



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 6, 2016 – 12:33 AM EST

PDB ID : 5LUF
EMDB ID: : EMD-4107
Title : Cryo-EM of bovine respirasome
Authors : Sousa, J.S.; Mills, D.J.; Vonck, J.; Kuehlbrandt, W.
Deposited on : 2016-09-08
Resolution : 9.10 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.

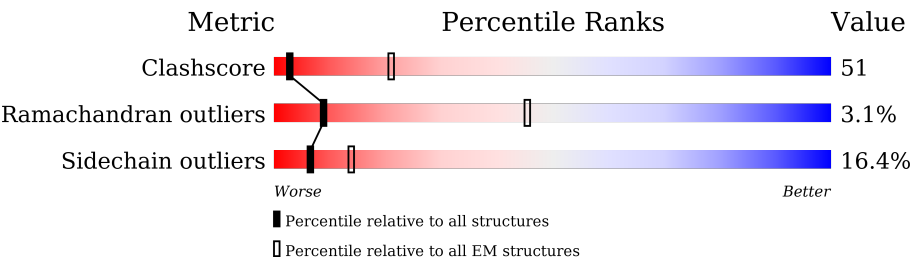
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 9.10 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	c	446	<div><div>70%26%.</div></div>
1	l	446	<div><div>70%26%.</div></div>
2	m	439	<div><div>73%20%.5%</div></div>
2	n	439	<div><div>75%19%.5%</div></div>
3	b	379	<div><div>69%28%.</div></div>
3	o	379	<div><div>74%23%.</div></div>
4	d	241	<div><div>78%18%.</div></div>
4	p	241	<div><div>76%22%.</div></div>
5	e	196	<div><div>28%9%.62%</div></div>


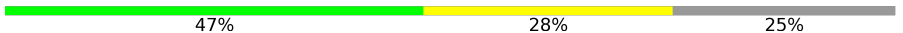




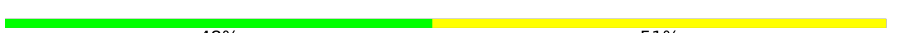


















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Mol	Chain	Length	Quality of chain
5	q	196	 63% 30% 6% .
6	f	110	 65% 28% . .
6	r	110	 65% 29% . .
7	g	81	 74% 22% .
7	s	81	 73% 26% .
8	h	78	 69% 13% 18%
8	t	78	 67% 15% 18%
9	i	78	 28% 12% . 58%
9	u	78	 31% 9% . 58%
10	j	62	 74% 24% .
10	v	62	 73% 26% .
11	k	56	 32% 7% 61%
11	w	56	 29% 9% . 61%
12	x	514	 92% 8%
13	y	227	 90% 10%
14	z	261	 90% 10%
15	1	147	 71% 24% . .
16	2	109	 78% 20% .
17	3	98	 66% 28% 6%
18	4	84	 62% 31% 6% .
19	5	85	 62% 20% 6% 12%
20	6	73	 79% 18% .
21	7	59	 69% 17% 5% . 5%
22	8	56	 66% 21% 13%
23	9	47	 81% 17% .




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Mol	Chain	Length	Quality of chain
24	0	46	
25	A	111	
26	B	143	
27	C	154	
28	D	384	
29	E	159	
30	F	411	
31	G	538	
32	H	313	
33	I	162	
34	J	171	
35	K	84	
36	L	601	
37	M	453	
38	N	345	
39	O	220	
40	P	303	
41	Q	85	
42	R	47	
43	S	80	
44	T	75	
45	V	71	
46	W	72	
47	X	330	
48	Y	106	

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Mol	Chain	Length	Quality of chain
49	a	142	 50% 50%
50	U	828	 22% 8% 70%
51	Z	625	 29% 13% 57%

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
54	FES	G	803	-	-	X	-
57	HEA	x	603	X	-	-	-
57	HEA	x	604	X	-	-	-
59	SF4	B	201	-	-	X	-
59	SF4	I	201	-	-	X	-
59	SF4	I	202	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 74493 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 Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	c	446	Total	C	N	O	S	0	0
			3458	2161	609	668	20		
1	l	446	Total	C	N	O	S	0	0
			3458	2161	609	668	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	m	419	Total	C	N	O	S	0	0
			3141	1972	556	606	7		
2	n	419	Total	C	N	O	S	0	0
			3141	1972	556	606	7		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	b	379	Total	C	N	O	S	0	0
			3011	2018	472	502	19		
3	o	379	Total	C	N	O	S	0	0
			3011	2018	472	502	19		

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	241	Total	C	N	O	S	0	0
			1919	1225	330	349	15		
4	p	241	Total	C	N	O	S	0	0
			1919	1225	330	349	15		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	75	Total	C	N	O	S	0	0
			566	352	94	118	2		
5	q	196	Total	C	N	O	S	0	0
			1518	956	263	291	8		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	106	Total	C	N	O	S	0	0
			916	579	166	169	2		
6	r	106	Total	C	N	O	S	0	0
			916	579	166	169	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	56	ASP	ASN	conflict	UNP P00129
r	56	ASP	ASN	conflict	UNP P00129

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	81	Total	C	N	O	S	0	0
			682	441	128	112	1		
7	s	81	Total	C	N	O	S	0	0
			682	441	128	112	1		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	64	Total	C	N	O	S	0	0
			524	316	96	107	5		
8	t	64	Total	C	N	O	S	0	0
			524	316	96	107	5		

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	33	Total	C	N	O	S	0	0
			248	152	51	44	1		
9	u	33	Total	C	N	O	S	0	0
			248	152	51	44	1		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	62	Total	C	N	O	0	0
			512	335	89	88		
10	v	62	Total	C	N	O	0	0
			512	335	89	88		

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	k	22	Total	C	N	O	0	0
			159	103	29	27		
11	w	22	Total	C	N	O	0	0
			159	103	29	27		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	22	GLN	SER	conflict	UNP P07552
k	34	SER	TRP	conflict	UNP P07552
k	38	SER	TRP	conflict	UNP P07552
w	22	GLN	SER	conflict	UNP P07552
w	34	SER	TRP	conflict	UNP P07552
w	38	SER	TRP	conflict	UNP P07552

- Molecule 12 is a protein called Cytochrome c oxidase subunit 1.

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

- Molecule 13 is a protein called Cytochrome c oxidase subunit 2.

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

- Molecule 14 is a protein called Cytochrome c oxidase subunit 3.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	238	GLY	ALA	conflict	UNP P00415

- Molecule 15 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1	144	Total	C	N	O	S	0	0
			1195	777	196	218	4		

- Molecule 16 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2	109	Total	C	N	O	S	0	0
			878	558	150	168	2		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	3	98	Total	C	N	O	S	0	0
			748	464	134	145	5		

- Molecule 18 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	4	84	Total	C	N	O	S	0	0
			672	431	129	111	1		

- Molecule 19 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	5	75	Total	C	N	O	S	0	0
			628	395	114	114	5		

- Molecule 20 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	6	73	Total	C	N	O	S	0	0
			598	388	107	99	4		

- Molecule 21 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	7	56	Total	C	N	O	S	0	0
			441	285	73	80	3		

- Molecule 22 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	8	49	Total	C	N	O	S	0	0
			384	250	65	67	2		

- Molecule 23 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	9	47	Total	C	N	O	S	0	0
			386	257	65	62	2		

- Molecule 24 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	0	43	Total	C	N	O	0	0
			335	223	53	59		

- Molecule 25 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	A	83	Total	C	N	O	0	0
			415	249	83	83		

- Molecule 26 is a protein called complex I.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	143	Total	C	N	O	S	0	0
			719	429	143	143	4		

- Molecule 27 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	C	154	Total	C	N	O	0	0
			770	462	154	154		

- Molecule 28 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	D	384	Total	C	N	O	0	0
			1920	1152	384	384		

- Molecule 29 is a protein called complex I.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	E	159	Total	C	N	O	S	0	0
			799	477	159	159	4		

- Molecule 30 is a protein called complex I.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	F	411	Total	C	N	O	S	0	0
			2059	1233	411	411	4		

- Molecule 31 is a protein called complex I.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	G	527	Total	C	N	O	S	0	0
			2651	1584	529	527	11		

- Molecule 32 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	H	285	Total	C	N	O	0	0
			1425	855	285	285		

- Molecule 33 is a protein called complex I.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	I	162	Total	C	N	O	S	0	0
			818	486	162	162	8		

- Molecule 34 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	J	131	Total	C	N	O	0	0
			655	393	131	131		

- Molecule 35 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	K	84	Total	C	N	O	0	0
			420	252	84	84		

- Molecule 36 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	L	558	Total	C	N	O	0	0
			2790	1674	558	558		

- Molecule 37 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	M	439	Total	C	N	O	0	0
			2195	1317	439	439		

- Molecule 38 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	N	326	Total	C	N	O	0	0
			1630	978	326	326		

- Molecule 39 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	O	181	Total	C	N	O	0	0
			905	543	181	181		

- Molecule 40 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	P	252	Total	C	N	O	0	0
			1260	756	252	252		

- Molecule 41 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	Q	69	Total	C	N	O	0	0
			345	207	69	69		

- Molecule 42 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	R	47	Total	C	N	O	0	0
			235	141	47	47		

- Molecule 43 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	S	80	Total	C	N	O	0	0
			400	240	80	80		

- Molecule 44 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	T	71	Total	C	N	O	0	0
			355	213	71	71		

- Molecule 45 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	V	71	Total	C	N	O	0	0
			355	213	71	71		

- Molecule 46 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	W	72	Total	C	N	O	0	0
			360	216	72	72		

- Molecule 47 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	X	329	Total	C	N	O	0	0
			1645	987	329	329		

- Molecule 48 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	Y	106	Total	C	N	O	0	0
			530	318	106	106		

- Molecule 49 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	a	71	Total	C	N	O	0	0
			355	213	71	71		

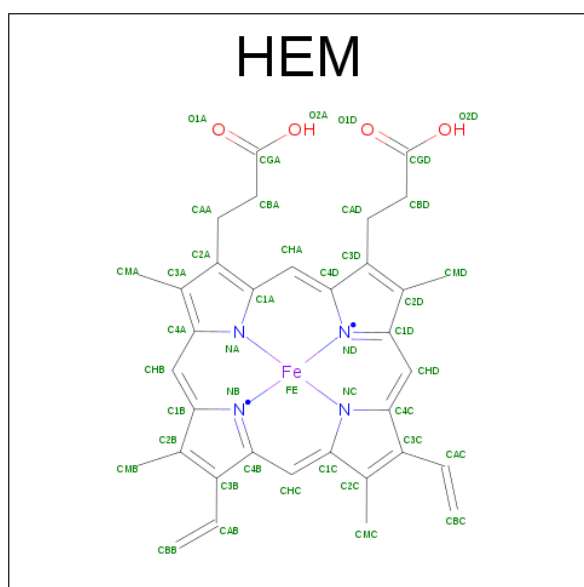
- Molecule 50 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	U	250	Total	C	N	O	0	0
			1250	750	250	250		

- Molecule 51 is a protein called complex I.

