



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:32 PM BST

PDB ID : 2YBB
EMDB ID: : EMD-1876
Title : Fitted model for bovine mitochondrial supercomplex I1III2IV1 by single particle cryo-EM (EMD-1876)
Authors : Althoff, T.; Mills, D.J.; Popot, J.-L.; Kuehlbrandt, W.
Deposited on : 2011-03-02
Resolution : 19.00 Å(reported)
Based on PDB ID : 3IAM,3M9C,1PP9,1BGY,1OCC,2B4Z

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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) : trunk27241

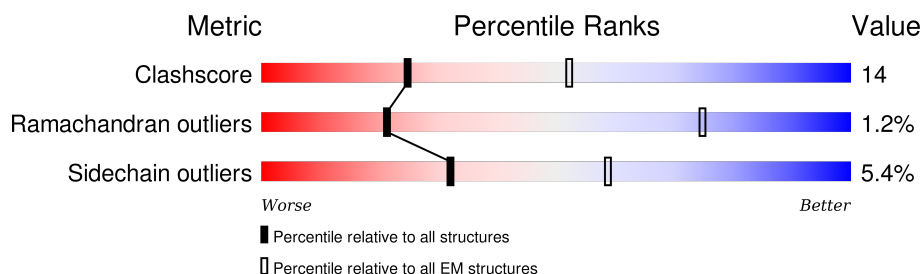
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 19.00 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.



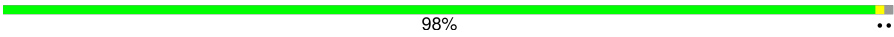

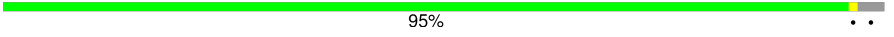

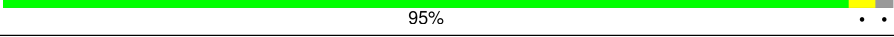

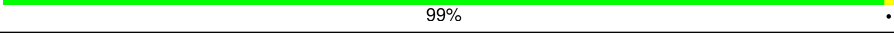

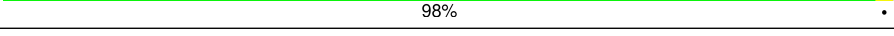

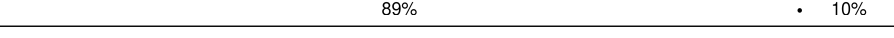
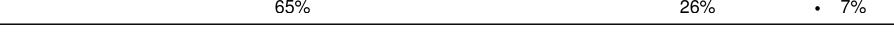

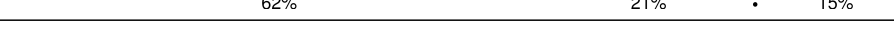

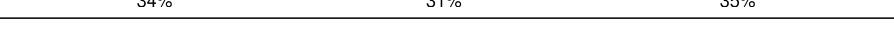
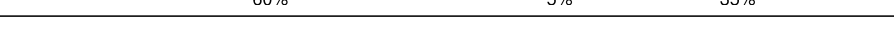

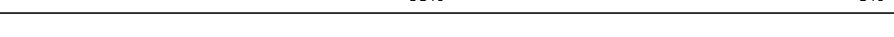






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	1	438	55% 39% 6%
2	2	181	56% 38% 5% .
3	3	783	49% 41% 6% .
4	4	409	44% 41% 7% 8%
5	5	207	52% 37% 6% 5%
6	6	181	40% 34% 6% 20%
7	7	129	63% 33% . .
8	8	182	42% 38% . 15%
9	A	446	78% 21% ..

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Mol	Chain	Length	Quality of chain
9	a	446	
10	B	439	
10	b	439	
11	C	379	
11	c	379	
12	D	241	
12	d	241	
13	E	196	
13	e	196	
14	F	110	
14	f	110	
15	G	81	
15	g	81	
16	H	78	
16	h	78	
17	I	65	
17	i	65	
18	J	62	
18	j	62	
19	K	56	
19	k	56	
20	L	514	
21	M	227	
22	N	261	
23	O	147	

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Mol	Chain	Length	Quality of chain
24	P	109	 78%19%.
25	Q	98	 63%31%6%
26	R	84	 58%32%8%. .
27	S	85	 60%22%6%12%
28	T	73	 75%21%.
29	U	59	 68%20%5%. . .
30	V	56	 64%23%13%
31	W	47	 81%17%.
32	X	46	 67%24%. 7%
33	Y	104	 80%19%.
34	m	474	 100%
35	n	391	 100%
36	o	378	 100%
37	p	281	 100%

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
38	SF4	8	183	-	-	X	-
49	HEA	L	515	X	-	-	-
49	HEA	L	516	X	-	-	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 72626 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-QUINONE OXIDOREDUCTASE SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	437	Total	C	N	O	S	0	0
			3417	2180	595	624	18		

- Molecule 2 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	179	Total	C	N	O	S	0	0
			1410	897	239	266	8		

- Molecule 3 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	754	Total	C	N	O	S	0	0
			5880	3743	1055	1051	31		

- Molecule 4 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	378	Total	C	N	O	S	0	0
			3018	1946	511	550	11		

- Molecule 5 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	196	Total	C	N	O	S	0	0
			1607	1043	273	288	3		

- Molecule 6 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	144	Total	C	N	O	S	0	0
			1102	700	192	197	13		

- Molecule 7 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	127	Total	C	N	O	S	0	0
			1031	664	183	181	3		

- Molecule 8 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	154	Total	C	N	O	S	0	0
			1193	759	201	222	11		

- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	443	Total	C	N	O	S	0	1
			3403	2121	602	660	20		
9	a	443	Total	C	N	O	S	0	1
			3403	2121	602	660	20		

- Molecule 10 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	424	Total	C	N	O	S	0	1
			3177	1996	562	612	7		
10	b	424	Total	C	N	O	S	0	0
			3180	1998	562	613	7		

- Molecule 11 is a protein called CYTOCHROME B.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	365	Total	C	N	O	S	0	0
			2892	1940	450	485	17		
11	c	370	Total	C	N	O	S	0	0
			2931	1968	455	490	18		

- Molecule 12 is a protein called CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	241	Total	C	N	O	S	0	0
			1919	1225	330	349	15		

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

- Molecule 13 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	196	Total	C	N	O	S	0	0
			1519	957	263	291	8		
13	e	196	Total	C	N	O	S	0	0
			1519	957	263	291	8		

- Molecule 14 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	99	Total	C	N	O	S	0	0
			861	545	155	159	2		
14	f	99	Total	C	N	O	S	0	0
			861	545	155	159	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	56	ASP	ASN	ENGINEERED MUTATION	UNP P00129
f	56	ASP	ASN	ENGINEERED MUTATION	UNP P00129

- Molecule 15 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	75	Total	C	N	O	S	0	2
			621	406	117	97	1		
15	g	76	Total	C	N	O	S	0	2
			626	409	118	98	1		

- Molecule 16 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	66	Total	C	N	O	S	0	0
			539	327	98	109	5		
16	h	66	Total	C	N	O	S	0	0
			539	327	98	109	5		

- Molecule 17 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	42	Total	C	N	O	S	0	0
			285	174	55	55	1		
17	i	42	Total	C	N	O	S	0	0
			285	174	55	55	1		

- Molecule 18 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	62	Total	C	N	O		0	0
			507	333	88	86			
18	j	62	Total	C	N	O		0	0
			507	333	88	86			

- Molecule 19 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 10.

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

- Molecule 20 is a protein called CYTOCHROME C OXIDASE SUBUNIT 1.

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

- Molecule 21 is a protein called CYTOCHROME C OXIDASE SUBUNIT 2.

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

- Molecule 22 is a protein called CYTOCHROME C OXIDASE SUBUNIT 3.

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

- Molecule 23 is a protein called CYTOCHROME C OXIDASE SUBUNIT 4 ISOFORM 1,

MITOCHONDRIAL.

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

- Molecule 24 is a protein called CYTOCHROME C OXIDASE SUBUNIT 5A, MITOCHONDRIAL.

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

- Molecule 25 is a protein called CYTOCHROME C OXIDASE SUBUNIT 5B, MITOCHONDRIAL.

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

- Molecule 26 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE VIA, CYTOCHROME C OXIDASE POLYPEPTIDE VB.

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

- Molecule 27 is a protein called CYTOCHROME C OXIDASE SUBUNIT 6B1.

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

- Molecule 28 is a protein called CYTOCHROME C OXIDASE SUBUNIT 6C.

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

- Molecule 29 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7A1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	57	Total	C	N	O	S	0	1
			442	285	74	80	3		

- Molecule 30 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7B, MITOCHONDRIAL.

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

- Molecule 31 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7C, MITOCHONDRIAL.

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

- Molecule 32 is a protein called CYTOCHROME C OXIDASE SUBUNIT 8B, MITOCHONDRIAL.

