



## wwPDB EM Map/Model Validation Report ⓘ

Sep 27, 2016 – 07:43 PM EDT

PDB ID : 5J8K  
EMDB ID: : EMD-8129  
Title : Architecture of supercomplex I-III<sub>2</sub>  
Authors : Letts, J.A.; Fiedorczuk, K.; Sazanov, L.A.  
Deposited on : 2016-04-08  
Resolution : 7.80 Å(reported)

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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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-20027939

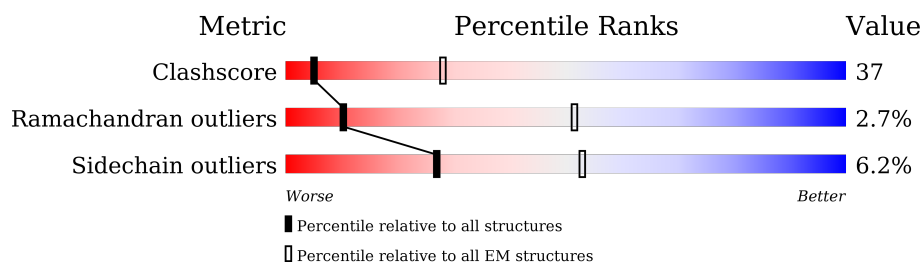
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.80 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.













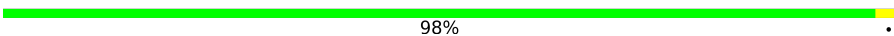







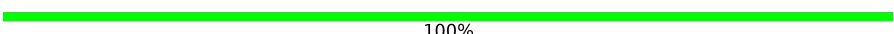
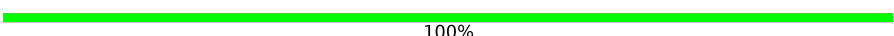

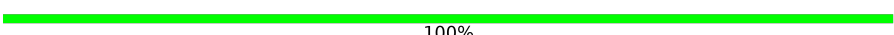
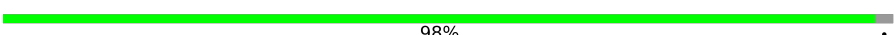
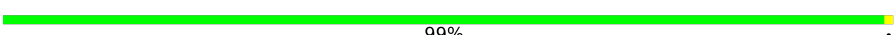

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	102	78% 22%
2	B	154	55% 45% .
3	C	194	59% 40% .
4	D	384	68% 32%
5	E	189	70% 30%
6	F	429	62% 37%
7	G	652	65% 34% .
8	H	297	69% 31%
9	I	171	61% 36% ..

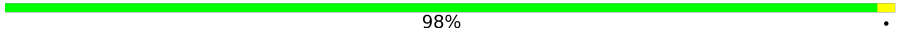

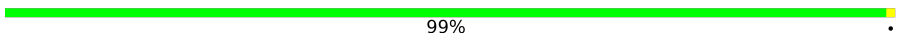
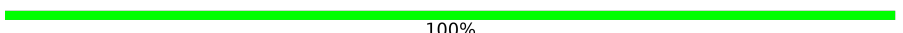
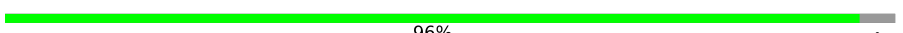






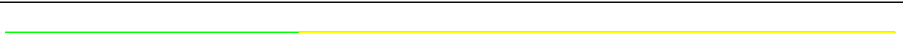



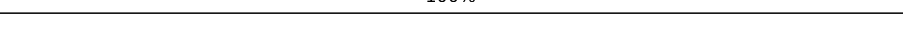
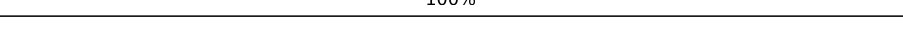
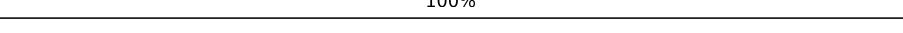
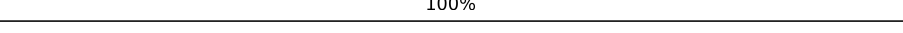
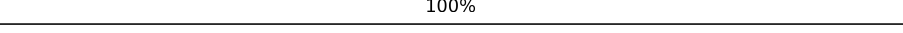
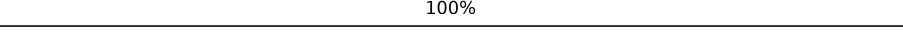




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Mol	Chain	Length	Quality of chain
10	J	171	
11	K	93	
12	L	575	
13	M	455	
14	N	345	
15	O	104	
16	P	85	
17	Q	66	
18	R	29	
19	S	80	
19	d	80	
20	T	53	
21	U	96	
22	V	112	
23	W	103	
24	X	309	
25	Y	322	
26	Z	119	
27	a	111	
28	b	92	
29	c	79	
30	e	55	
31	f	59	
32	g	130	
33	9	63	









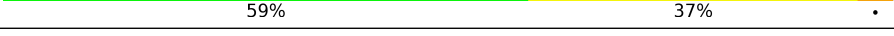

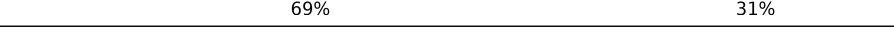
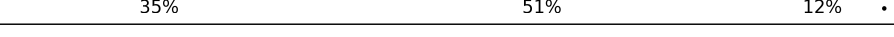

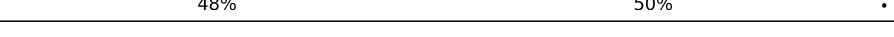



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Mol	Chain	Length	Quality of chain
33	h	63	 98%
33	z	63	 40% 59%
34	i	70	 99%
35	j	44	 100%
36	k	83	 96%
37	0	36	 83% 17%
38	1	30	 83% 17%
39	2	38	 74% 26%
40	3	28	 86% 14%
40	4	28	 79% 21%
41	5	34	 82% 18%
42	6	21	 33% 67%
43	7	39	 82% 18%
44	8	27	 67% 33%
45	y	46	 100%
46	x	13	 100%
47	w	24	 100%
48	v	18	 100%
49	u	16	 100%
50	t	12	 100%
51	AA	446	 49% 48%
51	AL	446	 50% 47%
52	AB	423	 51% 47%
52	AM	423	 52% 46%
53	AC	378	 58% 40%

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Mol	Chain	Length	Quality of chain
53	AN	378	
54	AD	241	
54	AO	241	
55	AE	196	
55	AP	196	
56	AF	105	
56	AQ	105	
57	AG	75	
57	AR	75	
58	AH	67	
58	AS	67	
59	AI	57	
59	AT	57	
60	AJ	60	
60	AU	60	
61	AK	51	
61	AV	51	

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
62	SF4	F	500	-	-	X	-
62	SF4	G	802	-	-	X	-
62	SF4	I	201	-	-	X	-
62	SF4	I	202	-	-	X	-
63	FES	E	201	-	-	X	-

## 2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 55850 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 COMPLEX I ND3.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	102	Total	C	N	O	0	0
			510	306	102	102		

- Molecule 2 is a protein called COMPLEX I PSST/NDUFS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	154	Total	C	N	O	S	0	0
			774	462	154	154	4		

- Molecule 3 is a protein called COMPLEX I 30KDA/NDUFS3.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	194	Total	C	N	O	0	0
			970	582	194	194		

- Molecule 4 is a protein called COMPLEX I 49KDA/NDUFS2.

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

- Molecule 5 is a protein called COMPLEX I 24KDA/NDUFV2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	189	Total	C	N	O	S	0	0
			949	567	189	189	4		

- Molecule 6 is a protein called COMPLEX I 51KDA/NDUFV1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	429	Total	C	N	O	S	0	0
			2149	1287	429	429	4		

- Molecule 7 is a protein called COMPLEX I 75KDA/NDUFS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	652	Total	C	N	O	S	0	0
			3276	1959	654	652	11		

- Molecule 8 is a protein called COMPLEX I ND1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	297	Total	C	N	O		0	0
			1485	891	297	297			

- Molecule 9 is a protein called COMPLEX I TYKY/NDUFS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	171	Total	C	N	O	S	0	0
			863	513	171	171	8		

- Molecule 10 is a protein called COMPLEX I ND6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	139	Total	C	N	O		0	0
			695	417	139	139			

- Molecule 11 is a protein called COMPLEX I ND4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	93	Total	C	N	O		0	0
			465	279	93	93			

- Molecule 12 is a protein called COMPLEX I ND5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	575	Total	C	N	O		0	0
			2875	1725	575	575			

- Molecule 13 is a protein called COMPLEX I ND4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	455	Total	C	N	O		0	0
			2275	1365	455	455			

- Molecule 14 is a protein called COMPLEX I ND2.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	345	Total	C	N	O	0	0
			1725	1035	345	345		

- Molecule 15 is a protein called COMPLEX I 18KDA/NDUFS6.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	104	Total	C	N	O	0	0
			520	312	104	104		

- Molecule 16 is a protein called COMPLEX I 13KDA/NDUFS6.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	85	Total	C	N	O	0	0
			425	255	85	85		

- Molecule 17 is a protein called COMPLEX I 15KDA/NDUFS5.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	66	Total	C	N	O	0	0
			330	198	66	66		

- Molecule 18 is a protein called COMPLEX I MWFE/NDUFA1.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	29	Total	C	N	O	0	0
			145	87	29	29		

- Molecule 19 is a protein called COMPLEX I B8/NDUFA2.

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

- Molecule 20 is a protein called COMPLEX I B9/NDUFA3.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	T	53	Total	C	N	O	0	0
			265	159	53	53		

- Molecule 21 is a protein called COMPLEX I B13/NDUFA5.



Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	96	Total	C	N	O	0	0
			480	288	96	96		

- Molecule 22 is a protein called COMPLEX I B14/NDUFA6.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	V	112	Total	C	N	O	0	0
			560	336	112	112		

- Molecule 23 is a protein called COMPLEX I PGIV/NDUFA8.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	W	103	Total	C	N	O	0	0
			515	309	103	103		

- Molecule 24 is a protein called COMPLEX I 39KDA/NDUFA9.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	258	Total	C	N	O	0	0
			1290	774	258	258		

- Molecule 25 is a protein called COMPLEX I 42KDA/NDUFA10.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	322	Total	C	N	O	0	0
			1595	951	322	322		

- Molecule 26 is a protein called COMPLEX I B14.7/NDUFA11.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Z	119	Total	C	N	O	0	0
			595	357	119	119		

- Molecule 27 is a protein called COMPLEX I B17.2/NDUFA12.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	a	111	Total	C	N	O	0	0
			555	333	111	111		

- Molecule 28 is a protein called COMPLEX I B16.6/NDUFA13.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	b	92	Total	C	N	O	0	0
			460	276	92	92		

- Molecule 29 is a protein called COMPLEX I SDAP/NDUFAB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	c	71	Total	C	N	O	0	0
			355	213	71	71		

- Molecule 30 is a protein called COMPLEX I B15/NDUFB4.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	e	55	Total	C	N	O	0	0
			275	165	55	55		

- Molecule 31 is a protein called COMPLEX I B18/NDUFB7.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	f	58	Total	C	N	O	0	0
			290	174	58	58		

- Molecule 32 is a protein called COMPLEX I B22/NDUFB9.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	g	130	Total	C	N	O	0	0
			650	390	130	130		

- Molecule 33 is a protein called COMPLEX I PDSW/NDUFB10.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	h	63	Total	C	N	O	0	0
			315	189	63	63		
33	9	63	Total	C	N	O	0	0
			315	189	63	63		
33	z	26	Total	C	N	O	0	0
			130	78	26	26		

- Molecule 34 is a protein called COMPLEX I ESSS/NDUFB11.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	i	70	Total	C	N	O	0	0
			350	210	70	70		

- Molecule 35 is a protein called COMPLEX I KFYI/NDUFC1.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	j	44	Total	C	N	O	0	0
			220	132	44	44		

- Molecule 36 is a protein called COMPLEX I B14.5B/NDUFC2.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	k	80	Total	C	N	O	0	0
			400	240	80	80		

- Molecule 37 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	0	36	Total	C	N	O	0	0
			180	108	36	36		

- Molecule 38 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	1	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 39 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	2	38	Total	C	N	O	0	0
			190	114	38	38		

- Molecule 40 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	3	28	Total	C	N	O	0	0
			140	84	28	28		
40	4	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 41 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	5	34	Total	C	N	O	0	0
			170	102	34	34		

- Molecule 42 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	6	21	Total	C	N	O	0	0
			105	63	21	21		

- Molecule 43 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	7	39	Total	C	N	O	0	0
			195	117	39	39		

- Molecule 44 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	8	27	Total	C	N	O	0	0
			135	81	27	27		

- Molecule 45 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 11.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	y	46	Total	C	N	O	0	0
			230	138	46	46		

- Molecule 46 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	x	13	Total	C	N	O	0	0
			65	39	13	13		

- Molecule 47 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 13.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	w	24	Total	C	N	O	0	0
			120	72	24	24		

- Molecule 48 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	v	18	Total	C	N	O	0	0
			90	54	18	18		

- Molecule 49 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	u	16	Total	C	N	O	0	0
			80	48	16	16		

- Molecule 50 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 16.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	t	12	Total	C	N	O	0	0
			60	36	12	12		

- Molecule 51 is a protein called COMPLEX III SUBUNIT 1 / CORE 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	AA	446	Total	C	N	O	0	0
			2198	1306	446	446		
51	AL	446	Total	C	N	O	0	0
			2198	1306	446	446		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	241	ILE	LEU	conflict	UNP W5Q5G6
AA	242	ARG	CYS	conflict	UNP W5Q5G6
AA	244	ARG	PRO	conflict	UNP W5Q5G6
AA	245	GLU	TRP	conflict	UNP W5Q5G6
AA	246	ASP	GLY	conflict	UNP W5Q5G6
AA	?	-	ALA	deletion	UNP W5Q5G6
AA	?	-	VAL	deletion	UNP W5Q5G6
AA	?	-	PRO	deletion	UNP W5Q5G6
AA	249	PRO	GLN	conflict	UNP W5Q5G6
AA	251	ALA	TRP	conflict	UNP W5Q5G6
AA	254	ALA	PRO	conflict	UNP W5Q5G6
AA	255	ILE	PHE	conflict	UNP W5Q5G6
AA	256	ALA	GLN	conflict	UNP W5Q5G6
AA	257	VAL	ILE	conflict	UNP W5Q5G6
AA	258	GLU	ARG	conflict	UNP W5Q5G6
AA	259	GLY	HIS	conflict	UNP W5Q5G6
AL	241	ILE	LEU	conflict	UNP W5Q5G6
AL	242	ARG	CYS	conflict	UNP W5Q5G6
AL	244	ARG	PRO	conflict	UNP W5Q5G6
AL	245	GLU	TRP	conflict	UNP W5Q5G6
AL	246	ASP	GLY	conflict	UNP W5Q5G6
AL	?	-	ALA	deletion	UNP W5Q5G6
AL	?	-	VAL	deletion	UNP W5Q5G6

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Chain	Residue	Modelled	Actual	Comment	Reference
AL	?	-	PRO	deletion	UNP W5Q5G6
AL	249	PRO	GLN	conflict	UNP W5Q5G6
AL	251	ALA	TRP	conflict	UNP W5Q5G6
AL	254	ALA	PRO	conflict	UNP W5Q5G6
AL	255	ILE	PHE	conflict	UNP W5Q5G6
AL	256	ALA	GLN	conflict	UNP W5Q5G6
AL	257	VAL	ILE	conflict	UNP W5Q5G6
AL	258	GLU	ARG	conflict	UNP W5Q5G6
AL	259	GLY	HIS	conflict	UNP W5Q5G6

- Molecule 52 is a protein called COMPLEX III SUBUNIT 2 / CORE 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	AB	423	Total	C	N	O	0	0
			2081	1235	423	423		
52	AM	423	Total	C	N	O	0	0
			2081	1235	423	423		

- Molecule 53 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	AC	378	Total	C	N	O	0	0
			1866	1110	378	378		
53	AN	378	Total	C	N	O	0	0
			1866	1110	378	378		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	185	SER	PHE	conflict	UNP P24959
AC	295	ILE	VAL	conflict	UNP P24959
AC	303	LEU	ILE	conflict	UNP P24959
AC	359	ILE	PHE	conflict	UNP P24959
AC	361	LEU	ILE	conflict	UNP P24959
AC	363	MET	LEU	conflict	UNP P24959
AN	185	SER	PHE	conflict	UNP P24959
AN	295	ILE	VAL	conflict	UNP P24959
AN	303	LEU	ILE	conflict	UNP P24959
AN	359	ILE	PHE	conflict	UNP P24959
AN	361	LEU	ILE	conflict	UNP P24959
AN	363	MET	LEU	conflict	UNP P24959

- Molecule 54 is a protein called COMPLEX III SUBUNIT 4 / CYTOCHROME C1.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	AD	241	Total	C	N	O	0	0
			1188	706	241	241		
54	AO	241	Total	C	N	O	0	0
			1188	706	241	241		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AD	139	THR	-	insertion	UNP W5Q0A9
AD	140	GLY	ARG	conflict	UNP W5Q0A9
AO	139	THR	-	insertion	UNP W5Q0A9
AO	140	GLY	ARG	conflict	UNP W5Q0A9

- Molecule 55 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	AE	196	Total	C	N	O	0	0
			967	575	196	196		
55	AP	196	Total	C	N	O	0	0
			967	575	196	196		

- Molecule 56 is a protein called COMPLEX III SUBUNIT 7 / 14KDA.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	AF	105	Total	C	N	O	0	0
			522	312	105	105		
56	AQ	105	Total	C	N	O	0	0
			522	312	105	105		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AF	56	ASP	ASN	conflict	UNP W5P642
AF	108	ALA	THR	conflict	UNP W5P642
AQ	56	ASP	ASN	conflict	UNP W5P642
AQ	108	ALA	THR	conflict	UNP W5P642

- Molecule 57 is a protein called COMPLEX III SUBUNIT 8 / QP-C.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	AG	75	Total	C	N	O	0	0
			371	221	75	75		
57	AR	75	Total	C	N	O	0	0
			371	221	75	75		

- Molecule 58 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	AH	67	Total	C	N	O	0	0
			335	201	67	67		
58	AS	67	Total	C	N	O	0	0
			335	201	67	67		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
59	AI	57	Total	C	N	O	0	0
			281	167	57	57		
59	AT	57	Total	C	N	O	0	0
			281	167	57	57		

- Molecule 60 is a protein called COMPLEX III SUBUNIT 9 / 7.2KDA.

Mol	Chain	Residues	Atoms				AltConf	Trace
60	AJ	60	Total	C	N	O	0	0
			297	177	60	60		
60	AU	60	Total	C	N	O	0	0
			297	177	60	60		

- Molecule 61 is a protein called COMPLEX III SUBUNIT 10 / 6.4KDA.