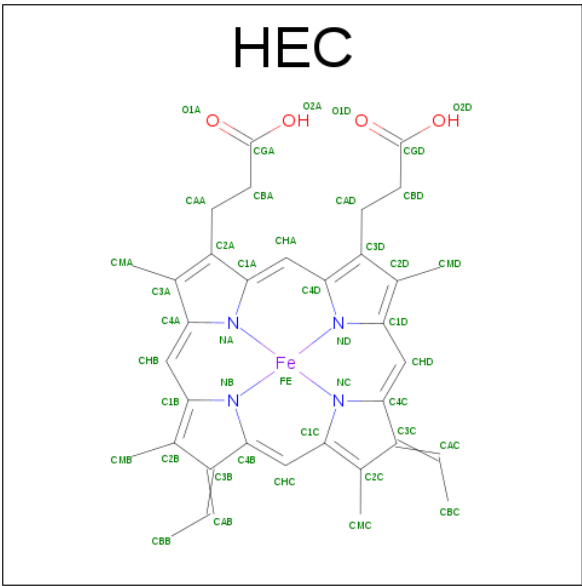
Mol	Chain	Residues	Atoms				AltConf	Trace
51	Z	266	Total	C	N	O	0	0
			1329	798	265	266		

- Molecule 52 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



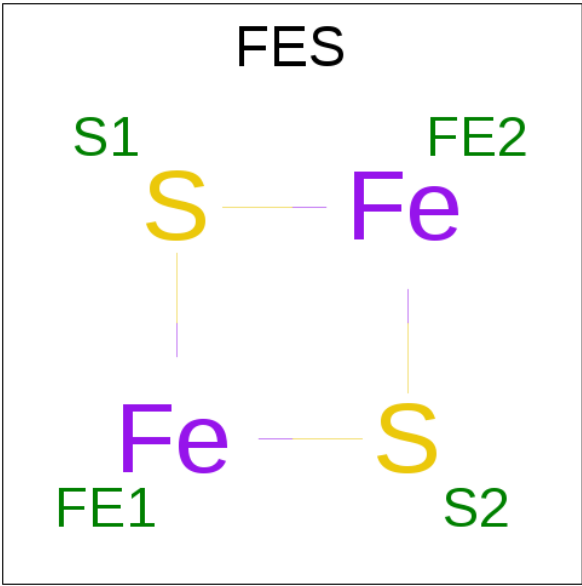
Mol	Chain	Residues	Atoms					AltConf
52	b	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
52	b	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
52	o	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
52	o	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

- Molecule 53 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



Mol	Chain	Residues	Atoms					AltConf
53	d	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
53	p	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
54	q	1	Total	Fe	S	0
			4	2	2	

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

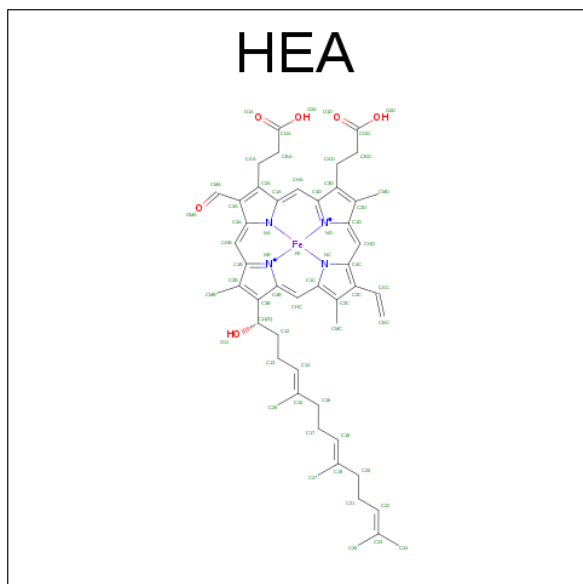
- Molecule 55 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 57 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).

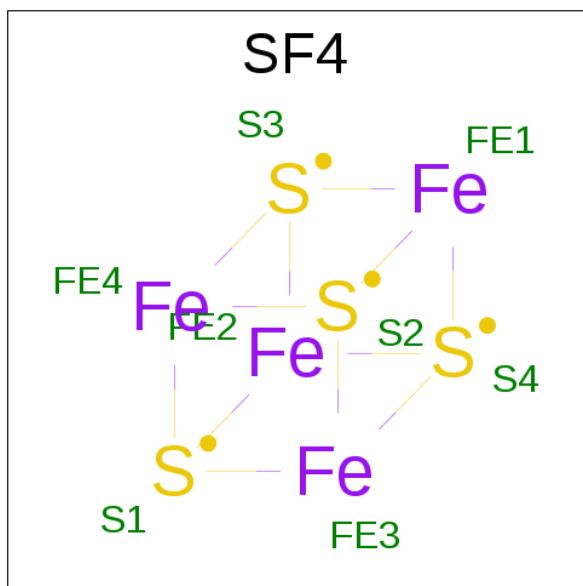


Mol	Chain	Residues	Atoms					AltConf
57	x	1	Total	C	Fe	N	O	0
			120	98	2	8	12	
57	x	1	Total	C	Fe	N	O	0
			120	98	2	8	12	

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	3	1	Total	Zn	0
			1	1	

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

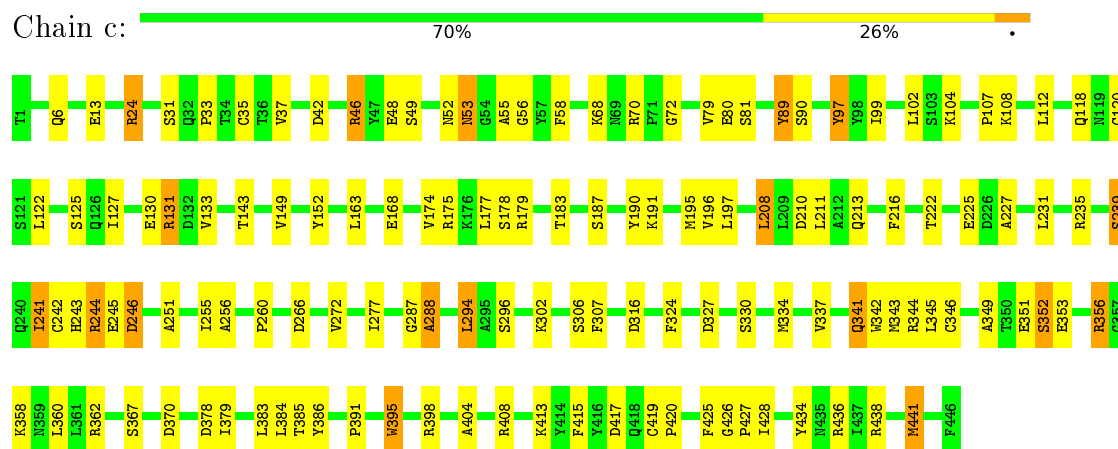


Mol	Chain	Residues	Atoms			AltConf
59	B	1	Total	Fe	S	0
			8	4	4	
59	F	1	Total	Fe	S	0
			8	4	4	
59	G	1	Total	Fe	S	0
			16	8	8	
59	G	1	Total	Fe	S	0
			16	8	8	
59	I	1	Total	Fe	S	0
			16	8	8	
59	I	1	Total	Fe	S	0
			16	8	8	

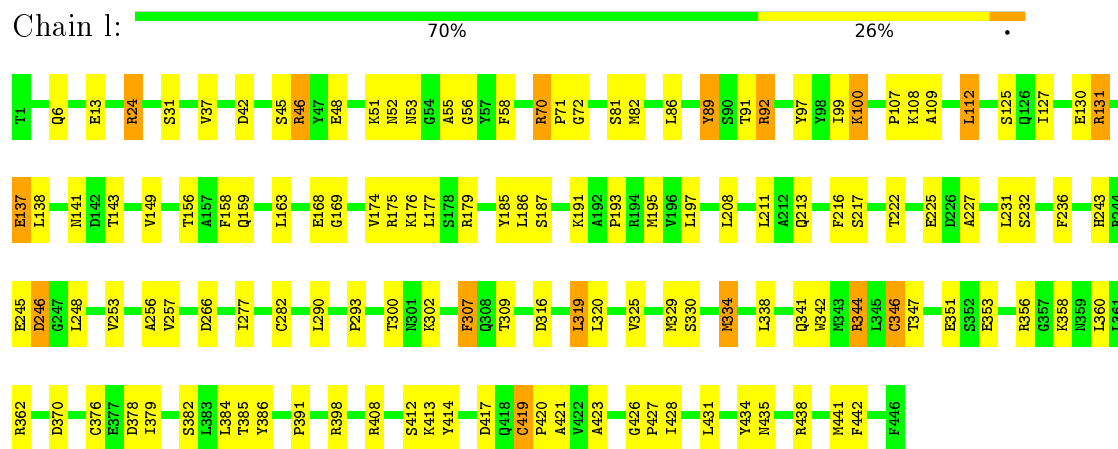
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

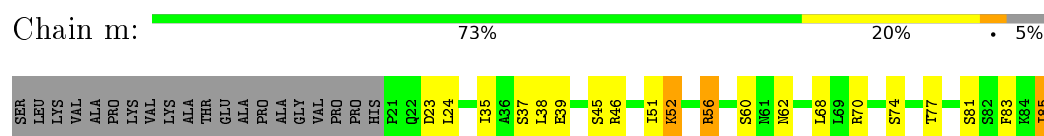
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

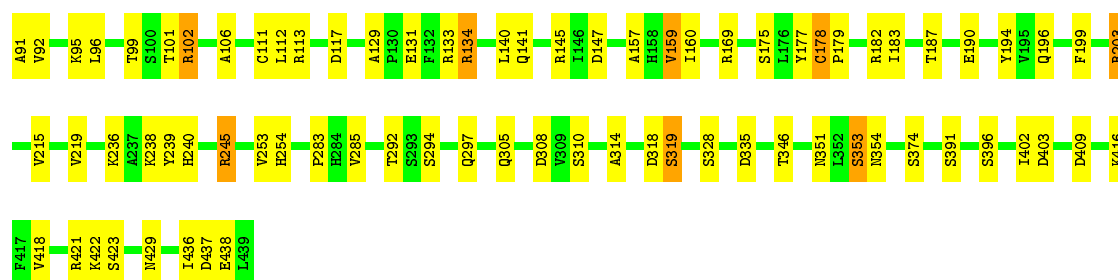


- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



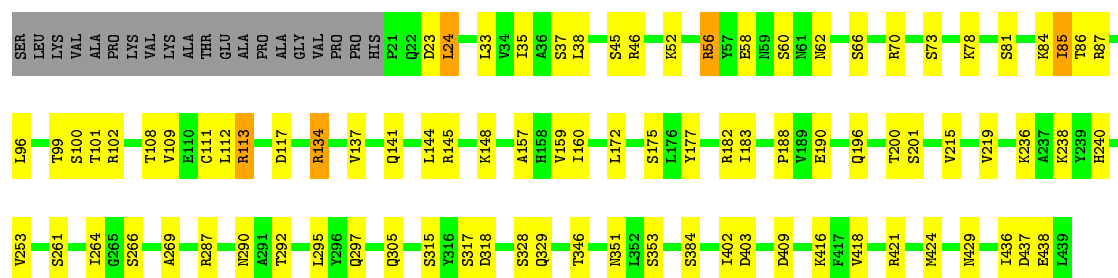
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial





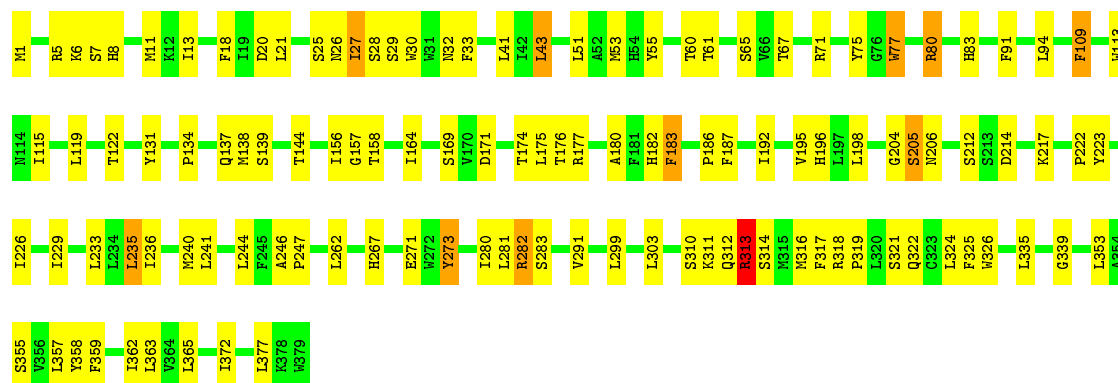
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain n: 75% 19% 5%



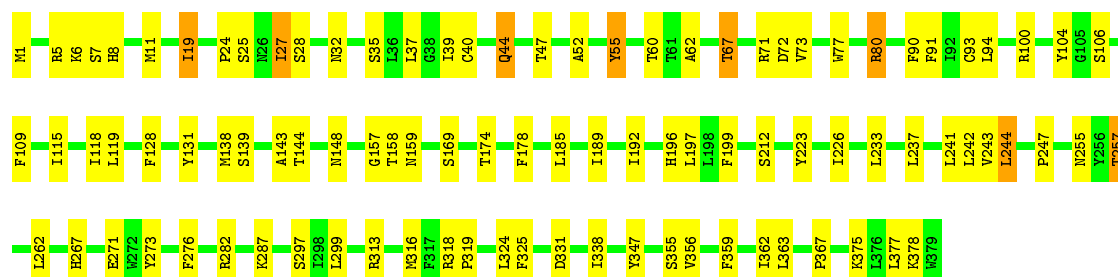
- Molecule 3: Cytochrome b

Chain b: 69% 28%

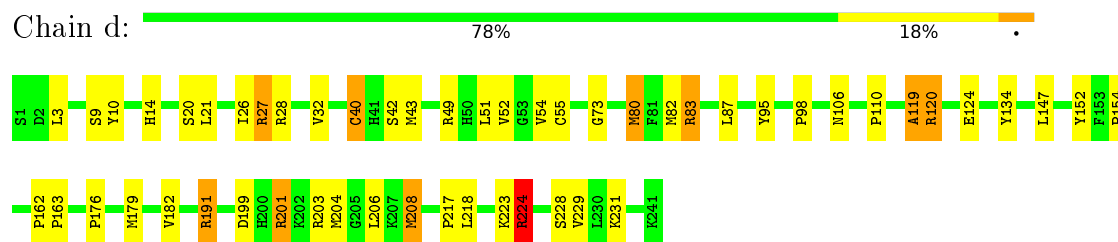


- Molecule 3: Cytochrome b

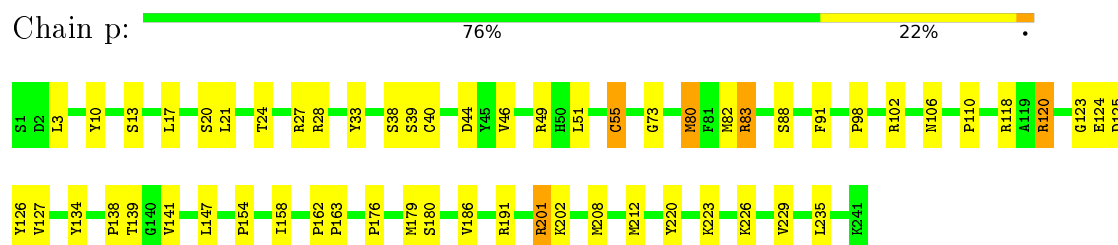
Chain o: 74% 23%



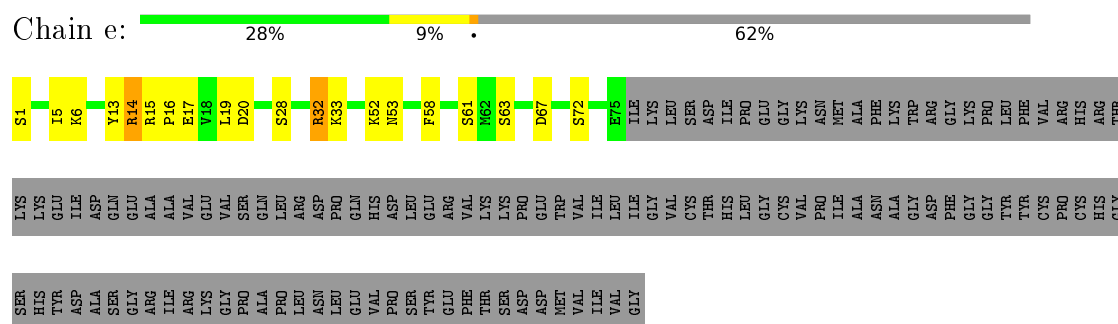
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



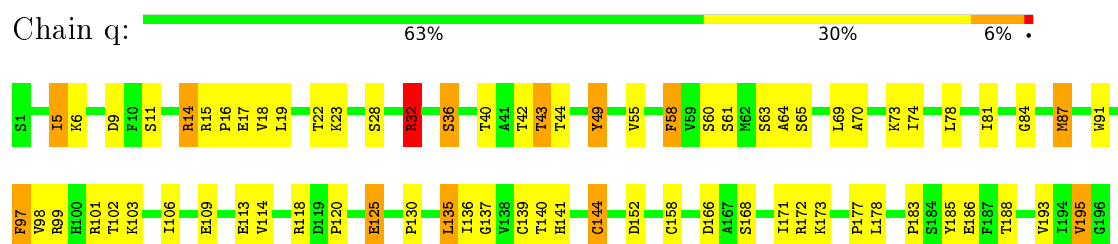
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



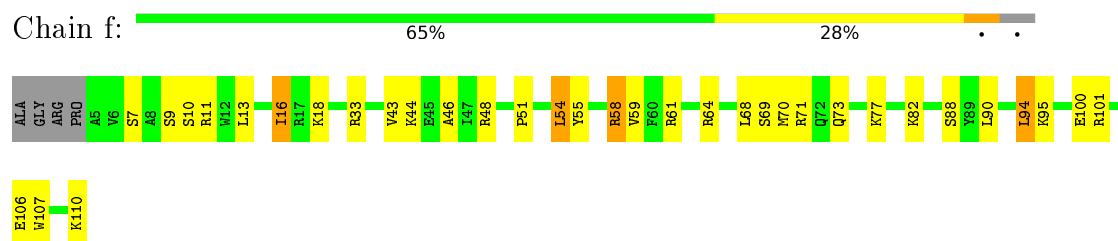
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

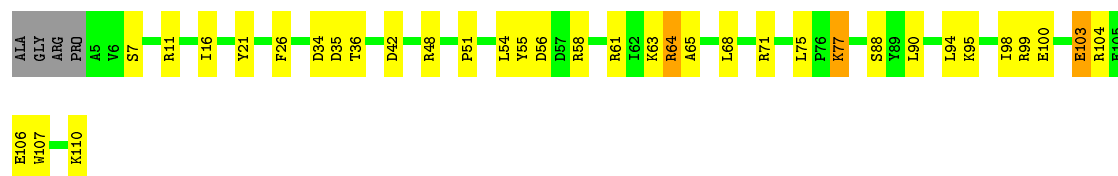


- Molecule 6: Cytochrome b-c1 complex subunit 7



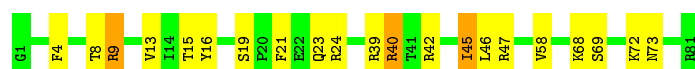
- Molecule 6: Cytochrome b-c1 complex subunit 7

Chain r: 



- Molecule 7: Cytochrome b-c1 complex subunit 8

Chain g: 



- Molecule 7: Cytochrome b-c1 complex subunit 8

Chain s: 



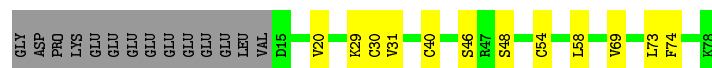
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain h: 



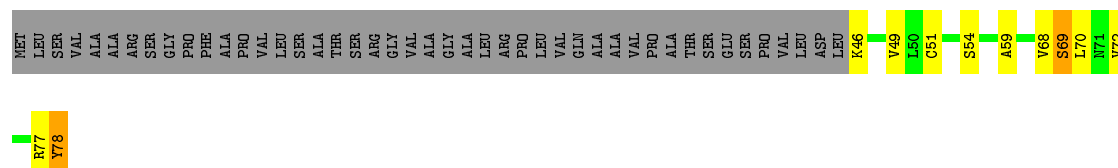
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain t: 



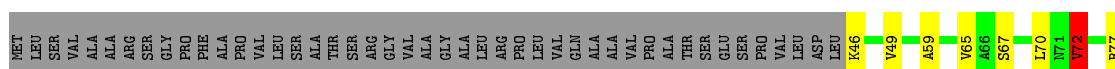
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain i: 



- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

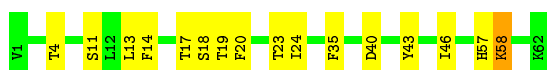
Chain u: 