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

- Molecule 33 is a protein called CYTOCHROME C.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Y	104	Total	C	N	O	S	7	0
			875	552	155	163	5		

- Molecule 34 is a protein called NADH\ : UBIQUINONE OXIDOREDUCTASE, MEMBRANE SUBUNIT L,.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	m	474	Total	C	N			0	0
			1422	948	474				

- Molecule 35 is a protein called NADH\ : UBIQUINONE OXIDOREDUCTASE, MEMBRANE SUBUNIT M,.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	n	391	Total	C	N			0	0
			1173	782	391				

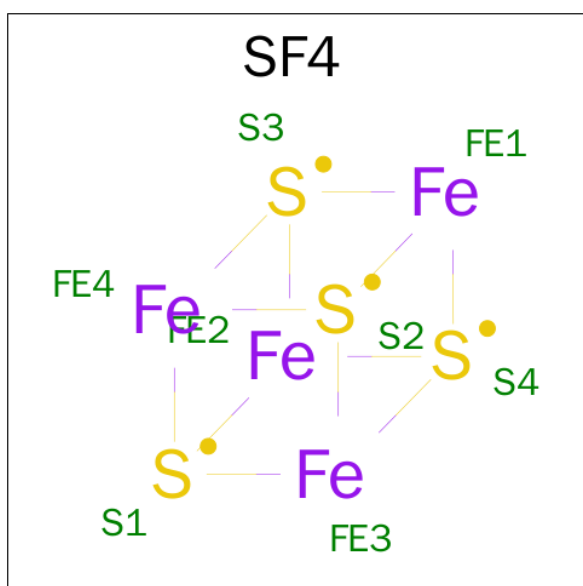
- Molecule 36 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT N.

Mol	Chain	Residues	Atoms			AltConf	Trace
36	o	378	Total	C	N	0	0
			1134	756	378		

- Molecule 37 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT K.

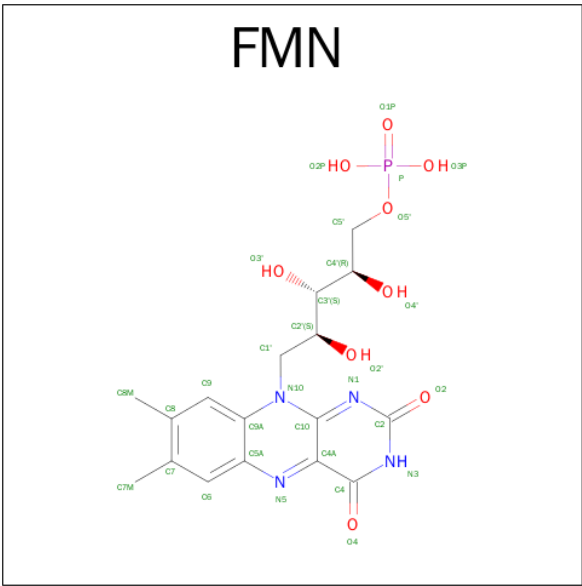
Mol	Chain	Residues	Atoms			AltConf	Trace
37	p	281	Total	C	N	0	0
			843	562	281		

- Molecule 38 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



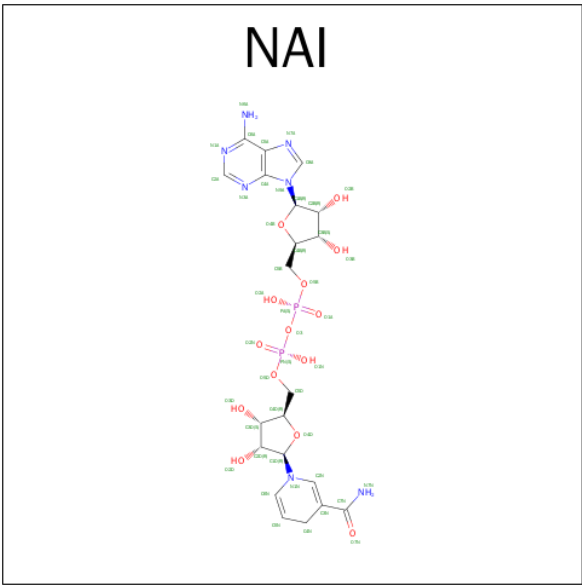
Mol	Chain	Residues	Atoms			AltConf
38	1	1	Total	Fe	S	0
			8	4	4	
38	3	1	Total	Fe	S	0
			24	12	12	
38	3	1	Total	Fe	S	0
			24	12	12	
38	3	1	Total	Fe	S	0
			24	12	12	
38	6	1	Total	Fe	S	0
			8	4	4	
38	8	1	Total	Fe	S	0
			16	8	8	
38	8	1	Total	Fe	S	0
			16	8	8	

- Molecule 39 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms					AltConf
39	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 40 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).

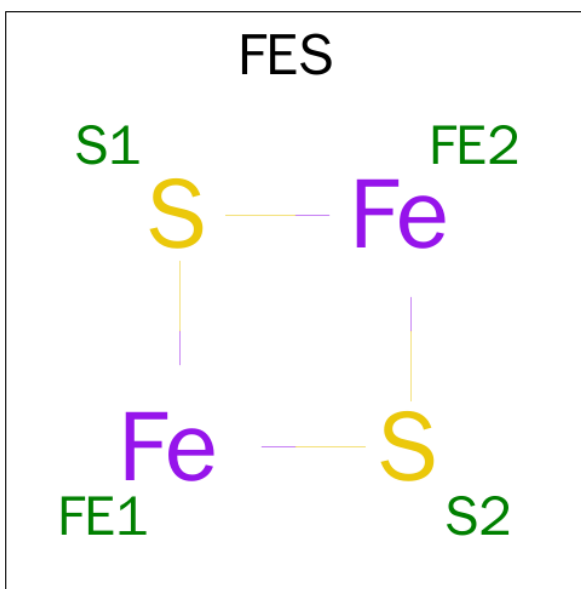


Mol	Chain	Residues	Atoms					AltConf
40	1	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 41 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
41	1	1	Total 1	Mg 1	0
41	4	1	Total 1	Mg 1	0
41	5	1	Total 1	Mg 1	0
41	2	1	Total 1	Mg 1	0
41	L	1	Total 1	Mg 1	0
41	3	2	Total 2	Mg 2	0

- Molecule 42 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).

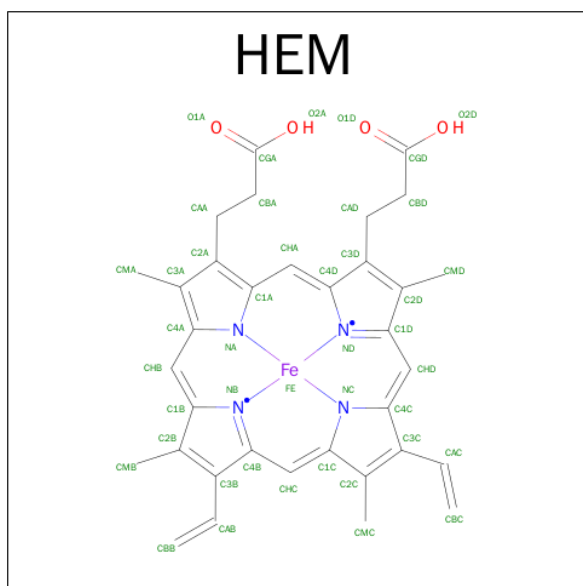


Mol	Chain	Residues	Atoms			AltConf
42	2	1	Total 4	Fe 2	S 2	0
42	3	1	Total 4	Fe 2	S 2	0
42	E	1	Total 4	Fe 2	S 2	0
42	e	1	Total 4	Fe 2	S 2	0

- Molecule 43 is CALCIUM ION (three-letter code: CA) (formula: Ca).