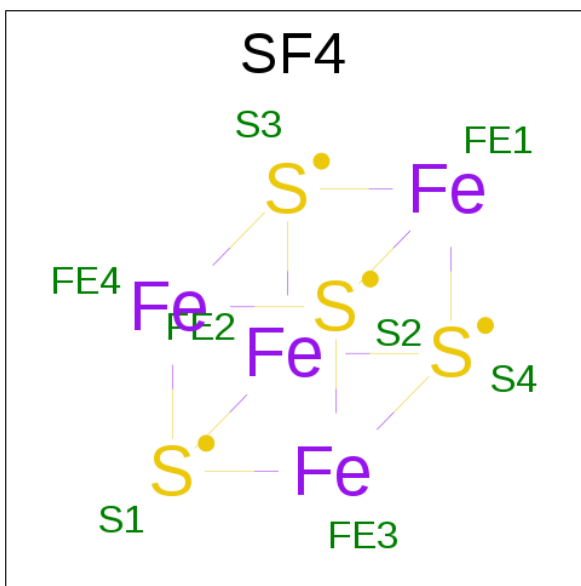
Mol	Chain	Residues	Atoms				AltConf	Trace
61	AK	51	Total	C	N	O	0	0
			250	148	51	51		
61	AV	51	Total	C	N	O	0	0
			250	148	51	51		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AK	22	GLN	SER	conflict	UNP W5PSD1
AV	22	GLN	SER	conflict	UNP W5PSD1

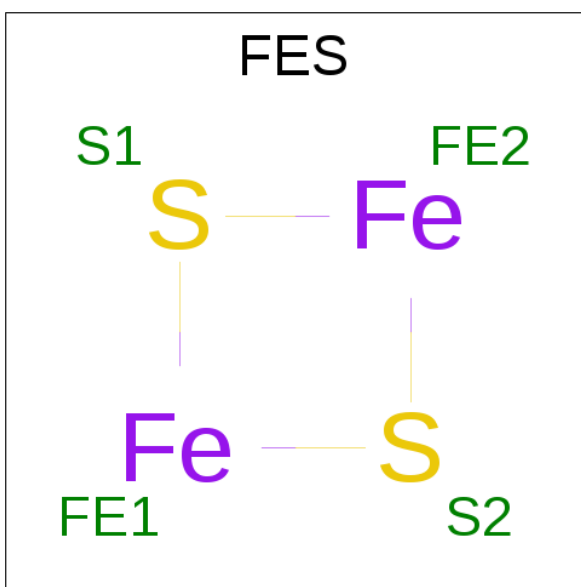


- Molecule 62 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



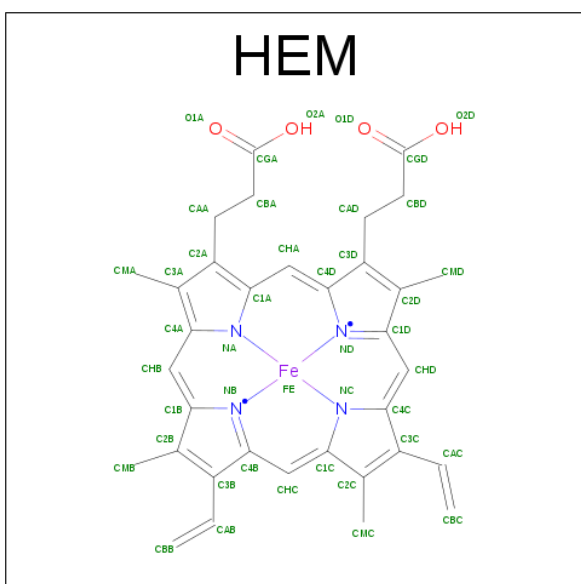
Mol	Chain	Residues	Atoms			AltConf
62	B	1	Total	Fe	S	0
			8	4	4	
62	F	1	Total	Fe	S	0
			8	4	4	
62	G	1	Total	Fe	S	0
			16	8	8	
62	G	1	Total	Fe	S	0
			16	8	8	
62	I	1	Total	Fe	S	0
			16	8	8	
62	I	1	Total	Fe	S	0
			16	8	8	

- Molecule 63 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



Mol	Chain	Residues	Atoms			AltConf
63	E	1	Total	Fe	S	0
			4	2	2	
63	G	1	Total	Fe	S	0
			4	2	2	
63	AE	1	Total	Fe	S	0
			4	2	2	
63	AP	1	Total	Fe	S	0
			4	2	2	

- Molecule 64 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).




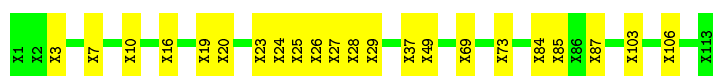
Mol	Chain	Residues	Atoms					AltConf
64	AC	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
64	AC	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
64	AD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
64	AN	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
64	AN	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
64	AO	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

### 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.

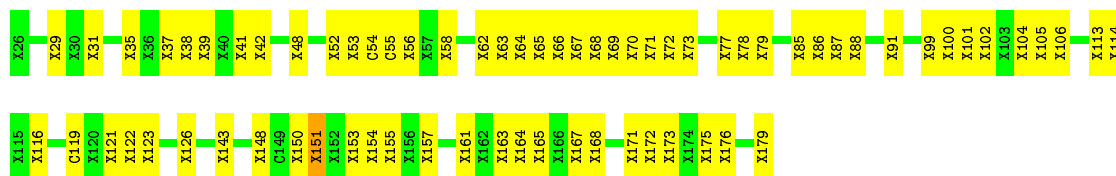
- Molecule 1: COMPLEX I ND3

Chain A: 



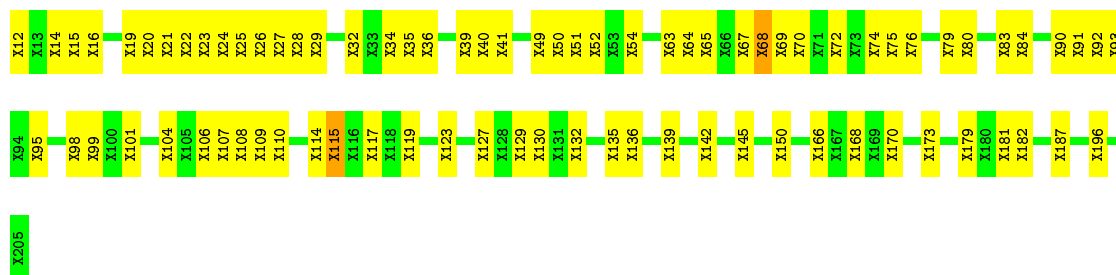
- Molecule 2: COMPLEX I PSST/NDUFS7

Chain B: 



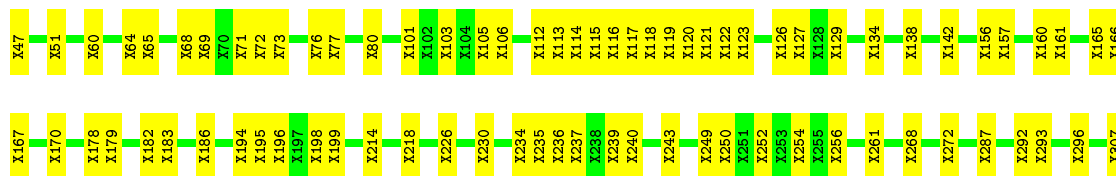
- Molecule 3: COMPLEX I 30KDA/NDUFS3

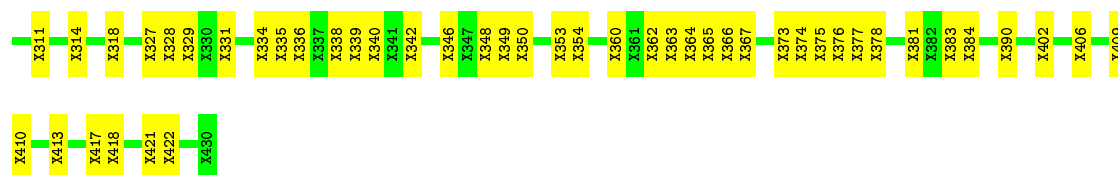
Chain C: 



- Molecule 4: COMPLEX I 49KDA/NDUFS2

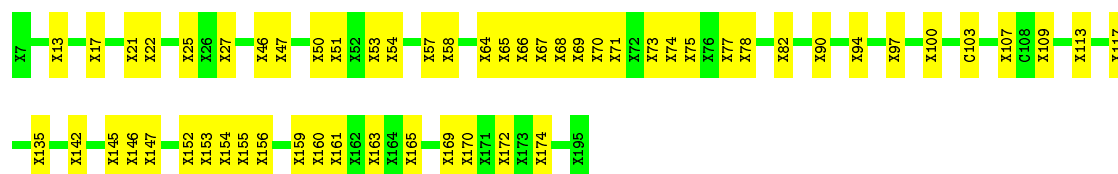
Chain D: 