Y78

- Molecule 10: Cytochrome b-c1 complex subunit 9

Chain j: 74% 24%



- Molecule 10: Cytochrome b-c1 complex subunit 9

Chain v: 73% 26%



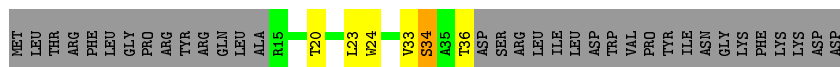
- Molecule 11: Cytochrome b-c1 complex subunit 10

Chain k: 32% 7% 61%



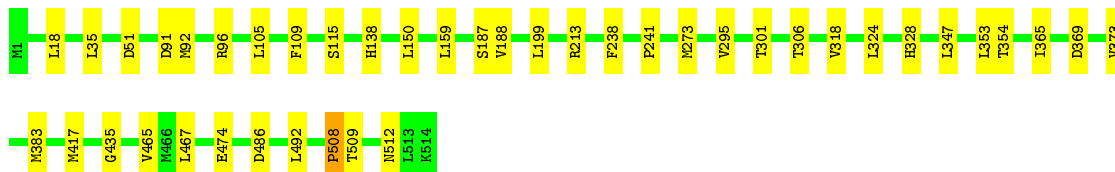
- Molecule 11: Cytochrome b-c1 complex subunit 10

Chain w: 29% 9% 61%



- Molecule 12: Cytochrome c oxidase subunit 1

Chain x: 92% 8%




- Molecule 13: Cytochrome c oxidase subunit 2

Chain y: 90% 10%



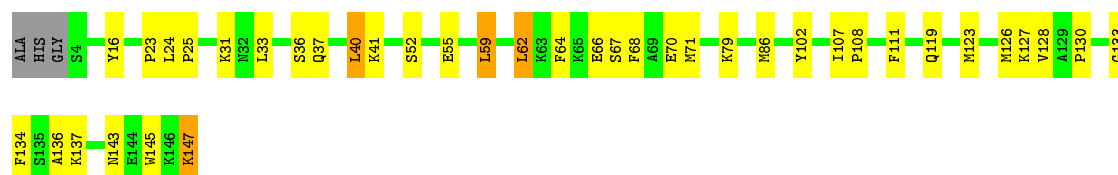
- Molecule 14: Cytochrome c oxidase subunit 3

Chain z:  90% 10%




- Molecule 15: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain 1:  71% 24%



- Molecule 16: Cytochrome c oxidase subunit 5A, mitochondrial

Chain 2:  78% 20%



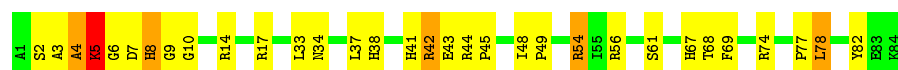
- Molecule 17: Cytochrome c oxidase subunit 5B, mitochondrial

Chain 3:  66% 28% 6%



- Molecule 18: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain 4:  62% 31% 6%




- Molecule 19: Cytochrome c oxidase subunit 6B1

Chain 5:  62% 20% 6% 12%

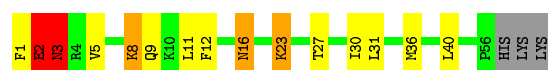


- Molecule 20: Cytochrome c oxidase subunit 6C

Chain 6:  79% 18%



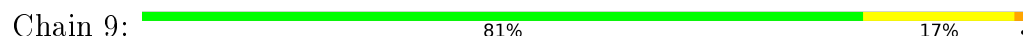
- Molecule 21: Cytochrome c oxidase subunit 7A1, mitochondrial



- Molecule 22: Cytochrome c oxidase subunit 7B, mitochondrial



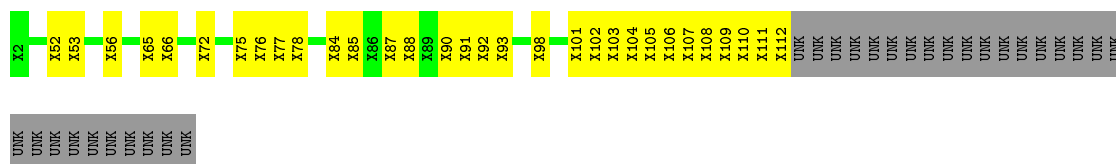
- Molecule 23: Cytochrome c oxidase subunit 7C, mitochondrial



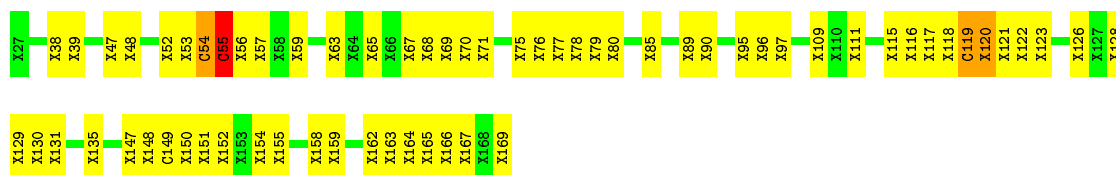
- Molecule 24: Cytochrome c oxidase subunit 8B, mitochondrial



