O35-C34-C32-C29
75	AH	403	CDL	CB4-OB6-CB5-C51
75	n	101	CDL	CA4-OA6-CA5-OA7
75	n	101	CDL	CA4-OA6-CA5-C11

There are no ring outliers.

41 monomers are involved in 365 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	A	501	SF4	6	0
70	A	502	FMN	17	0
75	AA	101	CDL	1	0
74	AC	301	FES	3	0
75	AG	101	CDL	29	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
76	AH	401	PEE	30	0
81	AH	402	HEC	5	0
75	AH	403	CDL	6	0
82	AJ	401	HEM	3	0
82	AJ	402	HEM	4	0
76	AJ	403	PEE	8	0
75	AJ	404	CDL	6	0
75	AJ	405	CDL	17	0
71	AL	501	PLX	3	0
75	AL	502	CDL	23	0
76	AL	503	PEE	38	0
75	AN	101	CDL	8	0
74	AP	301	FES	2	0
71	AQ	101	PLX	7	0
71	AT	101	PLX	3	0
76	AU	401	PEE	25	0
81	AU	402	HEC	7	0
75	AU	403	CDL	12	0
82	AV	401	HEM	7	0
82	AV	402	HEM	6	0
76	AV	403	PEE	21	0
75	AY	501	CDL	4	0
76	AY	502	PEE	22	0
69	B	301	SF4	1	0
69	B	302	SF4	2	0
71	B	303	PLX	1	0
72	E	201	8Q1	4	0
73	J	401	NDP	27	0
69	M	801	SF4	3	0
74	M	803	FES	1	0
74	O	301	FES	2	0
71	U	101	PLX	1	0
75	V	201	CDL	8	0
76	V	202	PEE	12	0
71	V	203	PLX	2	0
76	W	201	PEE	5	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.