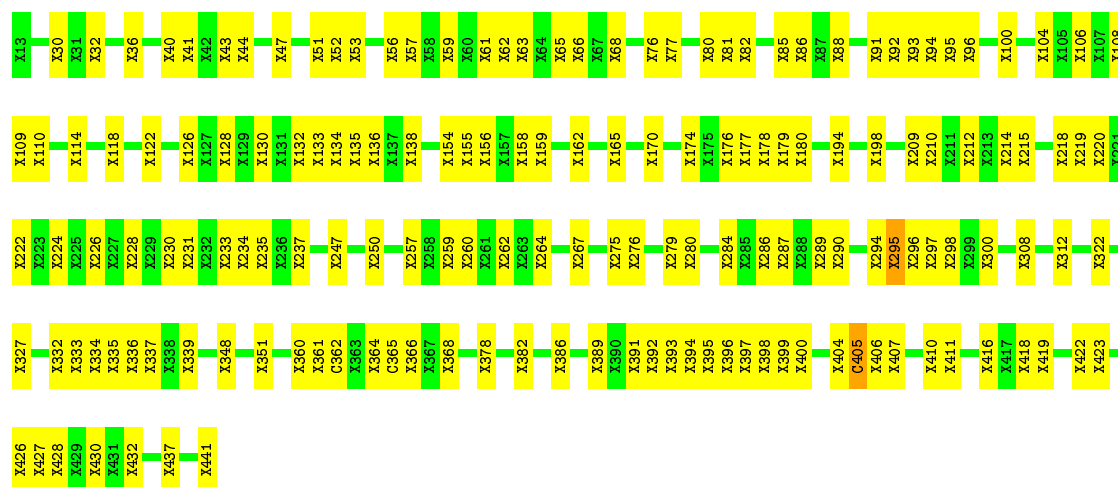
• Molecule 5: COMPLEX I 24KDA/NDUFV2

Chain E: 70% 30%



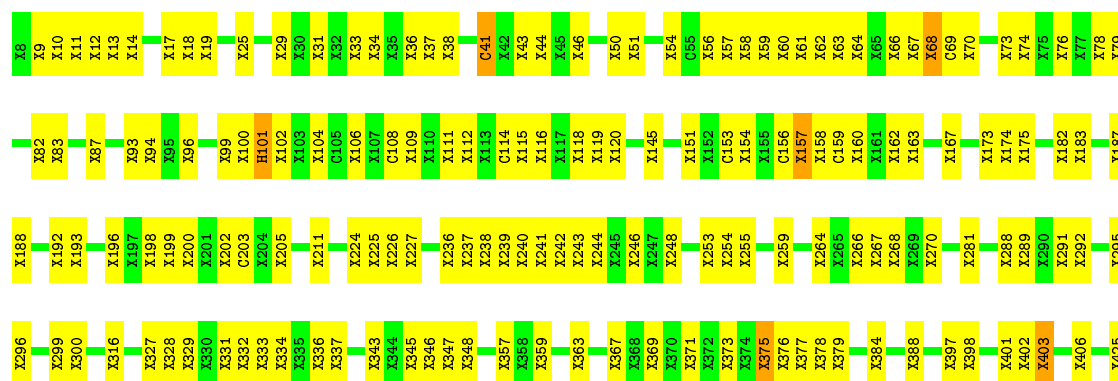
• Molecule 6: COMPLEX I 51KDA/NDUFV1

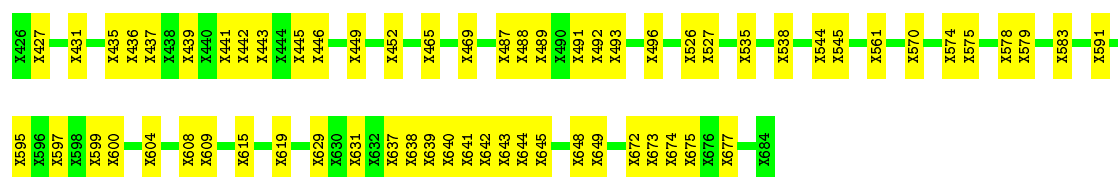
Chain F: 62% 37%



• Molecule 7: COMPLEX I 75KDA/NDUF81

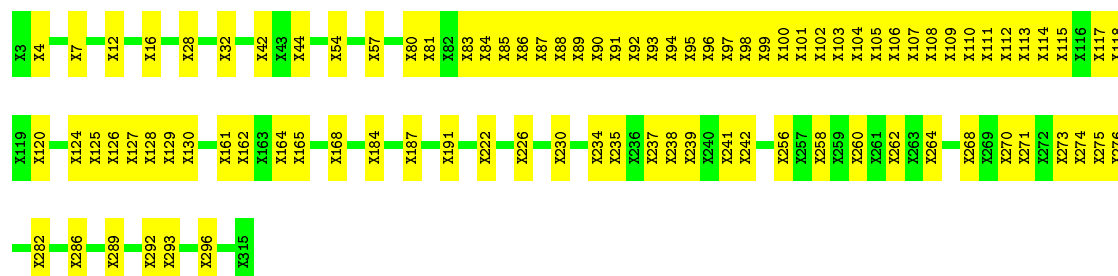
Chain G: 65% 34%





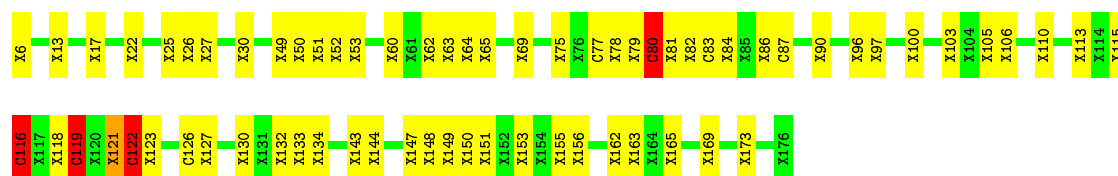
- Molecule 8: COMPLEX I ND1

Chain H: 69% 31%



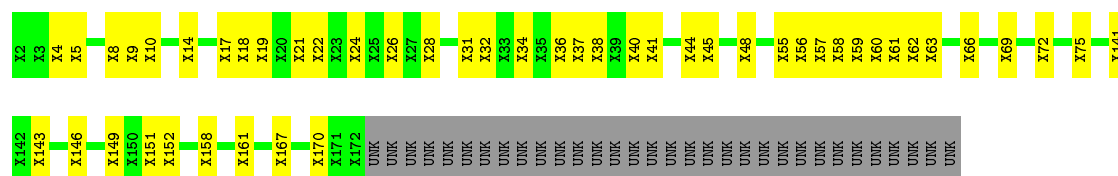
- Molecule 9: COMPLEX I TYKY/NDUFS8

Chain I: 61% 36% ..