- Molecule 25: complex I

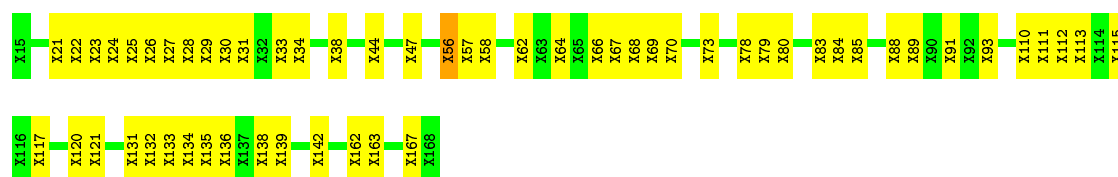


- Molecule 26: complex I



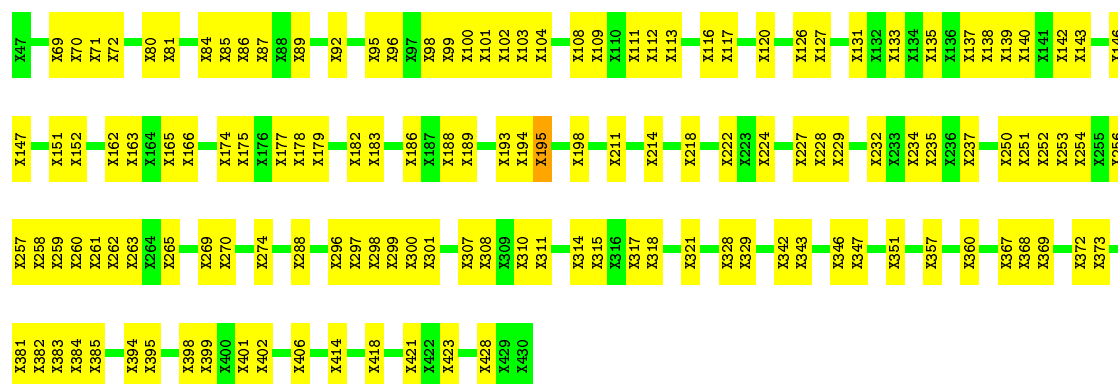
- Molecule 27: complex I





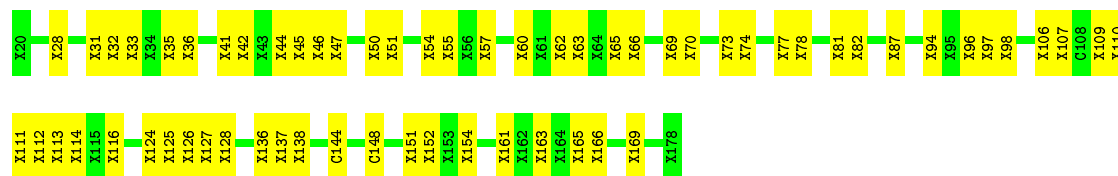
- Molecule 28: complex I

Chain D: 64% 36%



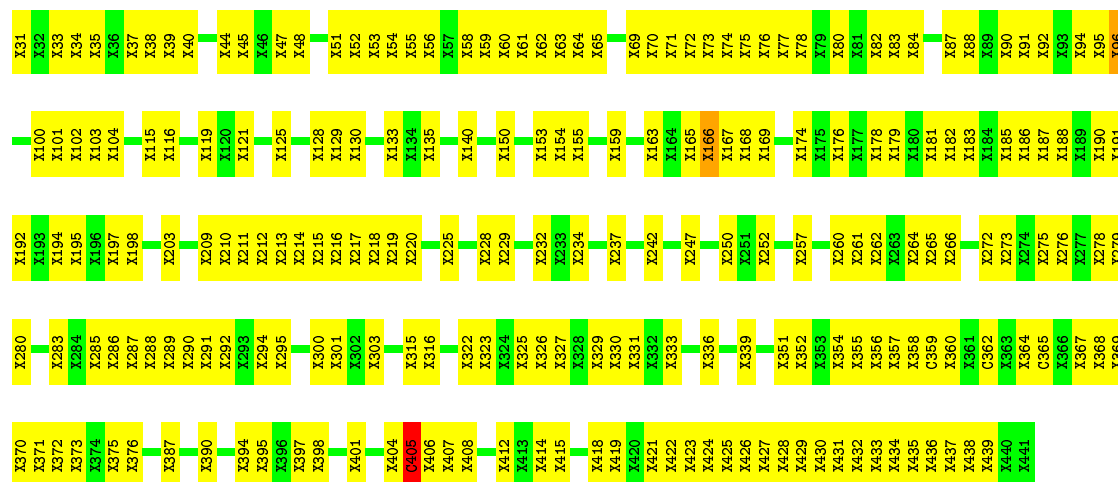
- Molecule 29: complex I

Chain E: 61% 39%

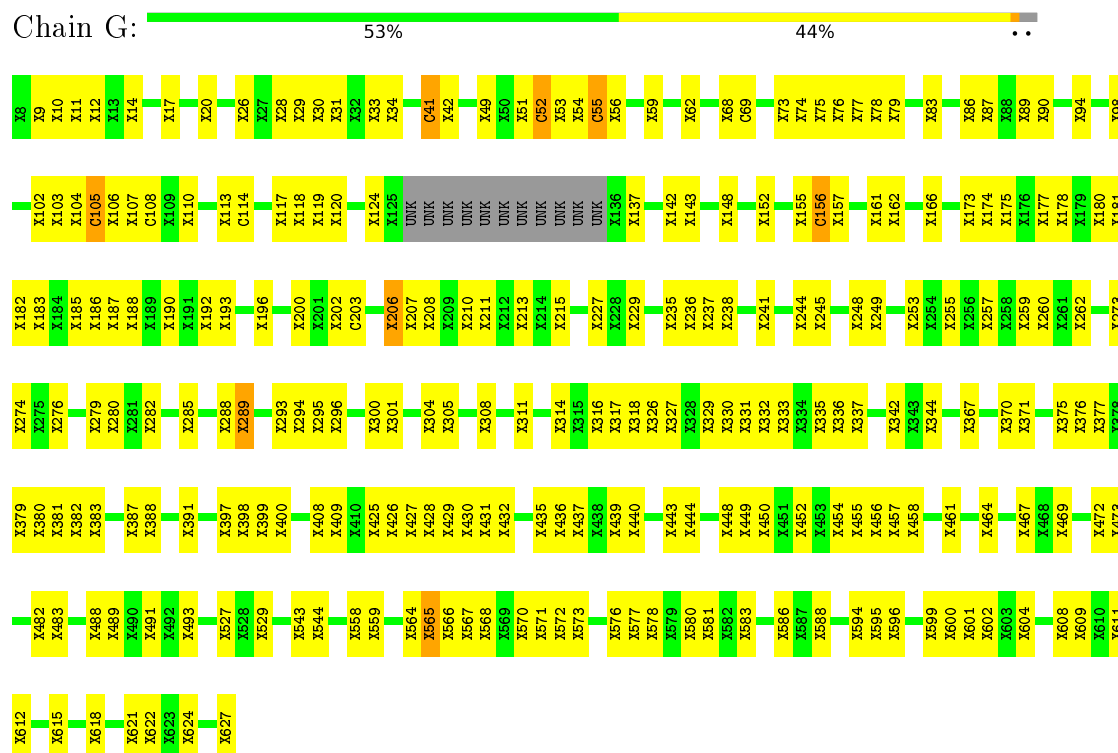


- Molecule 30: complex I

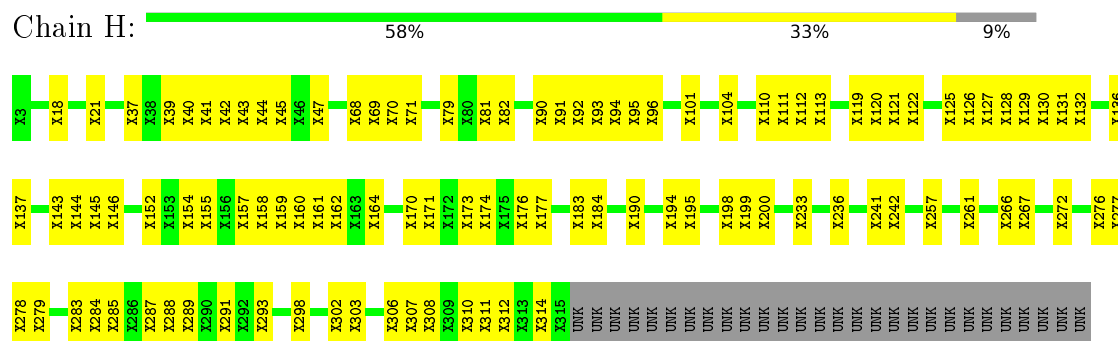
Chain F: 48% 51%



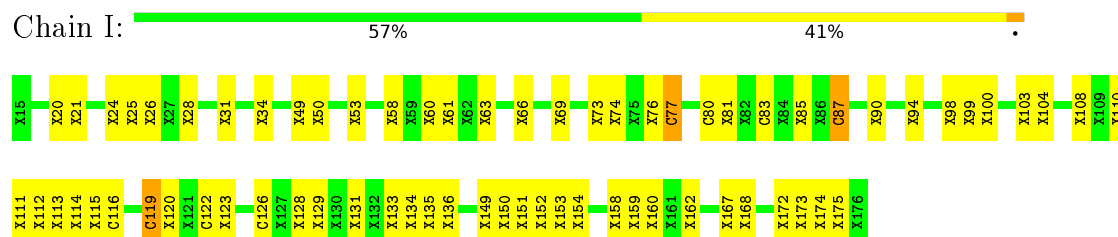
- Molecule 31: complex I



- Molecule 32: complex I

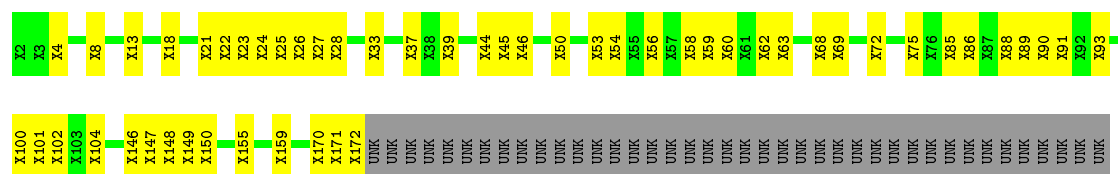


- Molecule 33: complex I



- Molecule 34: complex I

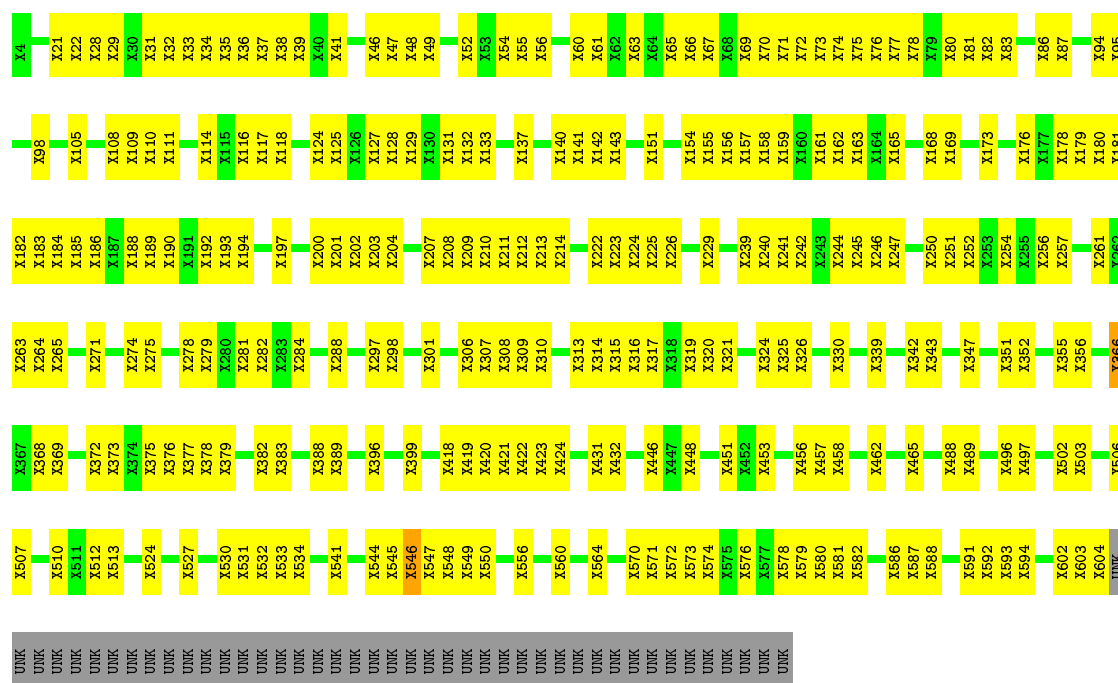




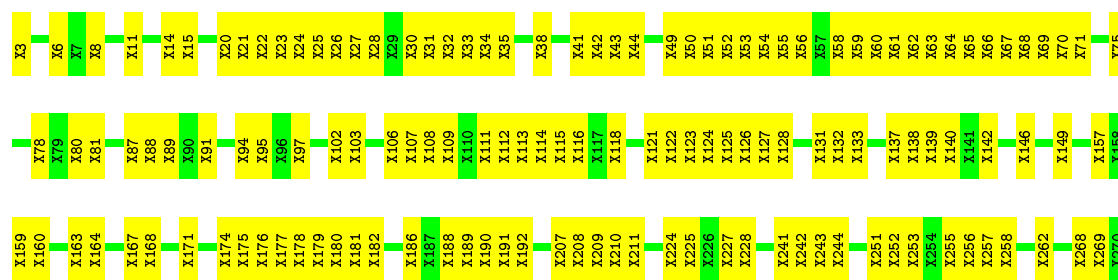
- Molecule 35: complex I

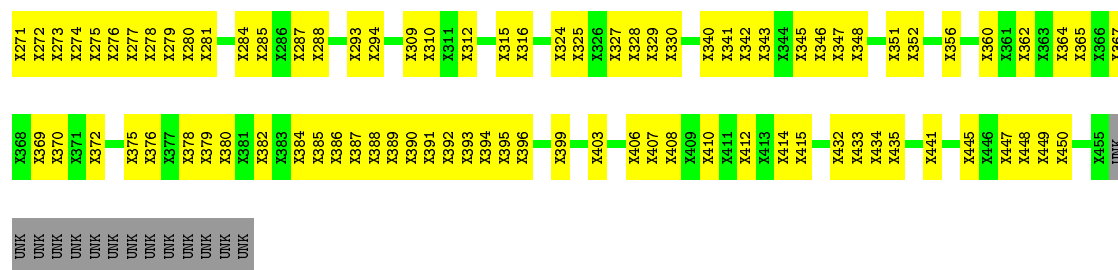


- Molecule 36: complex I

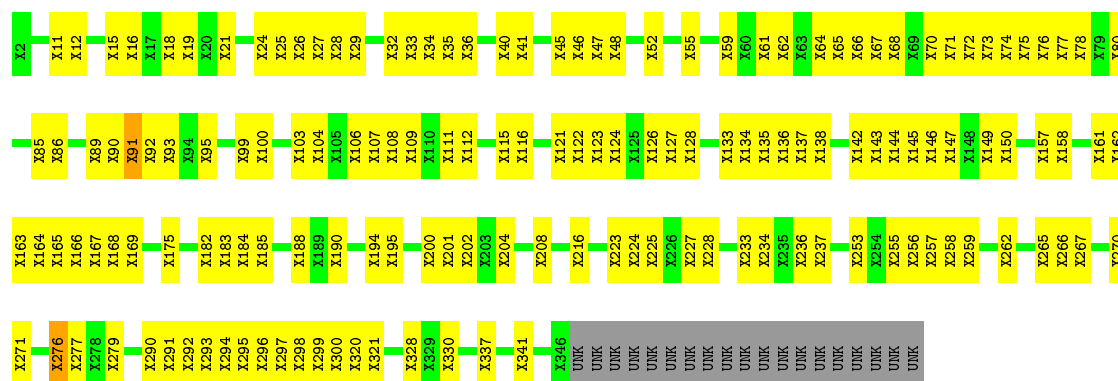


- Molecule 37: complex I

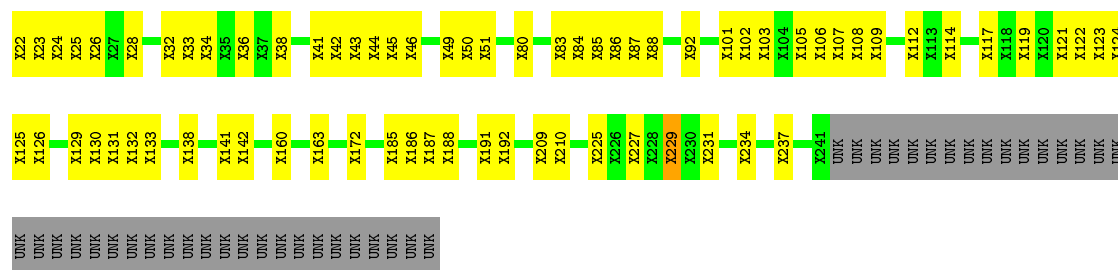




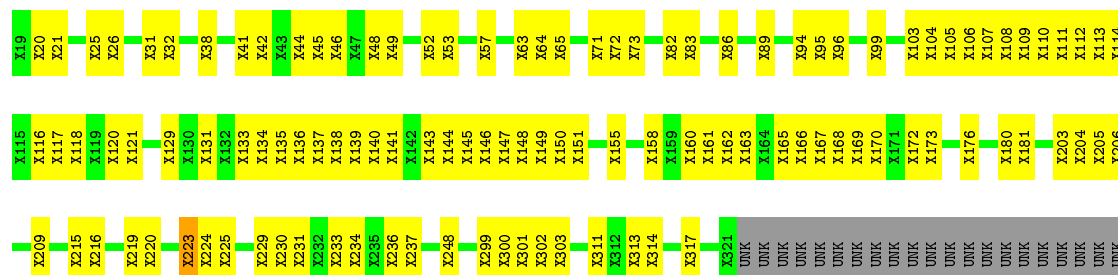
- Molecule 38: complex I



- Molecule 39: complex I



- Molecule 40: complex I



[illegible]

- Molecule 41: complex I

Chain Q: 60% 20% • 19%

[illegible]

- Molecule 42: complex I

Chain R:  45% 55%


X47
X50
X51
X59
X60
X61
X62
X63
X64
X65
X66
X67
X68
X69
X70
X75
X76
X77
X78
X79
X80
X81
X82
X86
X87
X88
X89
X90
X91
X92
X93

- Molecule 43: complex I

Chain S:  56% 43%

X17	X18	X19	X20	X21	X22	X23	X24	X25	X26	X27	X28	X29	X30	X31	X32	X33	X34	X35	X36	X37	X38	X39	X40	X41	X42	X43	X44	X45	X46	X47	X48	X49	X50	X51	X52	X53	X54	X55	X56	X57	X58	X59	X60	X61	X62	X63	X64	X65	X66	X67	X68	X69	X70	X71	X72	X73	X74	X75	X76	X77	X78	X79	X80	X81	X82	X83	X84	X85	X86	X87	X88	X89	X90	X91	X92	X93	X94	X95	X96	X97	X98	X99	X100	X101	X102	X103	X104	X105	X106	X107	X108	X109	X110	X111	X112	X113	X114	X115	X116	X117	X118	X119	X120	X121	X122	X123	X124	X125	X126	X127	X128	X129	X130	X131	X132	X133	X134	X135	X136	X137	X138	X139	X140	X141	X142	X143	X144	X145	X146	X147	X148	X149	X150	X151	X152	X153	X154	X155	X156	X157	X158	X159	X160	X161	X162	X163	X164	X165	X166	X167	X168	X169	X170	X171	X172	X173	X174	X175	X176	X177	X178	X179	X180	X181	X182	X183	X184	X185	X186	X187	X188	X189	X190	X191	X192	X193	X194	X195	X196	X197	X198	X199	X200	X201	X202	X203	X204	X205	X206	X207	X208	X209	X210	X211	X212	X213	X214	X215	X216	X217	X218	X219	X220	X221	X222	X223	X224	X225	X226	X227	X228	X229	X230	X231	X232	X233	X234	X235	X236	X237	X238	X239	X240	X241	X242	X243	X244	X245	X246	X247	X248	X249	X250	X251	X252	X253	X254	X255	X256	X257	X258	X259	X260	X261	X262	X263	X264	X265	X266	X267	X268	X269	X270	X271	X272	X273	X274	X275	X276	