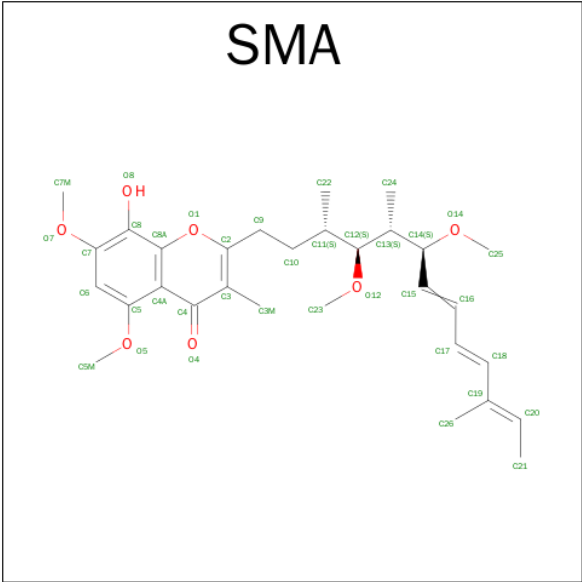
Mol	Chain	Residues	Atoms		AltConf
43	7	1	Total	Ca	0
			1	1	

- Molecule 44 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



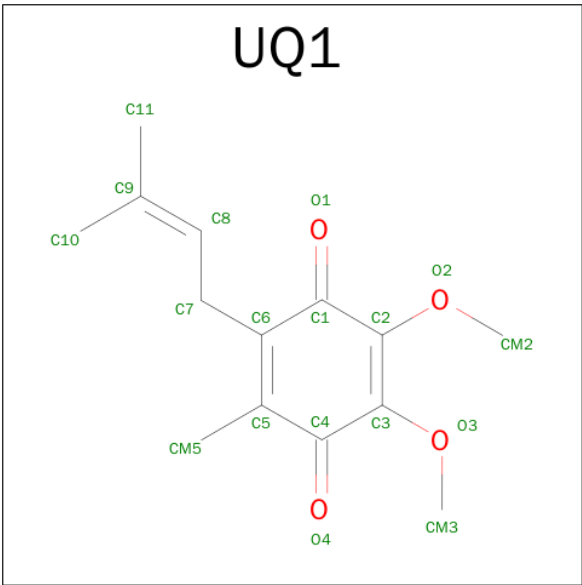
Mol	Chain	Residues	Atoms					AltConf
44	C	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
44	C	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
44	Y	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
44	c	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
44	c	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

- Molecule 45 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



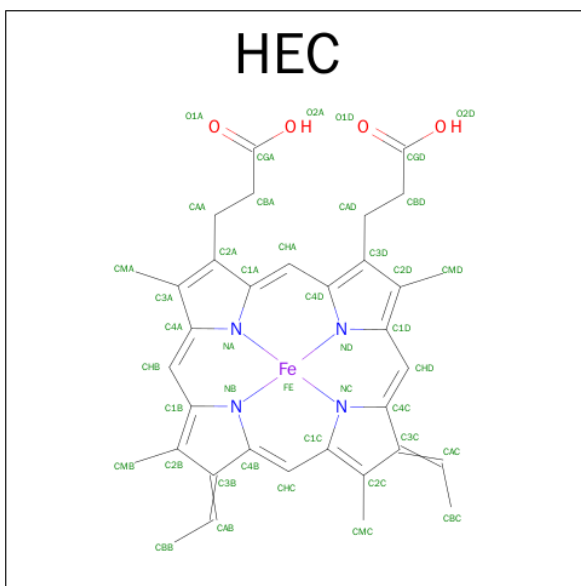
Mol	Chain	Residues	Atoms			AltConf
45	C	1	Total	C	O	0
			37	30	7	
45	c	1	Total	C	O	0
			37	30	7	

- Molecule 46 is UBIQUINONE-1 (three-letter code: UQ1) (formula: C₁₄H₁₈O₄).



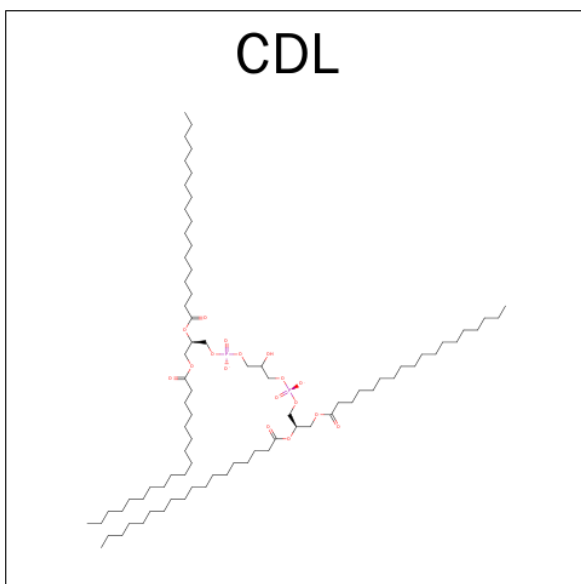
Mol	Chain	Residues	Atoms			AltConf
46	C	1	Total	C	O	0
			14	10	4	
46	c	1	Total	C	O	0
			14	10	4	

- Molecule 47 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 48 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



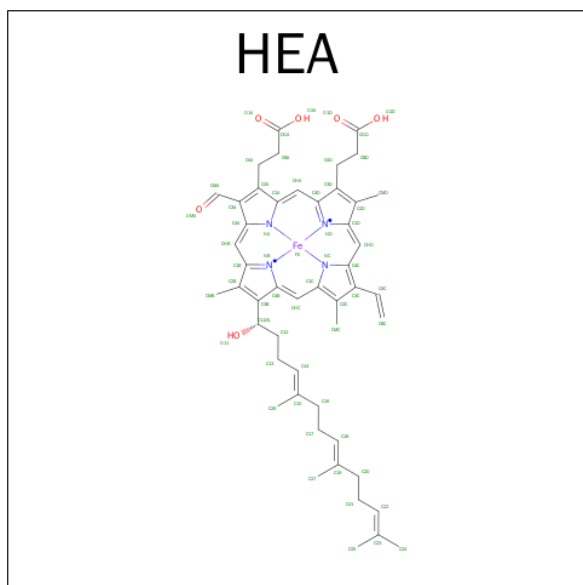
Mol	Chain	Residues	Atoms				AltConf
48	G	1	Total	C	O	P	0
			94	56	34	4	

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Mol	Chain	Residues	Atoms				AltConf
48	G	1	Total	C	O	P	0
			94	56	34	4	
48	d	1	Total	C	O	P	0
			50	31	17	2	
48	g	1	Total	C	O	P	0
			49	30	17	2	

- Molecule 49 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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

- Molecule 50 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
50	L	1	Total	Cu	0
			1	1	
50	M	2	Total	Cu	0
			2	2	

- Molecule 51 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
51	Q	1	Total 1	Zn 1	0

- Molecule 52 is water.

Mol	Chain	Residues	Atoms		AltConf
52	A	187	Total 187	O 187	0
52	B	149	Total 149	O 149	0
52	C	125	Total 125	O 125	0
52	D	118	Total 118	O 118	0
52	E	54	Total 54	O 54	0
52	F	57	Total 57	O 57	0
52	G	24	Total 24	O 24	0
52	H	14	Total 14	O 14	0
52	I	16	Total 16	O 16	0
52	J	5	Total 5	O 5	0
52	Y	161	Total 161	O 161	0
52	a	134	Total 134	O 134	0
52	b	130	Total 130	O 130	0
52	c	122	Total 122	O 122	0
52	d	109	Total 109	O 109	0
52	e	64	Total 64	O 64	0
52	f	73	Total 73	O 73	0
52	g	21	Total 21	O 21	0
52	h	16	Total 16	O 16	0

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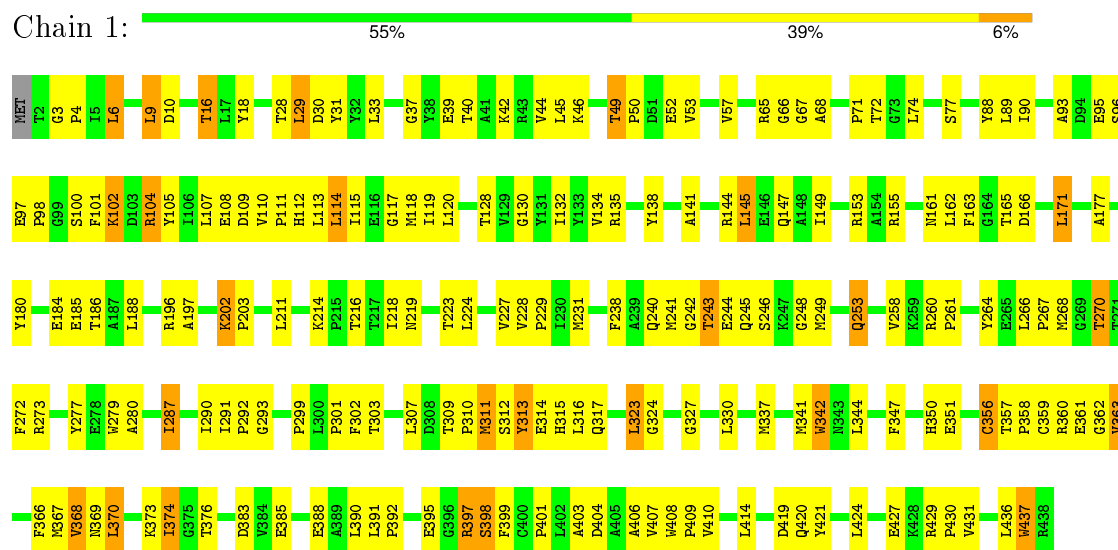
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Mol	Chain	Residues	Atoms		AltConf
52	i	10	Total 10	O 10	0
52	j	9	Total 9	O 9	0

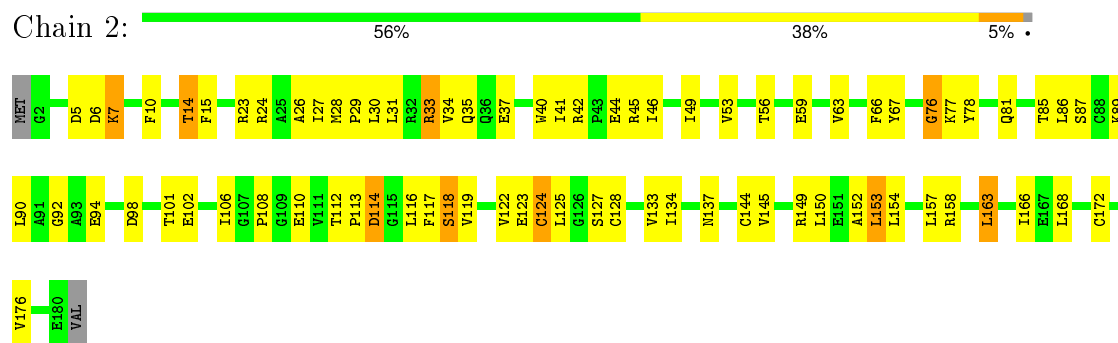
3 Residue-property plots

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.