- Molecule 10: COMPLEX I ND6

Chain J: 53% 28% 19%



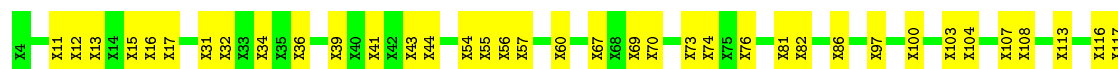
- Molecule 11: COMPLEX I ND4L

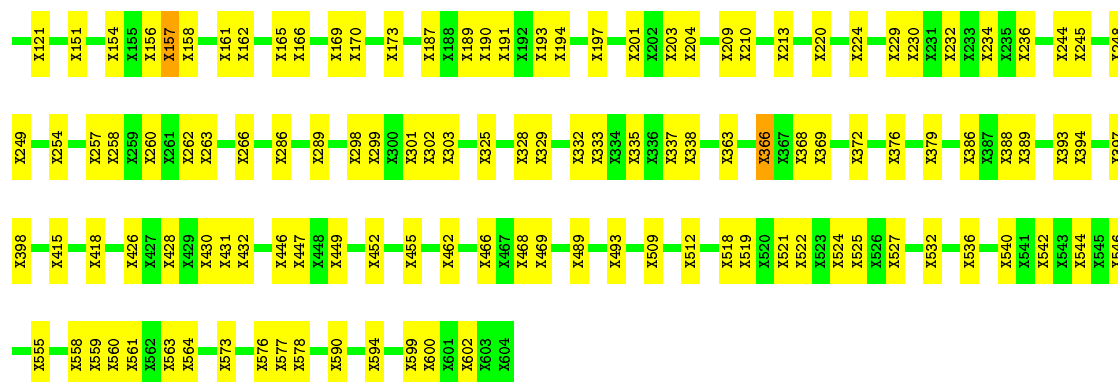
Chain K: 72% 28%



- Molecule 12: COMPLEX I ND5

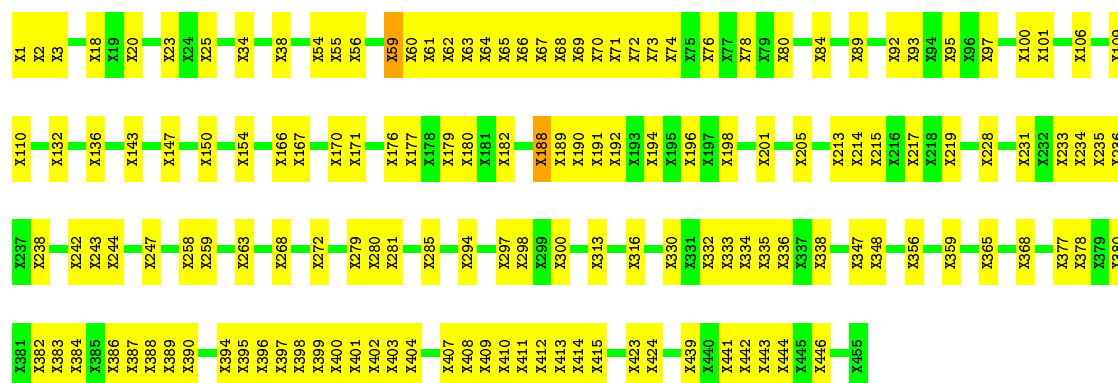
Chain L: 72% 27%





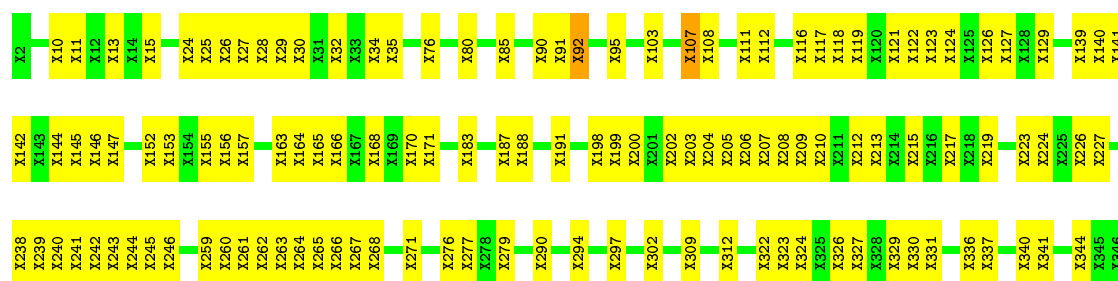
• Molecule 13: COMPLEX I ND4

Chain M: 67% 33%



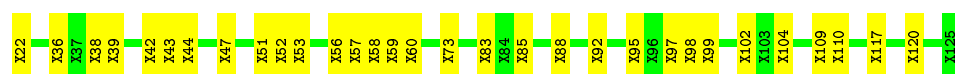
• Molecule 14: COMPLEX I ND2

Chain N: 64% 35%



• Molecule 15: COMPLEX I 18KDA/NDUFS6

Chain O: 70% 30%



• Molecule 16: COMPLEX I 13KDA/NDUFS6

Chain P: 72% 28%



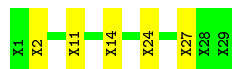
- Molecule 17: COMPLEX I 15KDA/NDUFS5

Chain Q: 64% 36%



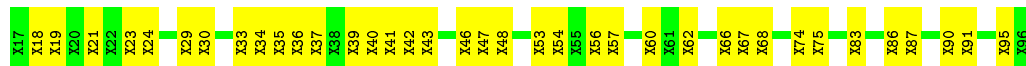
- Molecule 18: COMPLEX I MWFE/NDUFA1

Chain R: 83% 17%



- Molecule 19: COMPLEX I B8/NDUFA2

Chain S: 54% 46%



- Molecule 19: COMPLEX I B8/NDUFA2

Chain d: 98% 2%



- Molecule 20: COMPLEX I B9/NDUFA3

Chain T: 75% 25%



- Molecule 21: COMPLEX I B13/NDUFA5

Chain U: 92% 8%




- Molecule 22: COMPLEX I B14/NDUFA6

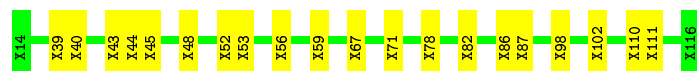
Chain V: 74% 25%





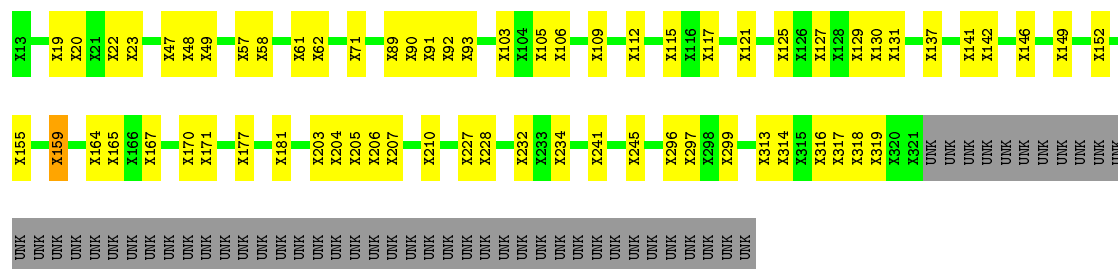
- Molecule 23: COMPLEX I PGIV/NDUFA8

Chain W:  81% 19%



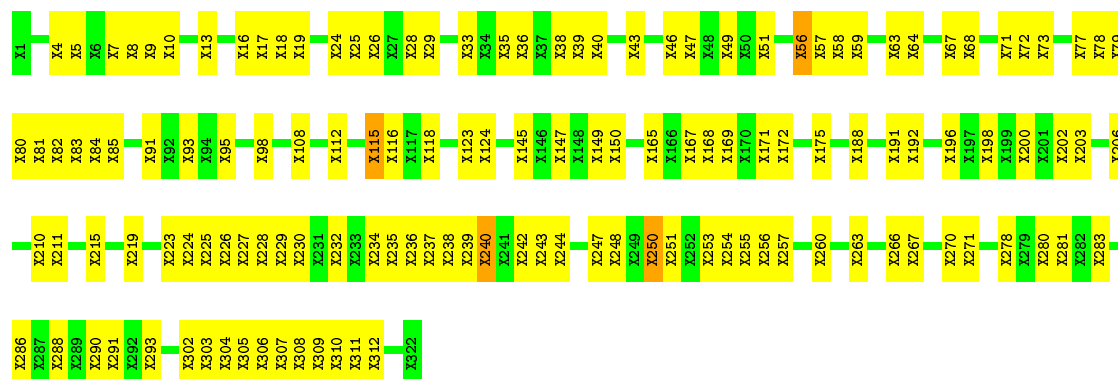
- Molecule 24: COMPLEX I 39KDA/NDUFA9

Chain X:  62% 21% 17%




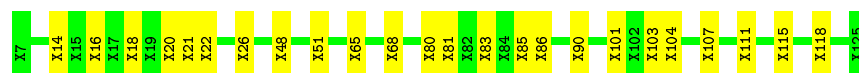
- Molecule 25: COMPLEX I 42KDA/NDUFA10

Chain Y:  58% 41% .



- Molecule 26: COMPLEX I B14.7/NDUFA11

Chain Z:  80% 20%



- Molecule 27: COMPLEX I B17.2/NDUFA12

Chain a:  100%

There are no outlier residues recorded for this chain.

- Molecule 28: COMPLEX I B16.6/NDUFA13

There are no outlier residues recorded for this chain.

- There are no outlier residues recorded for this chain.

- [illegible]

- Molecule 34: COMPLEX I ESSS/NDUFB11

Chain i:  99%



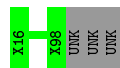
- Molecule 35: COMPLEX I KFYI/NDUFC1

Chain j:  100%


There are no outlier residues recorded for this chain.

- Molecule 36: COMPLEX I B14.5B/NDUFC2

Chain k:  96%




- Molecule 37: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 1

Chain 0:  83% 17%



- Molecule 38: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 2

Chain 1:  83% 17%




- Molecule 39: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 3

Chain 2:  74% 26%




- Molecule 40: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 4

Chain 3:  86% 14%



- Molecule 40: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 4

Chain 4:  79% 21%



- Molecule 41: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 5

Chain 5: 82% 18%



- Molecule 42: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 6

Chain 6: 33% 67%



- Molecule 43: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 7

Chain 7: 82% 18%



- Molecule 44: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 8

Chain 8: 67% 33%



- Molecule 45: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 11

Chain y: 100%

There are no outlier residues recorded for this chain.

- Molecule 46: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 12

Chain x: 100%

There are no outlier residues recorded for this chain.

- Molecule 47: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 13

Chain w: 100%

There are no outlier residues recorded for this chain.

- Molecule 48: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 14

Chain v: 100%

There are no outlier residues recorded for this chain.

- Molecule 49: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 15

Chain u:  100%

There are no outlier residues recorded for this chain.

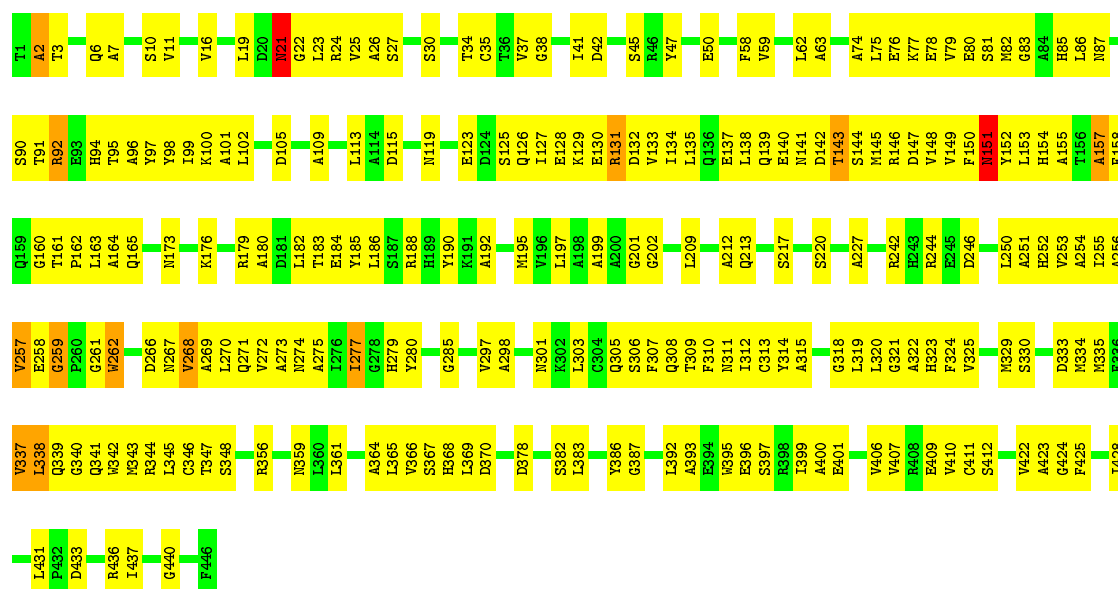
- Molecule 50: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 16

Chain t:  100%

There are no outlier residues recorded for this chain.