X277	X278	X279	X280	X281	X282	X283	X284	X285	X286	X287	X288	X289	X290	X291	X292	X293	X294	X295	X296	X297	X298	X299	X300	X301	X302	X303	X304	X305	X306	X307	X308	X309	X310	X311	X312	X313	X314	X315	X316	X317	X318	X319	X320	X321	X322	X323	X324	X325	X326	X327	X328	X329	X330	X331	X332	X333	X334	X335	X336	X337	X338	X339	X340	X341	X342	X343	X344	X345	X346	X347	X348	X349	X350	X351	X352	X353	X354	X355	X356	X357	X358	X359	X360	X361	X362	X363	X364	X365	X366	X367	X368	X369	X370	X371	X372	X373	X374	X375	X376	X377	X378	X379	X380	X381	X382	X383	X384	X385	X386	X387	X388	X389	X390	X391	X392	X393	X394	X395	X396	X397	X398	X399	X400	X401	X402	X403	X404	X405	X406	X407	X408	X409	X410	X411	X412	X413	X414	X415	X416	X417	X418	X419	X420	X421	X422	X423	X424	X425	X426	X427	X428	X429	X430	X431	X432	X433	X434	X435	X436	X437	X438	X439	X440	X441	X442	X443	X444	X445	X446	X447	X448	X449	X450	X451	X452	X453	X454	X455	X456	X457	X458	X459	X460	X461	X462	X463	X464	X465	X466	X467	X468	X469	X470	X471	X472	X473	X474	X475	X476	X477	X478	X479	X480	X481	X482	X483	X484	X485	X486	X487	X488	X489	X490	X491	X492	X493	X494	X495	X496	X497	X498	X499	X500	X501	X502	X503	X504	X505	X506	X507	X508	X509	X510	X511	X512	X513	X514	X515	X516	X517	X518	X519	X520	X521	X522	X523	X524	X525	X526	X527	X528	X529	X530	X531	X532	X533	X534	X535	X536	X537	X
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- Molecule 44: complex I

Chain T:  77% 17% 5%

Category	Count
X8	10
X40	20
X41	20
X42	20
X43	10
X46	20
X55	10
X59	20
X60	20
X61	20
X62	20
X63	20
X64	20
X65	20
X66	10
X70	20
X75	10
X32	20
UNK	20
UNK	20
UNK	20
UNK	20

- Molecule 45: complex I

Chain V: 59% 41%

X1	X2	X3	X8	X12	X23	X24	X25	X26	X27	X30	X31	X32	X33	X36	X37	X44	X45	X46	X47	X48	X51	X52	X53	X54	X55	X56	X57	X60	X66	X69	X70	X71
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- Molecule 46: complex I

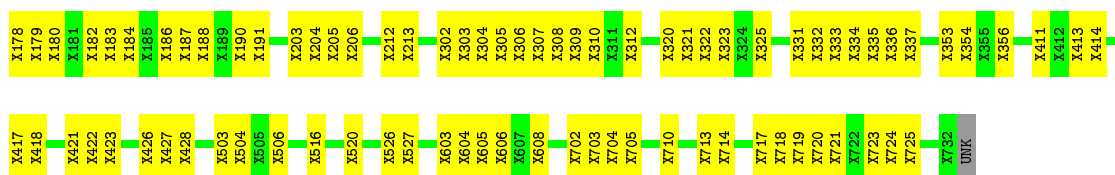
Chain W:  71% 28%

X1	X2	X3	X4	X5	X6	X7	X8	X9	X10	X11	X12	X13	X14	X15	X16	X17	X18	X19	X20	X21	X22	X23	X24	X25	X26	X27	X28	X29	X30	X31	X32	X33	X34	X35	X36	X37	X38	X39	X40	X41	X42	X43	X44	X45	X46	X47	X48	X49	X50	X51	X52	X53	X54	X55	X56	X57	X58	X59	X60	X61	X62	X63	X64	X65	X66	X67	X68	X69	X70	X71	X72	X73	X74	X75	X76	X77	X78	X79	X80	X81	X82	X83	X84	X85	X86	X87	X88	X89	X90	X91	X92	X93	X94	X95	X96	X97	X98	X99	X100
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- Molecule 47: complex I

Chain X:  63% 36%

X35 X40 X41 X42 X43 X44 X45 X46 X47 X48 X49 X56 X59 X89 X70 X71 X72 X73 X74 X75 X76 X77 X78 X79 X88 X89 X90 X91 X92 X93 X94 X95 X108 X110 X111 X112 X146 X156 X157 X158 X159 X160 X165 X166 X171 X172 X175 X176 X177