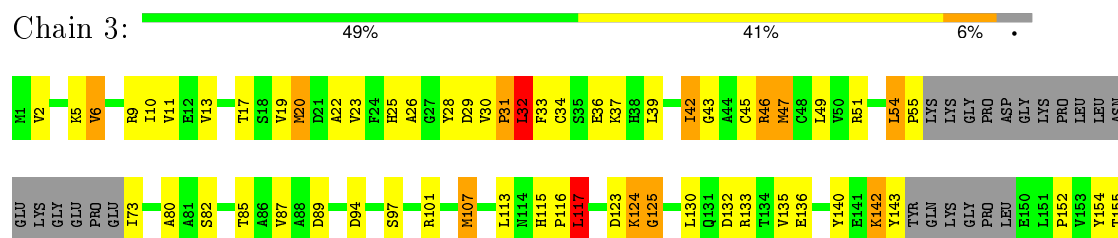
- Molecule 1: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 1

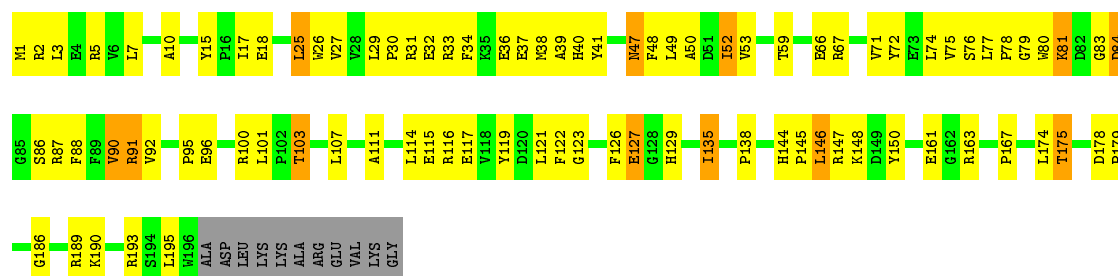


- Molecule 2: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 2

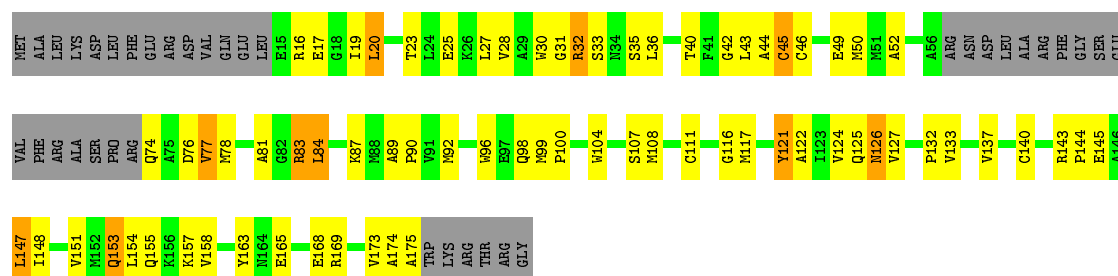


- Molecule 3: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 3

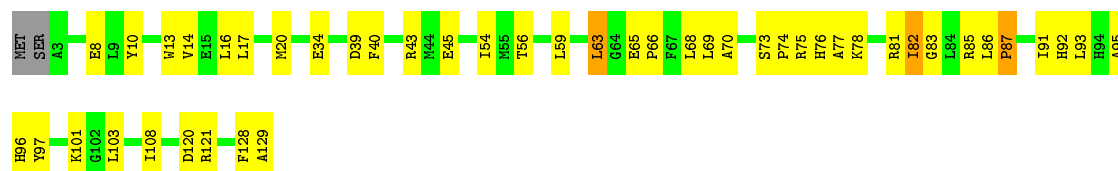




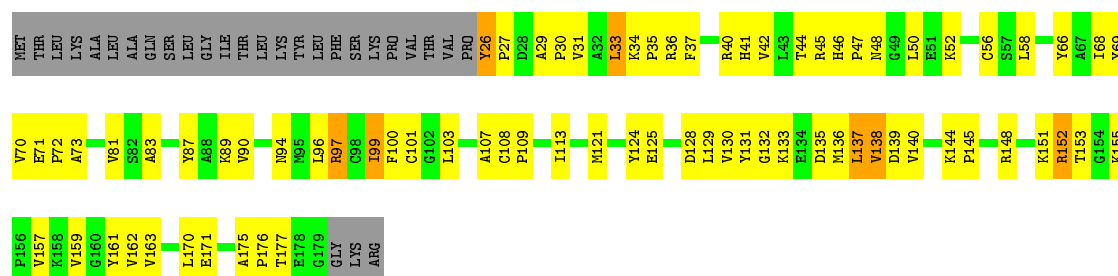
• Molecule 6: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 6



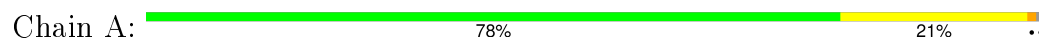
• Molecule 7: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 15

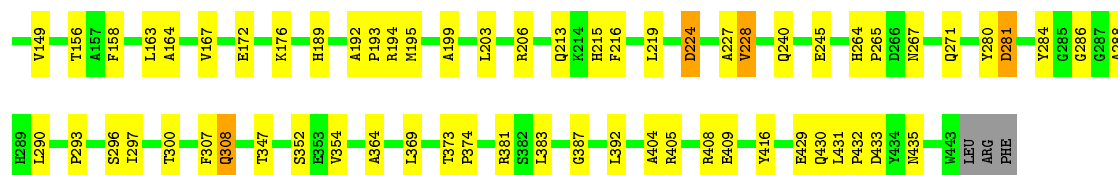


• Molecule 8: NADH-QUINONE OXIDOREDUCTASE SUBUNIT 9



• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL





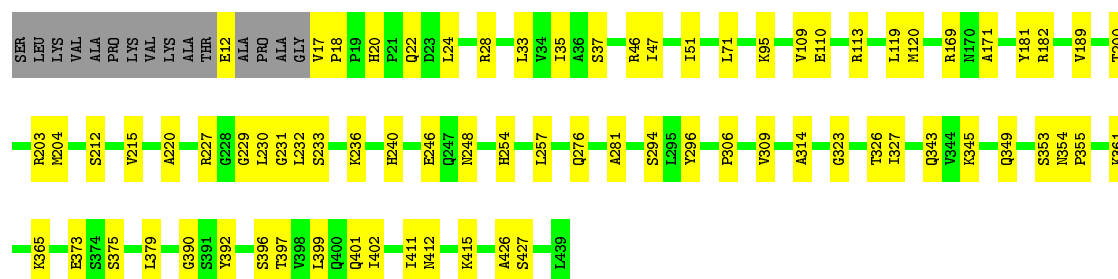
- Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL

Chain a: 98%



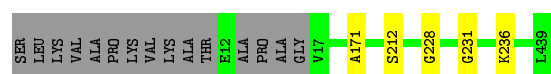
- Molecule 10: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL

Chain B: 79%



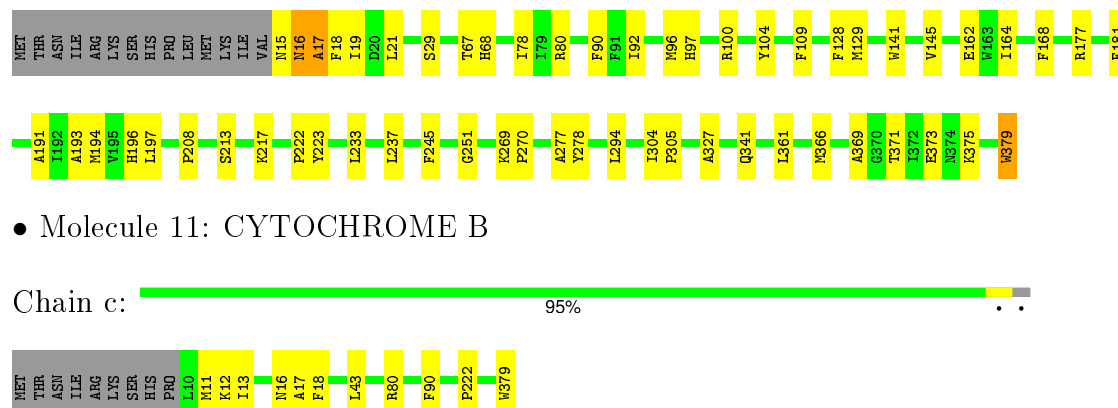
- Molecule 10: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL

Chain b: 95%



- Molecule 11: CYTOCHROME B

Chain C: 81%

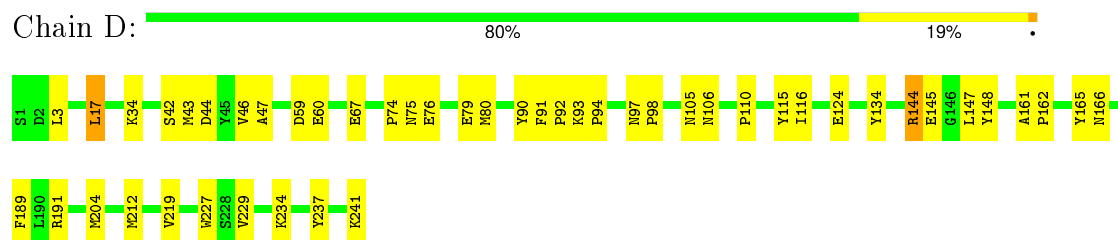


- Molecule 11: CYTOCHROME B

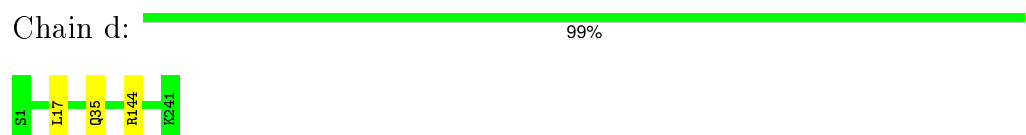
Chain c: 95%



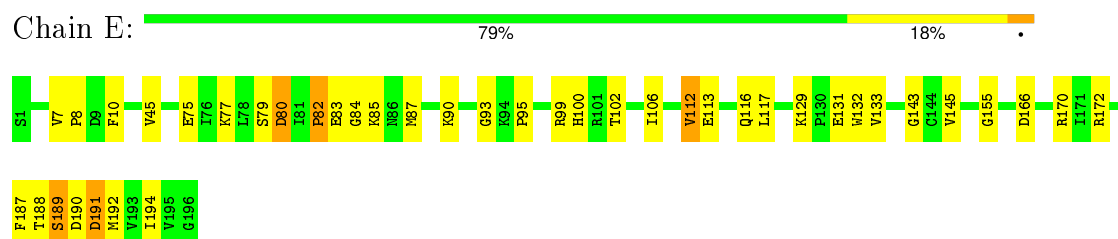
- Molecule 12: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL



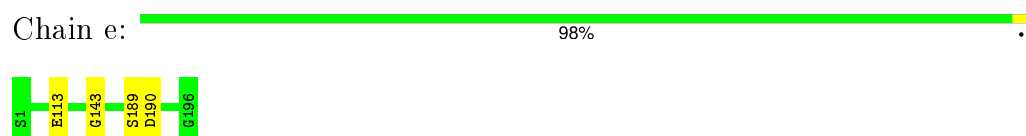
- Molecule 12: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL



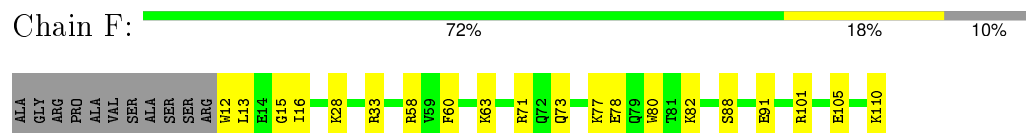
- Molecule 13: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL



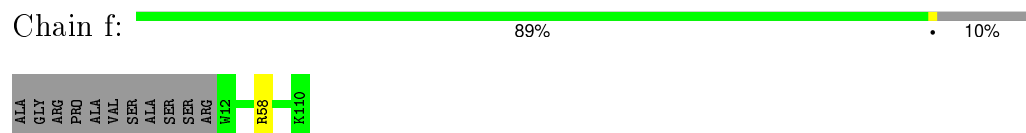
- Molecule 13: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL



- Molecule 14: CYTOCHROME B-C1 COMPLEX SUBUNIT 7



- Molecule 14: CYTOCHROME B-C1 COMPLEX SUBUNIT 7



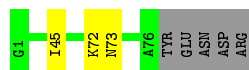
- Molecule 15: CYTOCHROME B-C1 COMPLEX SUBUNIT 8





- Molecule 15: CYTOCHROME B-C1 COMPLEX SUBUNIT 8

Chain g: 90% 6%



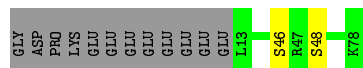
- Molecule 16: CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL

Chain H: 62% 21% 15%



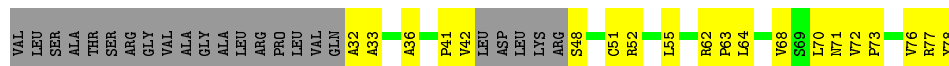
- Molecule 16: CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL

Chain h: 82% 15%



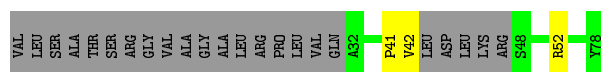
- Molecule 17: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

Chain I: 34% 31% 35%



- Molecule 17: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

Chain i: 60% 5% 35%



- Molecule 18: CYTOCHROME B-C1 COMPLEX SUBUNIT 9

Chain J: 63% 32% 5%



- Molecule 18: CYTOCHROME B-C1 COMPLEX SUBUNIT 9

Chain j: 95% 5%



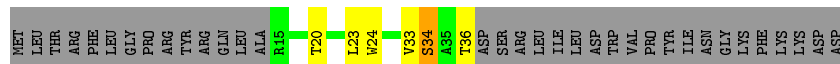
- Molecule 19: CYTOCHROME B-C1 COMPLEX SUBUNIT 10

Chain K: 



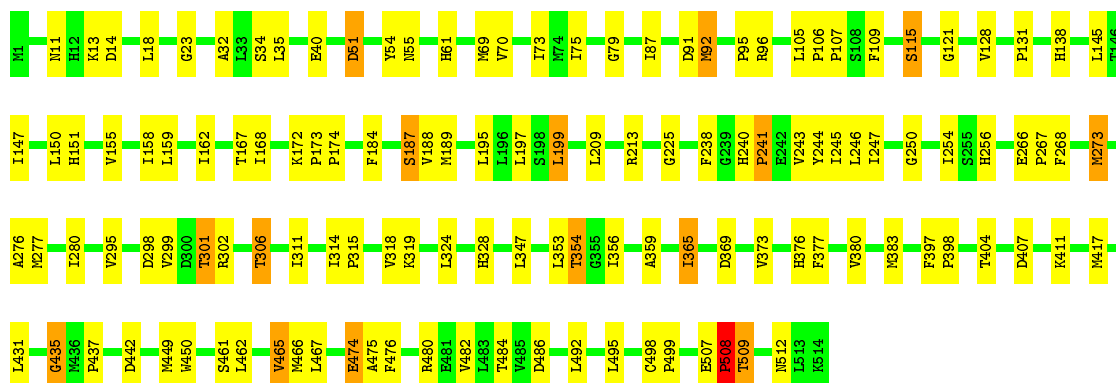
- Molecule 19: CYTOCHROME B-C1 COMPLEX SUBUNIT 10

Chain k: 



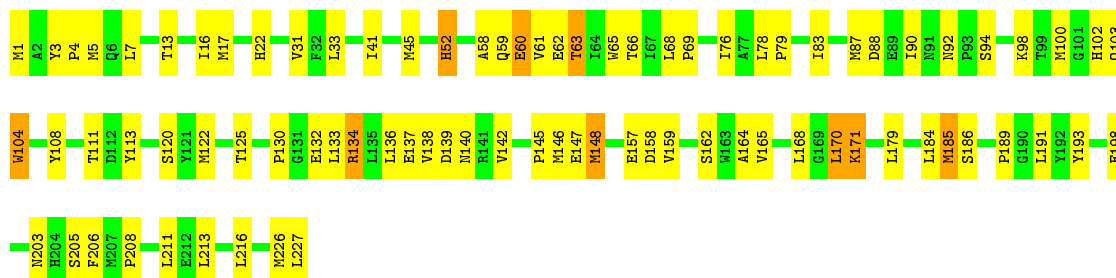
- Molecule 20: CYTOCHROME C OXIDASE SUBUNIT 1