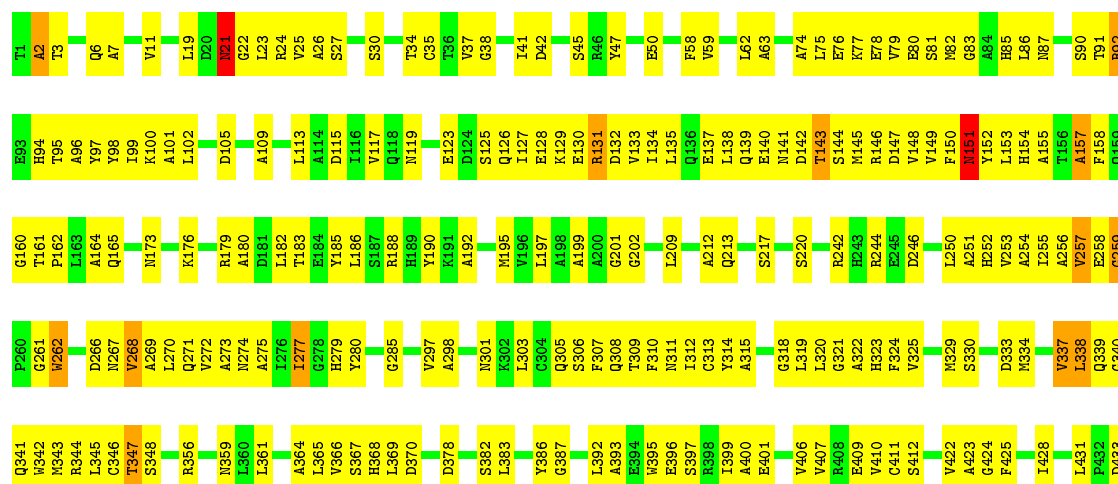
- Molecule 51: COMPLEX III SUBUNIT 1 / CORE 1

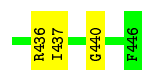
Chain AA:  49% 48%



- Molecule 51: COMPLEX III SUBUNIT 1 / CORE 1

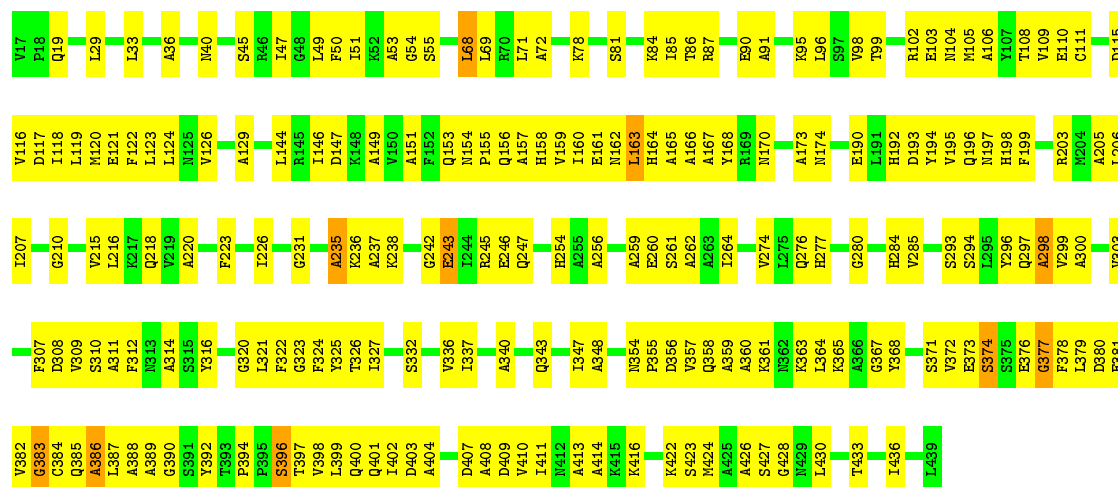
Chain AL:  50% 47%





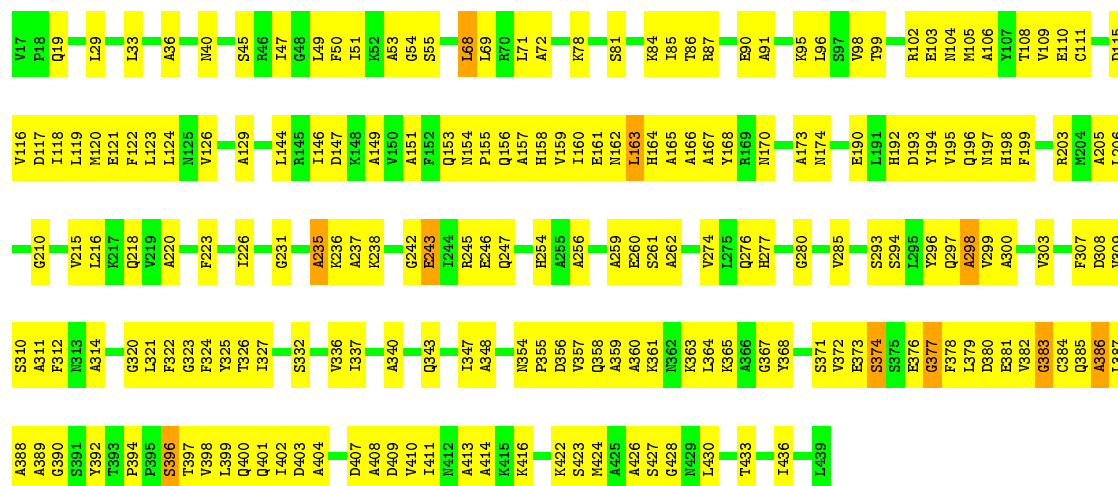
• Molecule 52: COMPLEX III SUBUNIT 2 / CORE 2

Chain AB: 51% 47%



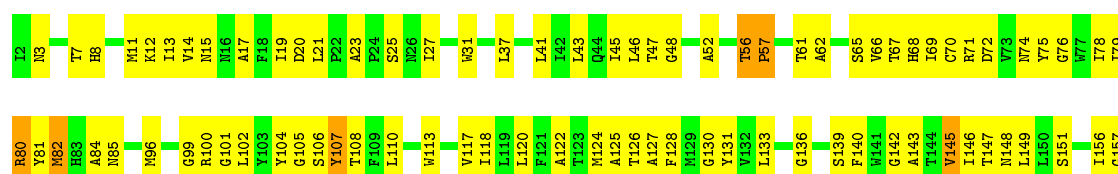
• Molecule 52: COMPLEX III SUBUNIT 2 / CORE 2

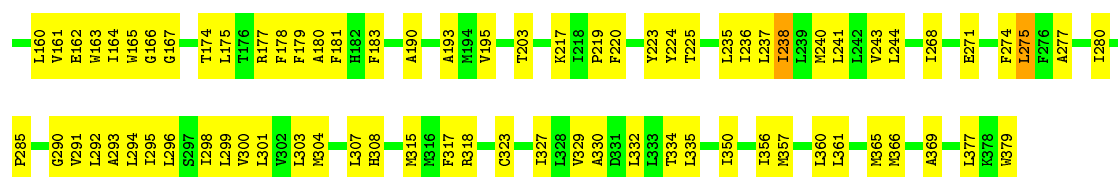
Chain AM: 52% 46%



• Molecule 53: Cytochrome b

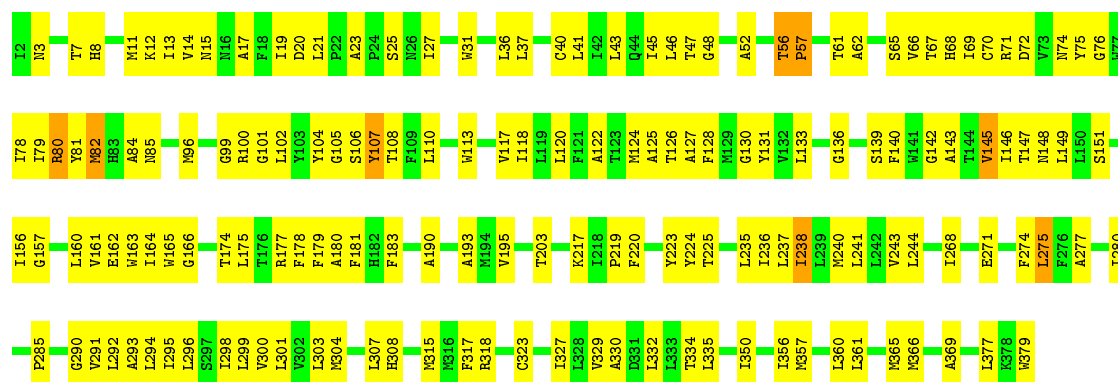
Chain AC: 58% 40%





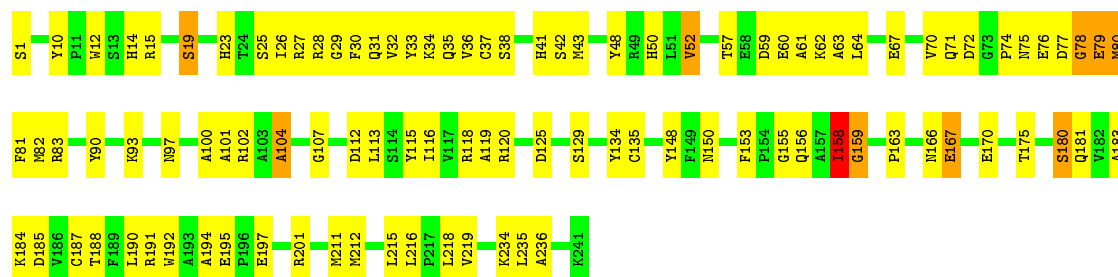
• Molecule 53: Cytochrome b

Chain AN: 58% 40%



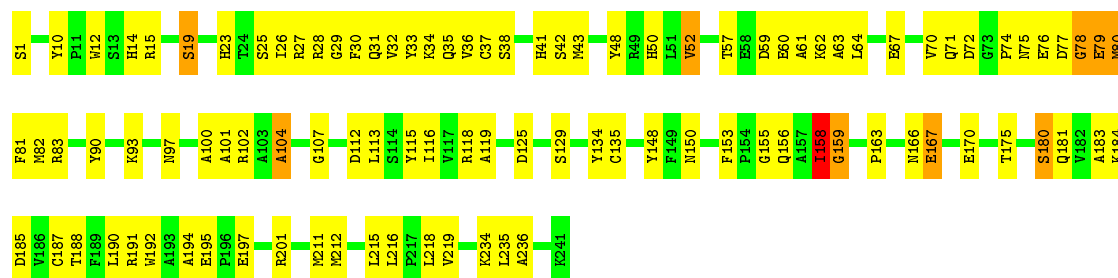
• Molecule 54: COMPLEX III SUBUNIT 4 / CYTOCHROME C1