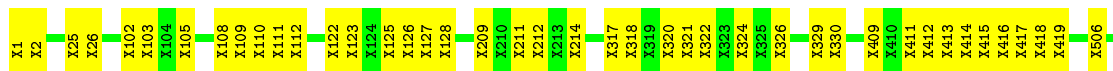
- Molecule 48: complex I

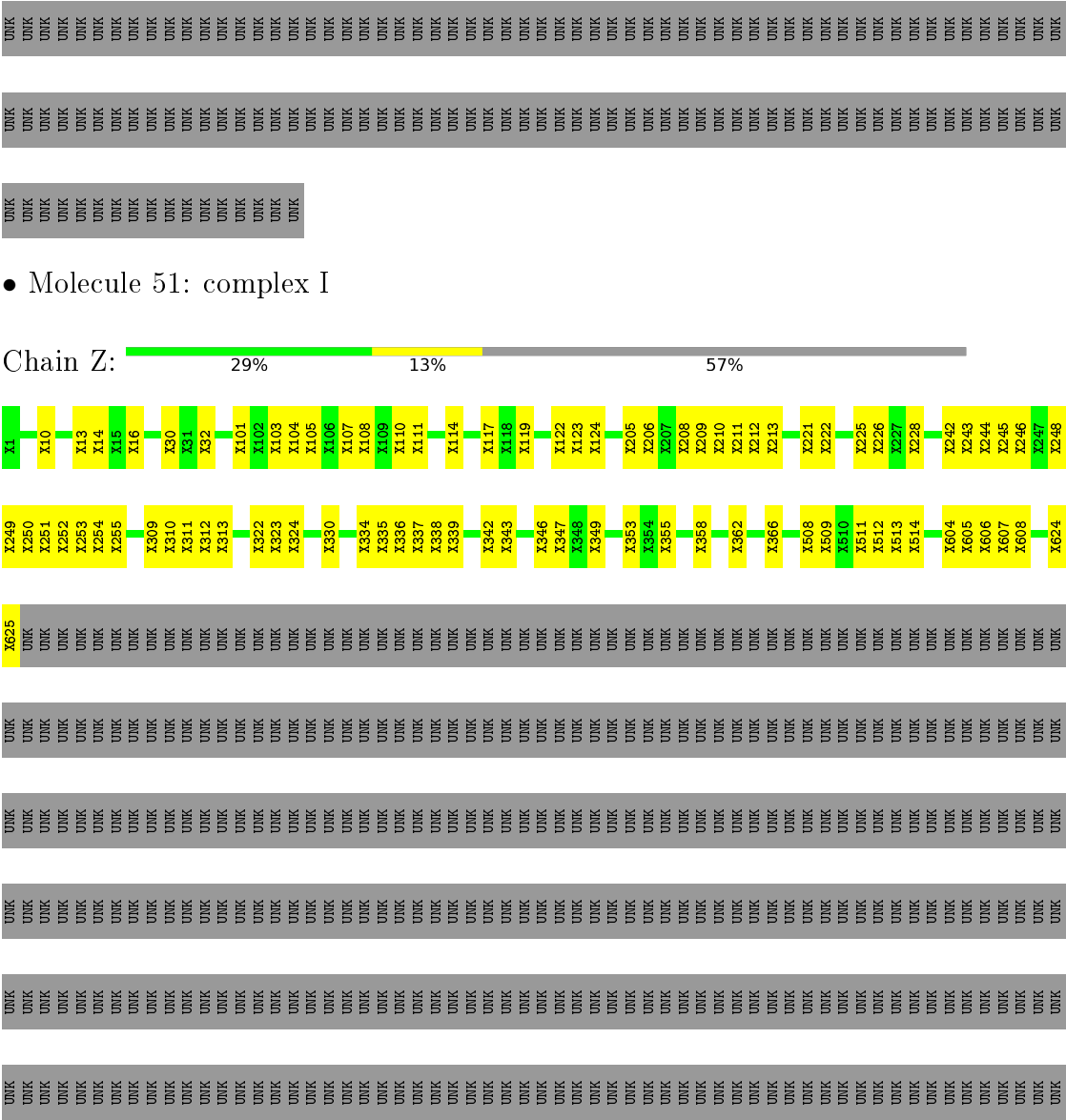


- Molecule 49: complex I



- Molecule 50: complex I





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	17093	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1.3	Depositor
Maximum defocus (nm)	4.3	Depositor
Magnification	57797	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SF4, MG, FES, HEC, HEM, 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	c	0.60	2/3531 (0.1%)	1.58	43/4792 (0.9%)
1	l	0.63	3/3531 (0.1%)	1.61	58/4792 (1.2%)
10	j	0.51	0/525	1.31	5/707 (0.7%)
10	v	0.51	0/525	1.42	6/707 (0.8%)
11	k	0.42	0/163	1.01	0/225
11	w	0.46	0/163	1.17	0/225
12	x	0.60	0/4164	0.76	1/5688 (0.0%)
13	y	0.57	0/1868	0.79	0/2544
14	z	0.56	0/2211	0.68	0/3023
15	1	0.57	0/1229	0.64	1/1658 (0.1%)
16	2	0.50	0/898	0.66	0/1218
17	3	0.56	0/765	0.81	0/1038
18	4	0.54	0/699	0.73	1/950 (0.1%)
19	5	0.55	0/648	0.73	0/877
2	m	0.51	0/3198	1.46	31/4336 (0.7%)
2	n	0.51	0/3198	1.33	11/4336 (0.3%)
20	6	0.60	0/611	0.65	0/810
21	7	0.61	0/451	0.72	0/610
22	8	0.57	0/398	0.66	0/546
23	9	0.63	0/399	0.62	0/534
24	0	0.51	0/345	0.65	0/470
26	B	1.57	1/21 (4.8%)	2.68	2/23 (8.7%)
29	E	0.77	0/20	1.58	0/20
3	b	0.71	2/3108 (0.1%)	1.73	62/4252 (1.5%)
3	o	0.69	3/3108 (0.1%)	1.62	50/4252 (1.2%)
30	F	2.57	1/20 (5.0%)	2.24	0/20
31	G	1.04	0/65	1.60	0/67
33	I	2.33	2/40 (5.0%)	1.47	0/40
4	d	0.55	0/1978	1.50	23/2684 (0.9%)
4	p	0.55	0/1978	1.40	24/2684 (0.9%)
5	e	0.60	0/574	1.62	7/775 (0.9%)
5	q	0.61	0/1551	1.68	28/2097 (1.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
6	f	0.57	0/935	1.56	18/1253 (1.4%)
6	r	0.57	0/935	1.66	24/1253 (1.9%)
7	g	0.61	1/704 (0.1%)	1.41	9/951 (0.9%)
7	s	0.59	0/704	1.30	5/951 (0.5%)
8	h	0.41	0/529	1.12	0/708
8	t	0.39	0/529	1.06	0/708
9	i	0.48	0/250	1.31	2/335 (0.6%)
9	u	0.48	0/250	1.32	1/335 (0.3%)
All	All	0.59	15/46819 (0.0%)	1.33	412/63494 (0.6%)

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
1	c	0	13
1	l	0	3
10	j	0	1
11	w	0	1
2	m	0	9
2	n	0	5
26	B	0	2
27	C	0	1
28	D	0	1
3	b	0	14
3	o	0	6
30	F	0	2
31	G	0	6
33	I	0	1
36	L	0	4
38	N	0	2
39	O	0	2
4	d	0	5
4	p	0	4
40	P	0	3
41	Q	0	1
43	S	0	1
46	W	0	1
47	X	0	1
5	e	0	1
5	q	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	f	0	2
7	g	0	2
7	s	0	3
8	t	0	1
9	i	0	1
9	u	0	1
All	All	0	109

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	F	405	CYS	CA-CB	-9.00	1.34	1.53
33	I	87	CYS	CA-CB	7.93	1.71	1.53
1	c	419	CYS	CB-SG	-7.15	1.70	1.82
33	I	77	CYS	CA-CB	6.97	1.69	1.53
1	l	253	VAL	C-O	6.79	1.36	1.23

The worst 5 of 412 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	l	46	ARG	NE-CZ-NH2	-19.32	110.64	120.30
2	m	70	ARG	NE-CZ-NH2	16.29	128.45	120.30
1	c	419	CYS	CA-CB-SG	16.22	143.19	114.00
4	d	120	ARG	NE-CZ-NH2	-16.20	112.20	120.30
2	m	245	ARG	NE-CZ-NH2	14.94	127.77	120.30

There are no chirality outliers.

5 of 109 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	c	118	GLN	Mainchain
1	c	122	LEU	Mainchain
1	c	196	VAL	Mainchain
1	c	210	ASP	Mainchain
1	c	53	ASN	Mainchain

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	c	3458	0	3356	0	0
1	l	3458	0	3353	0	0
2	m	3141	0	3123	0	0
2	n	3141	0	3123	0	0
3	b	3011	0	3076	0	0
3	o	3011	0	3076	0	0
4	d	1919	0	1868	0	0
4	p	1919	0	1868	0	0
5	e	566	0	564	0	0
5	q	1518	0	1499	0	0
6	f	916	0	909	0	0
6	r	916	0	909	0	0
7	g	682	0	679	0	0
7	s	682	0	679	0	0
8	h	524	0	504	0	0
8	t	524	0	504	0	0
9	i	248	0	265	0	0
9	u	248	0	265	0	0
10	j	512	0	518	0	0
10	v	512	0	518	0	0
11	k	159	0	159	0	0
11	w	159	0	159	0	0
12	x	4025	0	4003	0	0
13	y	1822	0	1834	0	0
14	z	2124	0	2044	0	0
15	1	1195	0	1183	30	0
16	2	878	0	868	20	0
17	3	748	0	728	21	0
18	4	672	0	645	23	0
19	5	628	0	582	18	0
20	6	598	0	612	10	0
21	7	441	0	437	11	0
22	8	384	0	366	6	0
23	9	386	0	388	7	0
24	0	335	0	352	11	0
25	A	415	0	88	27	0
26	B	719	0	161	91	0
27	C	770	0	163	63	0
28	D	1920	0	402	126	0
29	E	799	0	176	56	0
30	F	2059	0	444	263	0
31	G	2651	0	606	226	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	H	1425	0	295	99	0
33	I	818	0	195	65	0
34	J	655	0	138	44	0
35	K	420	0	89	14	0
36	L	2790	0	583	255	0
37	M	2195	0	455	208	0
38	N	1630	0	340	147	0
39	O	905	0	197	65	0
40	P	1260	0	271	144	0
41	Q	345	0	80	14	0
42	R	235	0	54	22	0
43	S	400	0	86	46	0
44	T	355	0	76	12	0
45	V	355	0	77	23	0
46	W	360	0	75	18	0
47	X	1645	0	351	102	0
48	Y	530	0	111	30	0
49	a	355	0	75	0	0
50	U	1250	0	272	63	0
51	Z	1329	0	280	70	0
52	b	86	0	60	0	0
52	o	86	0	60	0	0
53	d	43	0	30	0	0
53	p	43	0	30	0	0
54	E	4	0	0	0	0
54	G	4	0	0	3	0
54	q	4	0	0	0	0
55	x	1	0	0	0	0
55	y	2	0	0	0	0
56	x	1	0	0	0	0
57	x	120	0	108	0	0
58	3	1	0	0	0	0
59	B	8	0	0	6	0
59	F	8	0	0	1	0
59	G	16	0	0	0	0
59	I	16	0	0	5	0
All	All	74493	0	51444	2394	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 51.