Chain L: 



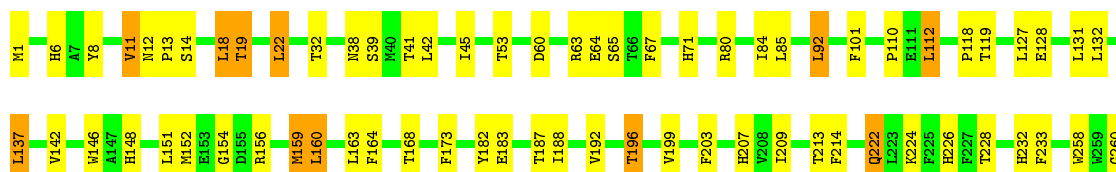
- Molecule 21: CYTOCHROME C OXIDASE SUBUNIT 2

Chain M: 



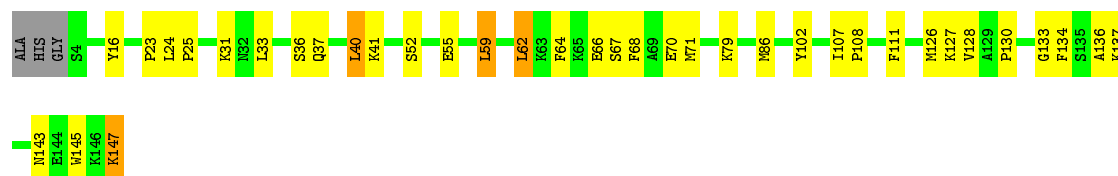
- Molecule 22: CYTOCHROME C OXIDASE SUBUNIT 3

Chain N: 




S261

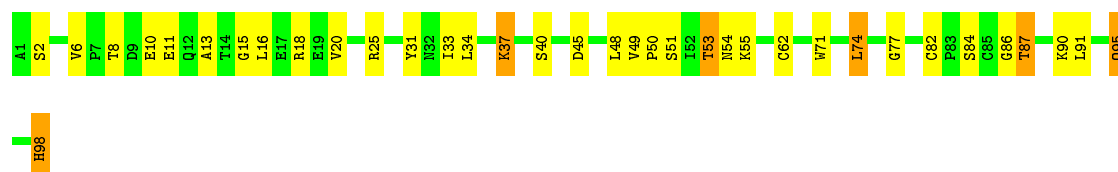
- Molecule 23: CYTOCHROME C OXIDASE SUBUNIT 4 ISOFORM 1, MITOCHONDRIAL

Chain O:  73% 22%

- Molecule 24: CYTOCHROME C OXIDASE SUBUNIT 5A, MITOCHONDRIAL

Chain P:  78% 19%

- Molecule 25: CYTOCHROME C OXIDASE SUBUNIT 5B, MITOCHONDRIAL

Chain Q:  63% 31% 6%

- Molecule 26: CYTOCHROME C OXIDASE POLYPEPTIDE VIA, CYTOCHROME C OXIDASE POLYPEPTIDE VB

Chain R:  58% 32% 8%

- Molecule 27: CYTOCHROME C OXIDASE SUBUNIT 6B1

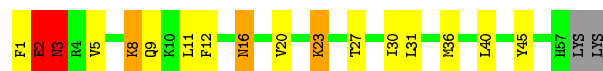
Chain S:  60% 22% 6% 12%

- Molecule 28: CYTOCHROME C OXIDASE SUBUNIT 6C

Chain T:  75% 21%

- Molecule 29: CYTOCHROME C OXIDASE SUBUNIT 7A1, MITOCHONDRIAL

Chain U:  68% 20% 5% . .




- Molecule 30: CYTOCHROME C OXIDASE SUBUNIT 7B, MITOCHONDRIAL

Chain V:  64% 23% 13%



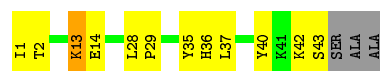
- Molecule 31: CYTOCHROME C OXIDASE SUBUNIT 7C, MITOCHONDRIAL

Chain W:  81% 17% .




- Molecule 32: CYTOCHROME C OXIDASE SUBUNIT 8B, MITOCHONDRIAL

Chain X:  67% 24% . 7%



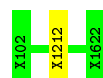
- Molecule 33: CYTOCHROME C

Chain Y:  80% 19% .



- Molecule 34: NADH\; UBIQUINONE OXIDOREDUCTASE, MEMBRANE SUBUNIT L,

Chain m:  100%



- Molecule 35: NADH\; UBIQUINONE OXIDOREDUCTASE, MEMBRANE SUBUNIT M,

Chain n:  100%

There are no outlier residues recorded for this chain.

- Molecule 36: NADH-QUINONE OXIDOREDUCTASE SUBUNIT N

Chain o:  100%

There are no outlier residues recorded for this chain.

- Molecule 37: NADH-QUINONE OXIDOREDUCTASE SUBUNIT K

Chain p:

100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE-FLIPPING ON EACH PARTICLE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CDL, SF4, NAI, ZN, FMN, SMA, FES, HEC, UQ1, HEM, CA, 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	1	0.45	1/3506 (0.0%)	0.63	2/4745 (0.0%)
10	B	0.32	0/3235	0.65	0/4387
10	b	0.31	0/3239	0.65	1/4393 (0.0%)
11	C	0.37	0/2986	0.65	1/4089 (0.0%)
11	c	0.35	0/3024	0.64	0/4137
12	D	0.34	0/1978	0.65	0/2684
12	d	0.34	0/1978	0.65	0/2684
13	E	0.32	0/1553	0.67	1/2100 (0.0%)
13	e	0.35	0/1553	0.69	1/2100 (0.0%)
14	F	0.32	0/878	0.64	0/1175
14	f	0.32	0/878	0.65	0/1175
15	G	0.32	0/642	0.65	0/869
15	g	0.34	0/647	0.68	0/876
16	H	0.31	0/544	0.60	0/729
16	h	0.31	0/544	0.56	0/729
17	I	0.32	0/285	0.66	0/384
17	i	0.32	0/285	0.69	0/384
18	J	0.37	0/520	0.65	0/699
18	j	0.36	0/520	0.65	0/699
19	K	0.42	0/163	1.01	0/225
19	k	0.46	0/163	1.17	0/225
2	2	0.45	0/1443	0.64	0/1958
20	L	0.60	0/4164	0.76	1/5688 (0.0%)
21	M	0.57	0/1868	0.79	0/2544
22	N	0.56	0/2211	0.68	0/3023
23	O	0.57	0/1229	0.64	1/1658 (0.1%)
24	P	0.50	0/898	0.66	0/1218
25	Q	0.56	0/765	0.81	0/1038
26	R	0.54	0/699	0.73	1/950 (0.1%)
27	S	0.55	0/648	0.73	0/877
28	T	0.60	0/611	0.65	0/810
29	U	0.61	0/451	0.72	0/610

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
3	3	0.43	0/6019	0.61	1/8163 (0.0%)
30	V	0.57	0/398	0.66	0/546
31	W	0.63	0/399	0.62	0/534
32	X	0.51	0/345	0.65	0/470
33	Y	0.31	0/891	0.60	0/1186
4	4	0.40	0/3096	0.59	2/4207 (0.0%)
5	5	0.44	0/1656	0.61	0/2246
6	6	0.48	0/1126	0.64	0/1528
7	7	0.43	0/1059	0.60	0/1429
8	8	0.48	0/1224	0.66	0/1663
9	A	0.32	0/3472	0.66	0/4714
9	a	0.33	0/3472	0.67	0/4714
All	All	0.43	1/67265 (0.0%)	0.66	12/91262 (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
19	k	0	1
34	m	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	356	CYS	CB-SG	-5.05	1.73	1.81