Chain AD: 58% 38%



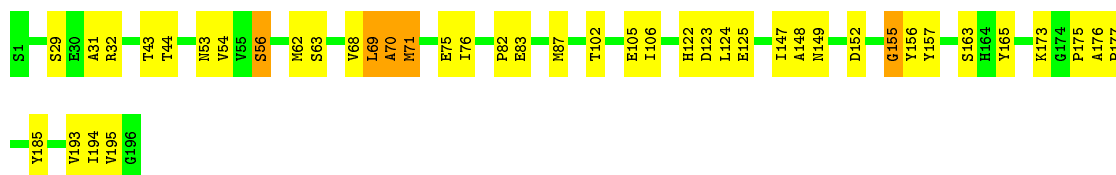
• Molecule 54: COMPLEX III SUBUNIT 4 / CYTOCHROME C1

Chain AO: 58% 38%



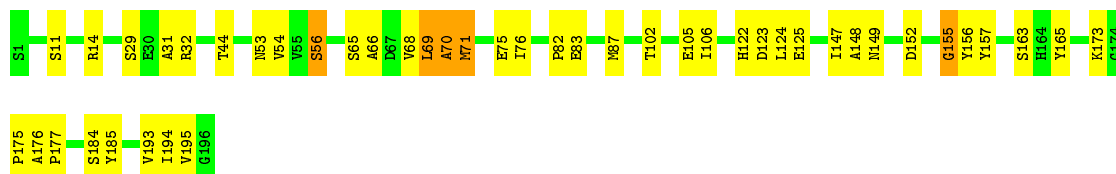
• Molecule 55: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AE: 78% 19%



- Molecule 55: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AP: 77% 20%



- Molecule 56: COMPLEX III SUBUNIT 7 / 14KDA

Chain AF: 53% 42%



- Molecule 56: COMPLEX III SUBUNIT 7 / 14KDA

Chain AQ: 53% 42%



- Molecule 57: COMPLEX III SUBUNIT 8 / QP-C

Chain AG: 59% 37%




- Molecule 57: COMPLEX III SUBUNIT 8 / QP-C

Chain AR: 59% 37%



- Molecule 58: Cytochrome b-c1 complex subunit 6



Chain AH:  67% 33%



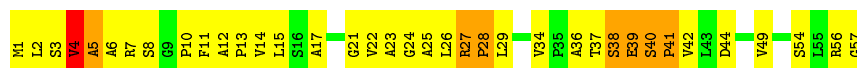
- Molecule 58: Cytochrome b-c1 complex subunit 6

Chain AS:  69% 31%



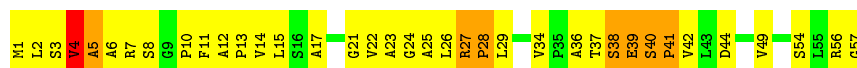
- Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AI:  35% 51% 12%



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

Chain AT:  35% 51% 12%



- Molecule 60: COMPLEX III SUBUNIT 9 / 7.2KDA

Chain AJ:  48% 50%




- Molecule 60: COMPLEX III SUBUNIT 9 / 7.2KDA

Chain AU:  52% 47%



- Molecule 61: COMPLEX III SUBUNIT 10 / 6.4KDA

Chain AK:  84% 16%



- Molecule 61: COMPLEX III SUBUNIT 10 / 6.4KDA

Chain AV:  88% 12%



## 4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images used	9844	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	47000	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: HEM, SF4, FES

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	$\# Z  > 2$
2	B	1.50	1/21 (4.8%)	0.85	0/23
5	E	0.76	0/20	0.79	0/20
51	AA	0.41	0/2197	0.68	3/3055 (0.1%)
51	AL	0.41	0/2197	0.67	3/3055 (0.1%)
52	AB	0.42	0/2080	0.66	1/2890 (0.0%)
52	AM	0.42	0/2080	0.65	1/2890 (0.0%)
53	AC	0.75	1/1865 (0.1%)	0.55	0/2595
53	AN	0.75	1/1865 (0.1%)	0.55	0/2595
54	AD	0.42	0/1187	0.69	1/1650 (0.1%)
54	AO	0.42	0/1187	0.69	1/1650 (0.1%)
55	AE	0.55	1/965 (0.1%)	1.17	2/1340 (0.1%)
55	AP	0.64	2/966 (0.2%)	1.19	3/1343 (0.2%)
56	AF	0.43	0/521	0.62	1/726 (0.1%)
56	AQ	0.43	0/521	0.62	1/726 (0.1%)
57	AG	0.38	0/370	0.52	0/514
57	AR	0.38	0/370	0.52	0/514
58	AH	0.37	0/334	0.47	0/466
58	AS	0.37	0/334	0.47	0/466
59	AI	0.50	0/280	1.17	4/388 (1.0%)
59	AT	0.50	0/280	1.17	4/388 (1.0%)
6	F	1.42	0/20	1.21	0/20
60	AJ	0.37	0/296	0.53	0/411
60	AU	0.37	0/296	0.53	0/411
61	AK	0.37	0/249	0.45	0/344
61	AV	0.38	0/249	0.45	0/344
7	G	0.82	0/65	1.24	2/67 (3.0%)
9	I	1.63	2/40 (5.0%)	2.16	2/40 (5.0%)
All	All	0.52	8/20855 (0.0%)	0.72	29/28931 (0.1%)

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
12	L	0	5
13	M	0	5
14	N	0	5
17	Q	0	1
18	R	0	1
19	d	0	2
2	B	0	2
22	V	0	1
23	W	0	1
24	X	0	3
25	Y	0	8
3	C	0	5
32	g	0	1
33	h	0	1
33	z	0	1
34	i	0	1
38	l	0	1
4	D	0	1
51	AA	0	13
51	AL	0	13
52	AB	0	17
52	AM	0	17
53	AC	0	2
53	AN	0	2
54	AD	0	8
54	AO	0	8
55	AE	0	3
55	AP	0	4
56	AF	0	5
56	AQ	0	5
57	AG	0	2
57	AR	0	2
59	AI	0	6
59	AT	0	6
6	F	0	3
60	AJ	0	1
60	AU	0	1
61	AK	0	1
61	AV	0	1
7	G	0	10
9	I	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	180

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	AC	56	THR	C-N	-26.50	0.83	1.34
53	AN	56	THR	C-N	-26.50	0.83	1.34
55	AP	44	THR	C-N	-10.59	1.09	1.34
9	I	122	CYS	CB-SG	-6.12	1.71	1.82
55	AP	56	SER	C-O	5.39	1.33	1.23

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	122	CYS	CA-CB-SG	-10.09	95.84	114.00
54	AO	159	GLY	N-CA-C	9.62	137.14	113.10
54	AD	159	GLY	N-CA-C	9.57	137.04	113.10
52	AB	231	GLY	N-CA-C	8.66	134.76	113.10
52	AM	231	GLY	N-CA-C	8.63	134.67	113.10

There are no chirality outliers.

5 of 180 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	151	UNK	Peptide
2	B	54	CYS	Peptide
3	C	115	UNK	Peptide
3	C	150	UNK	Peptide
3	C	68	UNK	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	510	0	109	17	0
2	B	774	0	177	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	970	0	232	56	0
4	D	1920	0	409	74	0
5	E	949	0	215	36	0
6	F	2149	0	466	97	0
7	G	3276	0	761	151	0
8	H	1485	0	307	69	0
9	I	863	0	207	55	0
10	J	695	0	144	32	0
11	K	465	0	100	14	0
12	L	2875	0	596	91	0
13	M	2275	0	466	93	0
14	N	1725	0	354	81	0
15	O	520	0	119	19	0
16	P	425	0	98	16	0
17	Q	330	0	69	15	0
18	R	145	0	31	2	0
19	S	400	0	82	24	0
19	d	400	0	87	0	0
20	T	265	0	55	7	0
21	U	480	0	107	4	0
22	V	560	0	119	15	0
23	W	515	0	111	10	0
24	X	1290	0	283	41	0
25	Y	1595	0	323	93	0
26	Z	595	0	124	15	0
27	a	555	0	129	0	0
28	b	460	0	103	0	0
29	c	355	0	76	0	0
30	e	275	0	58	0	0
31	f	290	0	61	0	0
32	g	650	0	136	0	0
33	9	315	0	70	5	0
33	h	315	0	65	0	0
33	z	130	0	29	0	0
34	i	350	0	81	0	0
35	j	220	0	47	0	0
36	k	400	0	86	0	0
37	0	180	0	39	3	0
38	1	150	0	32	2	0
39	2	190	0	41	5	0
40	3	140	0	33	2	0
40	4	140	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	5	170	0	37	4	0
42	6	105	0	23	9	0
43	7	195	0	42	22	0
44	8	135	0	29	5	0
45	y	230	0	48	0	0
46	x	65	0	15	0	0
47	w	120	0	27	0	0
48	v	90	0	20	0	0
49	u	80	0	18	0	0
50	t	60	0	15	0	0
51	AA	2198	0	1034	222	0
51	AL	2198	0	1034	198	0
52	AB	2081	0	1035	184	0
52	AM	2081	0	1035	182	0
53	AC	1866	0	827	128	0
53	AN	1866	0	827	123	0
54	AD	1188	0	533	100	0
54	AO	1188	0	533	99	0
55	AE	967	0	440	23	0
55	AP	967	0	440	21	0
56	AF	522	0	227	46	0
56	AQ	522	0	227	47	0
57	AG	371	0	162	22	0
57	AR	371	0	162	23	0
58	AH	335	0	141	13	0
58	AS	335	0	141	13	0
59	AI	281	0	142	37	0
59	AT	281	0	142	36	0
60	AJ	297	0	148	26	0
60	AU	297	0	148	24	0
61	AK	250	0	121	5	0
61	AV	250	0	121	4	0
62	B	8	0	0	1	0
62	F	8	0	0	3	0
62	G	16	0	0	5	0
62	I	16	0	0	14	0
63	AE	4	0	0	0	0
63	AP	4	0	0	0	0
63	E	4	0	0	3	0
63	G	4	0	0	1	0
64	AC	86	0	60	7	0
64	AD	43	0	30	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	AN	86	0	60	2	0
64	AO	43	0	30	11	0
All	All	55850	0	17341	2703	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 37.