The worst 5 of 2394 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)
26:B:148:UNK:CB	26:B:151:UNK:CA	1.77	1.59
30:F:405:CYS:CB	30:F:406:UNK:CB	1.78	1.56
30:F:405:CYS:HB2	30:F:406:UNK:CB	1.04	1.48
36:L:321:UNK:CB	36:L:324:UNK:CB	1.92	1.45
29:E:148:CYS:SG	30:F:103:UNK:CB	2.04	1.44

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	c	444/446 (100%)	355 (80%)	66 (15%)	23 (5%)	2	30
1	l	444/446 (100%)	370 (83%)	54 (12%)	20 (4%)	3	33
2	m	417/439 (95%)	341 (82%)	67 (16%)	9 (2%)	8	49
2	n	417/439 (95%)	344 (82%)	62 (15%)	11 (3%)	7	45
3	b	377/379 (100%)	303 (80%)	60 (16%)	14 (4%)	4	38
3	o	377/379 (100%)	316 (84%)	50 (13%)	11 (3%)	6	43
4	d	239/241 (99%)	188 (79%)	36 (15%)	15 (6%)	2	25
4	p	239/241 (99%)	195 (82%)	32 (13%)	12 (5%)	3	31
5	e	73/196 (37%)	57 (78%)	14 (19%)	2 (3%)	6	45
5	q	194/196 (99%)	148 (76%)	35 (18%)	11 (6%)	2	28
6	f	104/110 (94%)	89 (86%)	13 (12%)	2 (2%)	10	52
6	r	104/110 (94%)	87 (84%)	15 (14%)	2 (2%)	10	52
7	g	79/81 (98%)	63 (80%)	13 (16%)	3 (4%)	4	37
7	s	79/81 (98%)	60 (76%)	16 (20%)	3 (4%)	4	37
8	h	62/78 (80%)	52 (84%)	10 (16%)	0	100	100
8	t	62/78 (80%)	51 (82%)	10 (16%)	1 (2%)	12	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	i	31/78 (40%)	19 (61%)	10 (32%)	2 (6%)	1	25
9	u	31/78 (40%)	17 (55%)	11 (36%)	3 (10%)	1	14
10	j	60/62 (97%)	41 (68%)	13 (22%)	6 (10%)	1	14
10	v	60/62 (97%)	44 (73%)	12 (20%)	4 (7%)	1	24
11	k	20/56 (36%)	17 (85%)	2 (10%)	1 (5%)	3	31
11	w	20/56 (36%)	15 (75%)	3 (15%)	2 (10%)	1	14
12	x	512/514 (100%)	480 (94%)	28 (6%)	4 (1%)	24	69
13	y	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	15	60
14	z	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
15	1	142/147 (97%)	135 (95%)	7 (5%)	0	100	100
16	2	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
17	3	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	3	34
18	4	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	2	26
19	5	73/85 (86%)	64 (88%)	8 (11%)	1 (1%)	14	58
20	6	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
21	7	54/59 (92%)	48 (89%)	4 (7%)	2 (4%)	4	38
22	8	47/56 (84%)	41 (87%)	6 (13%)	0	100	100
23	9	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
24	0	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
26	B	4/143 (3%)	3 (75%)	0	1 (25%)	0	2
29	E	4/159 (2%)	3 (75%)	1 (25%)	0	100	100
30	F	4/411 (1%)	4 (100%)	0	0	100	100
31	G	12/538 (2%)	9 (75%)	1 (8%)	2 (17%)	0	5
33	I	8/162 (5%)	7 (88%)	0	1 (12%)	0	8
All	All	5719/7551 (76%)	4821 (84%)	718 (13%)	180 (3%)	9	42

5 of 180 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	c	327	ASP
1	c	426	GLY
1	c	427	PRO
2	m	141	GLN
2	m	183	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	c	370/370 (100%)	289 (78%)	81 (22%)	1	9
1	l	370/370 (100%)	286 (77%)	84 (23%)	1	8
2	m	328/343 (96%)	260 (79%)	68 (21%)	1	10
2	n	328/343 (96%)	262 (80%)	66 (20%)	1	11
3	b	327/327 (100%)	269 (82%)	58 (18%)	2	16
3	o	327/327 (100%)	276 (84%)	51 (16%)	3	21
4	d	206/206 (100%)	179 (87%)	27 (13%)	5	28
4	p	206/206 (100%)	179 (87%)	27 (13%)	5	28
5	e	65/168 (39%)	51 (78%)	14 (22%)	1	9
5	q	167/168 (99%)	123 (74%)	44 (26%)	0	5
6	f	96/98 (98%)	74 (77%)	22 (23%)	1	7
6	r	96/98 (98%)	78 (81%)	18 (19%)	2	13
7	g	71/71 (100%)	58 (82%)	13 (18%)	2	14
7	s	71/71 (100%)	57 (80%)	14 (20%)	1	12
8	h	61/74 (82%)	51 (84%)	10 (16%)	3	19
8	t	61/74 (82%)	51 (84%)	10 (16%)	3	19
9	i	27/60 (45%)	19 (70%)	8 (30%)	0	3
9	u	27/60 (45%)	20 (74%)	7 (26%)	0	5
10	j	52/52 (100%)	46 (88%)	6 (12%)	7	32
10	v	52/52 (100%)	43 (83%)	9 (17%)	2	17
11	k	15/46 (33%)	12 (80%)	3 (20%)	1	11
11	w	15/46 (33%)	11 (73%)	4 (27%)	0	5
12	x	427/427 (100%)	389 (91%)	38 (9%)	12	44
13	y	211/211 (100%)	191 (90%)	20 (10%)	11	41
14	z	226/226 (100%)	199 (88%)	27 (12%)	6	31
15	l	128/129 (99%)	120 (94%)	8 (6%)	22	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	2	95/95 (100%)	89 (94%)	6 (6%)	22	59
17	3	81/81 (100%)	76 (94%)	5 (6%)	23	60
18	4	68/68 (100%)	50 (74%)	18 (26%)	0	5
19	5	67/75 (89%)	58 (87%)	9 (13%)	5	27
20	6	58/58 (100%)	53 (91%)	5 (9%)	13	47
21	7	47/50 (94%)	40 (85%)	7 (15%)	4	23
22	8	39/46 (85%)	37 (95%)	2 (5%)	29	66
23	9	40/40 (100%)	38 (95%)	2 (5%)	30	66
24	0	37/38 (97%)	34 (92%)	3 (8%)	15	50
26	B	4/4 (100%)	2 (50%)	2 (50%)	0	0
29	E	4/4 (100%)	4 (100%)	0	100	100
30	F	4/4 (100%)	3 (75%)	1 (25%)	1	6
31	G	12/12 (100%)	8 (67%)	4 (33%)	0	2
33	I	8/8 (100%)	7 (88%)	1 (12%)	6	30
All	All	4894/5206 (94%)	4092 (84%)	802 (16%)	6	19

5 of 802 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	l	246	ASP
2	n	346	THR
16	2	80	GLU
1	l	330	SER
2	n	78	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 122 such sidechains are listed below:

Mol	Chain	Res	Type
1	l	213	GLN
2	n	304	HIS
19	5	25	GLN
1	l	240	GLN
2	n	62	ASN

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 22 ligands modelled in this entry, 5 are monoatomic - leaving 17 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	$\# Z > 2$
59	SF4	B	201	26	0,12,12	0.00	-	0,24,24	0.00	-
54	FES	E	201	29	0,4,4	0.00	-	0,4,4	0.00	-
59	SF4	F	501	30	0,12,12	0.00	-	0,24,24	0.00	-
59	SF4	G	801	31	0,12,12	0.00	-	0,24,24	0.00	-
59	SF4	G	802	31	0,12,12	0.00	-	0,24,24	0.00	-
54	FES	G	803	31	0,4,4	0.00	-	0,4,4	0.00	-
59	SF4	I	201	33	0,12,12	0.00	-	0,24,24	0.00	-
59	SF4	I	202	33	0,12,12	0.00	-	0,24,24	0.00	-
52	HEM	b	401	3	24,50,50	2.21	4 (16%)	16,82,82	3.46	6 (37%)
52	HEM	b	402	3	24,50,50	1.93	6 (25%)	16,82,82	2.79	6 (37%)
53	HEC	d	301	4	24,50,50	2.48	4 (16%)	19,82,82	2.59	7 (36%)
52	HEM	o	401	3	24,50,50	2.25	6 (25%)	16,82,82	3.12	10 (62%)
52	HEM	o	402	3	24,50,50	2.05	6 (25%)	16,82,82	2.35	9 (56%)
53	HEC	p	301	4	24,50,50	2.52	4 (16%)	19,82,82	2.65	9 (47%)
54	FES	q	201	5	0,4,4	0.00	-	0,4,4	0.00	-
57	HEA	x	603	12	40,67,67	1.49	5 (12%)	36,103,103	1.66	9 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	HEA	x	604	12	40,67,67	1.58	4 (10%)	36,103,103	1.47	8 (22%)

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
59	SF4	B	201	26	-	0/0/48/48	0/6/5/5
54	FES	E	201	29	-	0/0/4/4	0/1/1/1
59	SF4	F	501	30	-	0/0/48/48	0/6/5/5
59	SF4	G	801	31	-	0/0/48/48	0/6/5/5
59	SF4	G	802	31	-	0/0/48/48	0/6/5/5
54	FES	G	803	31	-	0/0/4/4	0/1/1/1
59	SF4	I	201	33	-	0/0/48/48	0/6/5/5
59	SF4	I	202	33	-	0/0/48/48	0/6/5/5
52	HEM	b	401	3	-	0/6/54/54	0/0/8/8
52	HEM	b	402	3	-	0/6/54/54	0/0/8/8
53	HEC	d	301	4	-	0/6/54/54	0/0/8/8
52	HEM	o	401	3	-	0/6/54/54	0/0/8/8
52	HEM	o	402	3	-	0/6/54/54	0/0/8/8
53	HEC	p	301	4	-	0/6/54/54	0/0/8/8
54	FES	q	201	5	-	0/0/4/4	0/1/1/1
57	HEA	x	603	12	3/3/7/16	0/24/76/76	0/0/8/8
57	HEA	x	604	12	3/3/7/16	0/24/76/76	0/0/8/8

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	b	401	HEM	C3B-C2B	-7.33	1.31	1.40
53	p	301	HEC	C3C-C2C	-7.25	1.33	1.40
53	d	301	HEC	C3B-C2B	-7.08	1.33	1.40
57	x	604	HEA	C3A-C2A	-6.97	1.31	1.40
53	p	301	HEC	C3B-C2B	-6.91	1.33	1.40

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	b	401	HEM	C3B-CAB-CBB	-9.03	108.23	126.40
53	d	301	HEC	CBC-CAC-C3C	-6.10	114.01	127.34
52	o	401	HEM	CMA-C3A-C4A	-6.09	117.95	128.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	p	301	HEC	CBB-CAB-C3B	-6.07	114.07	127.34
53	p	301	HEC	CBC-CAC-C3C	-5.54	115.23	127.34

5 of 6 chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	B	201	SF4	6	0
59	F	501	SF4	1	0
54	G	803	FES	3	0
59	I	201	SF4	2	0
59	I	202	SF4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
50	U	8
47	X	7
31	G	6
51	Z	6
36	L	5
39	O	3
40	P	2

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Mol	Chain	Number of breaks
34	J	2
32	H	2
44	T	2
41	Q	1
49	a	1
25	A	1
38	N	1
37	M	1

The worst 5 of 48 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	226:UNK	C	301:UNK	N	71.67
1	X	113:UNK	C	133:UNK	N	66.39
1	U	27:UNK	C	101:UNK	N	63.89
1	a	29:UNK	C	101:UNK	N	61.67
1	U	630:UNK	C	701:UNK	N	57.60