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	39	GLY	N-CA-C	-7.72	93.79	113.10
4	4	105	LEU	CA-CB-CG	7.21	131.89	115.30
10	b	228	GLY	N-CA-C	-6.96	95.71	113.10
23	O	133	GLY	N-CA-C	6.43	129.19	113.10
3	3	32	LEU	CA-CB-CG	5.91	128.89	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	k	24	TRP	Mainchain
34	m	1212	UNK	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	1	3417	0	3388	169	0
2	2	1410	0	1376	70	0
3	3	5880	0	5911	354	0
4	4	3018	0	3009	195	0
5	5	1607	0	1574	95	0
6	6	1102	0	1108	79	0
7	7	1031	0	1029	39	0
8	8	1193	0	1160	69	0
9	A	3403	0	3301	95	0
9	a	3403	0	3302	0	0
10	B	3177	0	3152	85	0
10	b	3180	0	3156	0	0
11	C	2892	0	2938	48	0
11	c	2931	0	2989	0	0
12	D	1919	0	1868	63	0
12	d	1919	0	1867	0	0
13	E	1519	0	1503	38	0
13	e	1519	0	1503	0	0
14	F	861	0	854	22	0
14	f	861	0	854	0	0
15	G	621	0	626	29	0
15	g	626	0	631	0	0
16	H	539	0	524	17	0
16	h	539	0	524	0	0
17	I	285	0	288	46	0
17	i	285	0	288	0	0
18	J	507	0	512	71	0
18	j	507	0	512	0	0
19	K	159	0	159	61	0
19	k	159	0	159	0	0
20	L	4025	0	4003	82	0
21	M	1822	0	1834	72	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	N	2124	0	2042	47	0
23	O	1195	0	1183	33	0
24	P	878	0	868	21	0
25	Q	748	0	728	26	0
26	R	672	0	645	30	0
27	S	628	0	582	22	0
28	T	598	0	612	14	0
29	U	442	0	439	14	0
30	V	384	0	366	9	0
31	W	386	0	388	8	0
32	X	335	0	352	12	0
33	Y	875	0	885	39	0
34	m	1422	0	52	0	0
35	n	1173	0	37	0	0
36	o	1134	0	36	0	0
37	p	843	0	24	0	0
38	1	8	0	0	0	0
38	3	24	0	0	3	0
38	6	8	0	0	1	0
38	8	16	0	0	2	0
39	1	31	0	19	6	0
40	1	44	0	27	6	0
41	1	1	0	0	0	0
41	2	1	0	0	0	0
41	3	2	0	0	0	0
41	4	1	0	0	0	0
41	5	1	0	0	0	0
41	L	1	0	0	0	0
42	2	4	0	0	0	0
42	3	4	0	0	1	0
42	E	4	0	0	0	0
42	e	4	0	0	0	0
43	7	1	0	0	0	0
44	C	86	0	60	5	0
44	Y	43	0	30	7	0
44	c	86	0	60	0	0
45	C	37	0	42	1	0
45	c	37	0	42	0	0
46	C	14	0	9	2	0
46	c	14	0	9	0	0
47	D	43	0	30	6	0
47	d	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	G	94	0	76	5	0
48	d	50	0	44	0	0
48	g	49	0	42	0	0
49	L	120	0	108	7	0
50	L	1	0	0	0	0
50	M	2	0	0	0	0
51	Q	1	0	0	0	0
52	A	187	0	0	11	0
52	B	149	0	0	3	0
52	C	125	0	0	4	0
52	D	118	0	0	2	0
52	E	54	0	0	2	0
52	F	57	0	0	3	0
52	G	24	0	0	1	0
52	H	14	0	0	0	0
52	I	16	0	0	2	0
52	J	5	0	0	0	0
52	Y	161	0	0	18	0
52	a	134	0	0	0	0
52	b	130	0	0	0	0
52	c	122	0	0	0	0
52	d	109	0	0	0	0
52	e	64	0	0	0	0
52	f	73	0	0	0	0
52	g	21	0	0	0	0
52	h	16	0	0	0	0
52	i	10	0	0	0	0
52	j	9	0	0	0	0
All	All	72626	0	65769	1833	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 14.

The worst 5 of 1833 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)
18:J:29:LEU:HD21	19:K:34:SER:CB	69.19	1.63
18:J:29:LEU:CD2	19:K:34:SER:HB2	70.77	1.42
9:A:408:ARG:NH2	19:K:15:ARG:HG2	78.17	1.38
12:D:106:ASN:HB2	52:Y:350:HOH:O	51.68	1.29
12:D:145:GLU:OE1	33:Y:27:LYS:HD3	63.63	1.28

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	435/438 (99%)	380 (87%)	48 (11%)	7 (2%)	12	56
2	2	177/181 (98%)	151 (85%)	22 (12%)	4 (2%)	8	48
3	3	748/783 (96%)	624 (83%)	101 (14%)	23 (3%)	5	42
4	4	374/409 (91%)	331 (88%)	34 (9%)	9 (2%)	7	47
5	5	194/207 (94%)	166 (86%)	24 (12%)	4 (2%)	9	50
6	6	140/181 (77%)	114 (81%)	21 (15%)	5 (4%)	4	38
7	7	125/129 (97%)	111 (89%)	13 (10%)	1 (1%)	24	69
8	8	152/182 (84%)	129 (85%)	22 (14%)	1 (1%)	26	71
9	A	441/446 (99%)	425 (96%)	14 (3%)	2 (0%)	34	77
9	a	441/446 (99%)	424 (96%)	16 (4%)	1 (0%)	52	86
10	B	418/439 (95%)	409 (98%)	8 (2%)	1 (0%)	52	86
10	b	420/439 (96%)	406 (97%)	12 (3%)	2 (0%)	34	77
11	C	363/379 (96%)	354 (98%)	6 (2%)	3 (1%)	24	69
11	c	366/379 (97%)	353 (96%)	8 (2%)	5 (1%)	14	58
12	D	239/241 (99%)	234 (98%)	5 (2%)	0	100	100
12	d	239/241 (99%)	235 (98%)	4 (2%)	0	100	100
13	E	194/196 (99%)	183 (94%)	7 (4%)	4 (2%)	9	50
13	e	194/196 (99%)	184 (95%)	9 (5%)	1 (0%)	34	77
14	F	97/110 (88%)	96 (99%)	1 (1%)	0	100	100
14	f	97/110 (88%)	96 (99%)	1 (1%)	0	100	100
15	G	73/81 (90%)	72 (99%)	1 (1%)	0	100	100
15	g	74/81 (91%)	69 (93%)	4 (5%)	1 (1%)	14	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	H	64/78 (82%)	61 (95%)	3 (5%)	0	100	100
16	h	64/78 (82%)	62 (97%)	1 (2%)	1 (2%)	12	56
17	I	38/65 (58%)	36 (95%)	1 (3%)	1 (3%)	7	45
17	i	38/65 (58%)	36 (95%)	1 (3%)	1 (3%)	7	45
18	J	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	11	55
18	j	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	11	55
19	K	20/56 (36%)	17 (85%)	2 (10%)	1 (5%)	3	31
19	k	20/56 (36%)	15 (75%)	3 (15%)	2 (10%)	1	14
20	L	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	24	69
21	M	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	15	60
22	N	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
23	O	142/147 (97%)	135 (95%)	7 (5%)	0	100	100
24	P	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
25	Q	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	3	34
26	R	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	2	26
27	S	73/85 (86%)	64 (88%)	8 (11%)	1 (1%)	14	58
28	T	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
29	U	54/59 (92%)	48 (89%)	4 (7%)	2 (4%)	4	38
30	V	47/56 (84%)	41 (87%)	6 (13%)	0	100	100
31	W	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
32	X	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
33	Y	109/104 (105%)	106 (97%)	3 (3%)	0	100	100
All	All	8228/8726 (94%)	7616 (93%)	511 (6%)	101 (1%)	21	61

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	4	PRO
2	2	108	PRO
3	3	6	VAL
3	3	117	LEU
3	3	216	PHE

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	1	355/356 (100%)	321 (90%)	34 (10%)	10	40
2	2	150/152 (99%)	135 (90%)	15 (10%)	9	38
3	3	607/628 (97%)	560 (92%)	47 (8%)	16	52
4	4	326/355 (92%)	296 (91%)	30 (9%)	11	43
5	5	167/175 (95%)	155 (93%)	12 (7%)	18	55
6	6	117/149 (78%)	107 (92%)	10 (8%)	13	48
7	7	104/106 (98%)	96 (92%)	8 (8%)	16	52
8	8	126/150 (84%)	111 (88%)	15 (12%)	6	31
9	A	364/370 (98%)	359 (99%)	5 (1%)	74	89
9	a	364/370 (98%)	359 (99%)	5 (1%)	74	89
10	B	332/343 (97%)	332 (100%)	0	100	100
10	b	332/343 (97%)	330 (99%)	2 (1%)	90	95
11	C	312/327 (95%)	307 (98%)	5 (2%)	70	88
11	c	316/327 (97%)	310 (98%)	6 (2%)	65	86
12	D	206/206 (100%)	203 (98%)	3 (2%)	72	88
12	d	206/206 (100%)	203 (98%)	3 (2%)	72	88
13	E	168/168 (100%)	167 (99%)	1 (1%)	90	95
13	e	168/168 (100%)	166 (99%)	2 (1%)	78	90
14	F	90/98 (92%)	89 (99%)	1 (1%)	80	91
14	f	90/98 (92%)	89 (99%)	1 (1%)	80	91
15	G	66/71 (93%)	65 (98%)	1 (2%)	72	88
15	g	66/71 (93%)	64 (97%)	2 (3%)	48	77
16	H	63/74 (85%)	61 (97%)	2 (3%)	46	76
16	h	63/74 (85%)	62 (98%)	1 (2%)	70	88
17	I	28/51 (55%)	27 (96%)	1 (4%)	42	74
17	i	28/51 (55%)	26 (93%)	2 (7%)	18	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	J	51/52 (98%)	49 (96%)	2 (4%)	39	72
18	j	51/52 (98%)	49 (96%)	2 (4%)	39	72
19	K	15/46 (33%)	12 (80%)	3 (20%)	1	11
19	k	15/46 (33%)	11 (73%)	4 (27%)	0	5
20	L	427/427 (100%)	389 (91%)	38 (9%)	12	44
21	M	211/211 (100%)	191 (90%)	20 (10%)	11	41
22	N	226/226 (100%)	199 (88%)	27 (12%)	6	31
23	O	128/129 (99%)	120 (94%)	8 (6%)	22	59
24	P	95/95 (100%)	89 (94%)	6 (6%)	22	59
25	Q	81/81 (100%)	76 (94%)	5 (6%)	23	60
26	R	68/68 (100%)	50 (74%)	18 (26%)	0	5
27	S	67/75 (89%)	58 (87%)	9 (13%)	5	27
28	T	58/58 (100%)	53 (91%)	5 (9%)	13	47
29	U	47/50 (94%)	40 (85%)	7 (15%)	4	23
30	V	39/46 (85%)	37 (95%)	2 (5%)	29	66
31	W	40/40 (100%)	38 (95%)	2 (5%)	30	66
32	X	37/38 (97%)	34 (92%)	3 (8%)	15	50
33	Y	91/84 (108%)	90 (99%)	1 (1%)	80	91
All	All	6961/7311 (95%)	6585 (95%)	376 (5%)	32	64