The worst 5 of 2703 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)
54:AO:37:CYS:CA	64:AO:301:HEM:HAB	1.54	1.36
6:F:298:UNK:O	6:F:334:UNK:HA	1.35	1.25
52:AM:307:PHE:HA	52:AM:327:ILE:O	1.33	1.25
43:7:33:UNK:HA	51:AA:227:ALA:N	1.50	1.25
53:AC:56:THR:C	53:AC:57:PRO:CA	2.05	1.24

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	
2	B	4/154 (3%)	4 (100%)	0	0	100	100
5	E	4/189 (2%)	2 (50%)	2 (50%)	0	100	100
6	F	4/429 (1%)	4 (100%)	0	0	100	100
7	G	12/652 (2%)	6 (50%)	4 (33%)	2 (17%)	0	5
9	I	8/171 (5%)	4 (50%)	3 (38%)	1 (12%)	0	8
51	AA	444/446 (100%)	369 (83%)	68 (15%)	7 (2%)	12	56
51	AL	444/446 (100%)	370 (83%)	67 (15%)	7 (2%)	12	56
52	AB	421/423 (100%)	370 (88%)	46 (11%)	5 (1%)	16	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	AM	421/423 (100%)	369 (88%)	47 (11%)	5 (1%)	16	61
53	AC	376/378 (100%)	288 (77%)	73 (19%)	15 (4%)	4	35
53	AN	376/378 (100%)	287 (76%)	74 (20%)	15 (4%)	4	35
54	AD	239/241 (99%)	180 (75%)	52 (22%)	7 (3%)	6	43
54	AO	239/241 (99%)	180 (75%)	52 (22%)	7 (3%)	6	43
55	AE	192/196 (98%)	148 (77%)	36 (19%)	8 (4%)	3	34
55	AP	194/196 (99%)	151 (78%)	35 (18%)	8 (4%)	3	35
56	AF	103/105 (98%)	86 (84%)	17 (16%)	0	100	100
56	AQ	103/105 (98%)	86 (84%)	17 (16%)	0	100	100
57	AG	73/75 (97%)	59 (81%)	11 (15%)	3 (4%)	3	35
57	AR	73/75 (97%)	59 (81%)	11 (15%)	3 (4%)	3	35
58	AH	65/67 (97%)	53 (82%)	12 (18%)	0	100	100
58	AS	65/67 (97%)	53 (82%)	12 (18%)	0	100	100
59	AI	55/57 (96%)	31 (56%)	17 (31%)	7 (13%)	0	8
59	AT	55/57 (96%)	31 (56%)	17 (31%)	7 (13%)	0	8
60	AJ	58/60 (97%)	47 (81%)	10 (17%)	1 (2%)	11	55
60	AU	58/60 (97%)	47 (81%)	10 (17%)	1 (2%)	11	55
61	AK	49/51 (96%)	44 (90%)	4 (8%)	1 (2%)	9	51
61	AV	49/51 (96%)	44 (90%)	4 (8%)	1 (2%)	9	51
All	All	4184/5793 (72%)	3372 (81%)	701 (17%)	111 (3%)	10	45

5 of 111 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
51	AA	143	THR
52	AB	436	ILE
54	AD	79	GLU
55	AE	70	ALA
55	AE	177	PRO

### 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	
2	B	4/4 (100%)	4 (100%)	0	100	100
5	E	4/4 (100%)	4 (100%)	0	100	100
6	F	4/4 (100%)	4 (100%)	0	100	100
7	G	12/12 (100%)	12 (100%)	0	100	100
9	I	8/8 (100%)	6 (75%)	2 (25%)	1	6
All	All	32/32 (100%)	30 (94%)	2 (6%)	27	59

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	116	CYS
9	I	119	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
64	HEM	AC	401	-	24,50,50	3.40	13 (54%)	16,82,82	3.26	2 (12%)
64	HEM	AC	402	-	24,50,50	2.87	14 (58%)	16,82,82	2.78	8 (50%)
64	HEM	AD	301	-	24,50,50	3.21	15 (62%)	16,82,82	2.64	5 (31%)
63	FES	AE	201	-	0,4,4	0.00	-	0,4,4	0.00	-
64	HEM	AN	401	-	24,50,50	3.38	13 (54%)	16,82,82	3.26	2 (12%)
64	HEM	AN	402	-	24,50,50	2.87	14 (58%)	16,82,82	2.78	8 (50%)
64	HEM	AO	301	-	24,50,50	3.22	15 (62%)	16,82,82	2.64	5 (31%)
63	FES	AP	201	-	0,4,4	0.00	-	0,4,4	0.00	-
62	SF4	B	201	2	0,12,12	0.00	-	0,24,24	0.00	-
63	FES	E	201	5	0,4,4	0.00	-	0,4,4	0.00	-
62	SF4	F	500	6	0,12,12	0.00	-	0,24,24	0.00	-
62	SF4	G	801	7	0,12,12	0.00	-	0,24,24	0.00	-
62	SF4	G	802	7	0,12,12	0.00	-	0,24,24	0.00	-
63	FES	G	803	7	0,4,4	0.00	-	0,4,4	0.00	-
62	SF4	I	201	9	0,12,12	0.00	-	0,24,24	0.00	-
62	SF4	I	202	9	0,12,12	0.00	-	0,24,24	0.00	-

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
64	HEM	AC	401	-	-	0/6/54/54	0/0/8/8
64	HEM	AC	402	-	-	0/6/54/54	0/0/8/8
64	HEM	AD	301	-	-	0/6/54/54	0/0/8/8
63	FES	AE	201	-	-	0/0/4/4	0/1/1/1
64	HEM	AN	401	-	-	0/6/54/54	0/0/8/8
64	HEM	AN	402	-	-	0/6/54/54	0/0/8/8
64	HEM	AO	301	-	-	0/6/54/54	0/0/8/8
63	FES	AP	201	-	-	0/0/4/4	0/1/1/1
62	SF4	B	201	2	-	0/0/48/48	0/6/5/5
63	FES	E	201	5	-	0/0/4/4	0/1/1/1
62	SF4	F	500	6	-	0/0/48/48	0/6/5/5
62	SF4	G	801	7	-	0/0/48/48	0/6/5/5
62	SF4	G	802	7	-	0/0/48/48	0/6/5/5
63	FES	G	803	7	-	0/0/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	SF4	I	201	9	-	0/0/48/48	0/6/5/5
62	SF4	I	202	9	-	0/0/48/48	0/6/5/5

The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	AC	401	HEM	C3C-C2C	-7.20	1.31	1.40
64	AN	401	HEM	C3C-C2C	-7.19	1.31	1.40
64	AC	401	HEM	C3B-C2B	-6.71	1.31	1.40
64	AN	401	HEM	C3B-C2B	-6.67	1.31	1.40
64	AO	301	HEM	C3C-C2C	-6.14	1.32	1.40

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	AC	401	HEM	C3B-CAB-CBB	-9.12	108.06	126.40
64	AN	401	HEM	C3B-CAB-CBB	-9.10	108.09	126.40
64	AN	401	HEM	C3C-CAC-CBC	-8.62	109.06	126.40
64	AC	401	HEM	C3C-CAC-CBC	-8.62	109.06	126.40
64	AD	301	HEM	C3C-CAC-CBC	-7.64	111.03	126.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
64	AC	401	HEM	7	0
64	AD	301	HEM	8	0
64	AN	401	HEM	2	0
64	AO	301	HEM	11	0
62	B	201	SF4	1	0
63	E	201	FES	3	0
62	F	500	SF4	3	0
62	G	801	SF4	1	0
62	G	802	SF4	4	0
63	G	803	FES	1	0
62	I	201	SF4	9	0
62	I	202	SF4	5	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
7	G	3
12	L	3
24	X	2
55	AP	1
10	J	1
36	k	1
55	AE	1
8	H	1
29	c	1
53	AC	1
1	A	1
53	AN	1

The worst 5 of 17 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	107:UNK	C	140:UNK	N	31.95
1	X	250:UNK	C	285:UNK	N	27.39
1	G	632:UNK	C	637:UNK	N	21.00
1	X	185:UNK	C	203:UNK	N	20.68
1	A	37:UNK	C	49:UNK	N	20.22