5 of 376 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	8	163	VAL
20	L	241	PRO
9	a	149	VAL
9	A	308	GLN
18	J	8	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
20	L	360	ASN
22	N	207	HIS
10	b	412	ASN

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Mol	Chain	Res	Type
20	L	512	ASN
22	N	6	HIS

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 42 ligands modelled in this entry, 12 are monoatomic - leaving 30 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	$\# Z > 2$
38	SF4	1	439	1	0,12,12	0.00	-	0,24,24	0.00	-
39	FMN	1	440	-	32,33,33	1.44	4 (12%)	34,50,50	1.99	6 (17%)
40	NAI	1	441	-	41,48,48	3.78	27 (65%)	46,73,73	1.92	4 (8%)
42	FES	2	182	2	0,4,4	0.00	-	0,4,4	0.00	-
38	SF4	3	784	3	0,12,12	0.00	-	0,24,24	0.00	-
38	SF4	3	785	3	0,12,12	0.00	-	0,24,24	0.00	-
38	SF4	3	786	3	0,12,12	0.00	-	0,24,24	0.00	-
42	FES	3	787	3	0,4,4	0.00	-	0,4,4	0.00	-
38	SF4	6	182	6	0,12,12	0.00	-	0,24,24	0.00	-
38	SF4	8	183	8	0,12,12	0.00	-	0,24,24	0.00	-
38	SF4	8	184	8	0,12,12	0.00	-	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	SMA	C	2001	-	35,38,38	1.82	6 (17%)	39,52,52	1.81	3 (7%)
46	UQ1	C	2002	-	14,14,18	2.13	8 (57%)	18,20,25	0.52	0
44	HEM	C	501	11	24,50,50	2.07	6 (25%)	16,82,82	1.49	4 (25%)
44	HEM	C	502	11	24,50,50	2.13	7 (29%)	16,82,82	2.11	5 (31%)
47	HEC	D	501	12	24,50,50	2.00	5 (20%)	19,82,82	3.04	5 (26%)
42	FES	E	501	13	0,4,4	0.00	-	0,4,4	0.00	-
48	CDL	G	2003	-	49,49,99	1.09	4 (8%)	51,61,111	1.12	4 (7%)
48	CDL	G	2004	-	43,43,99	1.12	2 (4%)	45,55,111	1.25	4 (8%)
49	HEA	L	515	20	40,67,67	1.49	5 (12%)	36,103,103	1.66	8 (22%)
49	HEA	L	516	20	40,67,67	1.58	4 (10%)	36,103,103	1.48	9 (25%)
44	HEM	Y	500	33	24,50,50	1.66	4 (16%)	16,82,82	2.87	8 (50%)
45	SMA	c	3001	-	35,38,38	2.02	8 (22%)	39,52,52	1.84	3 (7%)
46	UQ1	c	3002	-	14,14,18	1.94	8 (57%)	18,20,25	0.38	0
44	HEM	c	501	11	24,50,50	2.24	7 (29%)	16,82,82	1.24	2 (12%)
44	HEM	c	502	11	24,50,50	2.32	8 (33%)	16,82,82	1.72	4 (25%)
48	CDL	d	3003	-	49,49,99	1.08	4 (8%)	51,61,111	1.18	4 (7%)
47	HEC	d	501	12	24,50,50	2.04	4 (16%)	19,82,82	2.58	3 (15%)
42	FES	e	501	13	0,4,4	0.00	-	0,4,4	0.00	-
48	CDL	g	3004	-	48,48,99	1.14	4 (8%)	50,60,111	1.14	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	SF4	1	439	1	-	0/0/48/48	0/6/5/5
39	FMN	1	440	-	-	0/18/18/18	0/3/3/3
40	NAI	1	441	-	-	0/25/72/72	0/5/5/5
42	FES	2	182	2	-	0/0/4/4	0/1/1/1
38	SF4	3	784	3	-	0/0/48/48	0/6/5/5
38	SF4	3	785	3	-	0/0/48/48	0/6/5/5
38	SF4	3	786	3	-	0/0/48/48	0/6/5/5
42	FES	3	787	3	-	0/0/4/4	0/1/1/1
38	SF4	6	182	6	-	0/0/48/48	0/6/5/5
38	SF4	8	183	8	-	0/0/48/48	0/6/5/5
38	SF4	8	184	8	-	0/0/48/48	0/6/5/5
45	SMA	C	2001	-	-	0/33/34/34	0/2/2/2
46	UQ1	C	2002	-	-	0/4/28/33	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	HEM	C	501	11	-	0/6/54/54	0/0/8/8
44	HEM	C	502	11	-	0/6/54/54	0/0/8/8
47	HEC	D	501	12	-	0/6/54/54	0/0/8/8
42	FES	E	501	13	-	0/0/4/4	0/1/1/1
48	CDL	G	2003	-	-	0/58/58/110	0/0/0/0
48	CDL	G	2004	-	-	0/52/52/110	0/0/0/0
49	HEA	L	515	20	3/3/7/16	0/24/76/76	0/0/8/8
49	HEA	L	516	20	3/3/7/16	0/24/76/76	0/0/8/8
44	HEM	Y	500	33	-	0/6/54/54	0/0/8/8
45	SMA	c	3001	-	-	0/33/34/34	0/2/2/2
46	UQ1	c	3002	-	-	0/4/28/33	0/1/1/1
44	HEM	c	501	11	-	0/6/54/54	0/0/8/8
44	HEM	c	502	11	-	0/6/54/54	0/0/8/8
48	CDL	d	3003	-	-	0/58/58/110	0/0/0/0
47	HEC	d	501	12	-	0/6/54/54	0/0/8/8
42	FES	e	501	13	-	0/0/4/4	0/1/1/1
48	CDL	g	3004	-	-	0/57/57/110	0/0/0/0

The worst 5 of 125 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	1	441	NAI	C2B-C1B	-9.32	1.38	1.53
49	L	516	HEA	C3A-C2A	-7.06	1.31	1.40
47	d	501	HEC	C3C-C2C	-6.16	1.34	1.40
47	D	501	HEC	C3B-C2B	-5.94	1.34	1.40
40	1	441	NAI	C2B-C3B	-5.72	1.38	1.53

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	1	441	NAI	N3A-C2A-N1A	-9.78	121.19	128.87
47	D	501	HEC	CBB-CAB-C3B	-8.90	107.89	127.34
47	d	501	HEC	CBB-CAB-C3B	-8.75	108.22	127.34
47	D	501	HEC	CBC-CAC-C3C	-8.03	109.79	127.34
45	c	3001	SMA	C9-C10-C11	-7.19	105.90	114.79

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
49	L	516	HEA	ND
49	L	516	HEA	NA

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Mol	Chain	Res	Type	Atom
49	L	516	HEA	NB
49	L	515	HEA	ND
49	L	515	HEA	NA

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	1	440	FMN	6	0
40	1	441	NAI	6	0
38	3	784	SF4	1	0
38	3	785	SF4	1	0
38	3	786	SF4	1	0
42	3	787	FES	1	0
38	6	182	SF4	1	0
38	8	183	SF4	2	0
45	C	2001	SMA	1	0
46	C	2002	UQ1	2	0
44	C	501	HEM	2	0
44	C	502	HEM	3	0
47	D	501	HEC	6	0
48	G	2004	CDL	5	0
49	L	515	HEA	3	0
49	L	516	HEA	4	0
44	Y	500	HEM	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.