



Full wwPDB EM Validation Report ⓘ

Oct 12, 2024 – 08:42 pm BST

PDB ID : 5J8K
EMDB ID : EMD-8129
Title : Architecture of supercomplex I-III₂
Authors : Letts, J.A.; Fiedorczuk, K.; Sazanov, L.A.
Deposited on : 2016-04-08
Resolution : 7.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

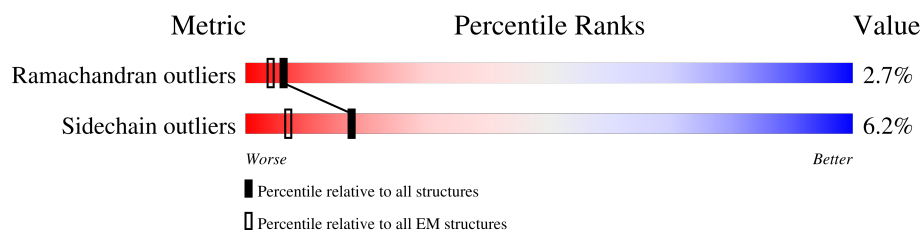
1 Overall quality at a glance

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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	102	
2	B	154	
3	C	194	
4	D	384	
5	E	189	
6	F	429	
7	G	652	
8	H	297	
9	I	171	

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Mol	Chain	Length	Quality of chain
10	J	171	<div> <div>37%</div> <div>81%</div> <div>19%</div> </div>
11	K	93	<div> <div>29%</div> <div>100%</div> </div>
12	L	575	<div> <div>33%</div> <div>99%</div> </div>
13	M	455	<div> <div>25%</div> <div>99%</div> </div>
14	N	345	<div> <div>22%</div> <div>99%</div> </div>
15	O	104	<div> <div>46%</div> <div>100%</div> </div>
16	P	85	<div> <div>47%</div> <div>100%</div> </div>
17	Q	66	<div> <div>24%</div> <div>98%</div> </div>
18	R	29	<div> <div>55%</div> <div>97%</div> </div>
19	S	80	<div> <div>44%</div> <div>100%</div> </div>
19	d	80	<div> <div>39%</div> <div>98%</div> </div>
20	T	53	<div> <div>28%</div> <div>100%</div> </div>
21	U	96	<div> <div>19%</div> <div>100%</div> </div>
22	V	112	<div> <div>35%</div> <div>99%</div> </div>
23	W	103	<div> <div>23%</div> <div>99%</div> </div>
24	X	309	<div> <div>39%</div> <div>83%</div> <div>17%</div> </div>
25	Y	322	<div> <div>28%</div> <div>98%</div> </div>
26	Z	119	<div> <div>55%</div> <div>100%</div> </div>
27	a	111	<div> <div>32%</div> <div>100%</div> </div>
28	b	92	<div> <div>27%</div> <div>100%</div> </div>
29	c	79	<div> <div>44%</div> <div>90%</div> <div>10%</div> </div>
30	e	55	<div> <div>22%</div> <div>100%</div> </div>
31	f	59	<div> <div>29%</div> <div>98%</div> </div>
32	g	130	<div> <div>23%</div> <div>99%</div> </div>
33	9	63	<div> <div>30%</div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
33	h	63	14% 98%
33	z	63	13% 40% 59%
34	i	70	24% 99%
35	j	44	34% 100%
36	k	83	27% 96%
37	0	36	44% 100%
38	1	30	37% 97%
39	2	38	26% 100%
40	3	28	18% 100%
40	4	28	54% 100%
41	5	34	50% 100%
42	6	21	10% 100%
43	7	39	18% 100%
44	8	27	15% 100%
45	y	46	11% 100%
46	x	13	15% 100%
47	w	24	8% 100%
48	v	18	22% 100%
49	u	16	62% 100%
50	t	12	17% 100%
51	AA	446	36% 95%
51	AL	446	55% 95%
52	AB	423	45% 95% 5%
52	AM	423	62% 95% 5%
53	AC	378	34% 95% 5%

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Mol	Chain	Length	Quality of chain
53	AN	378	<div>48%</div> <div>95%</div> <div>5%</div>
54	AD	241	<div>51%</div> <div>94%</div> <div>6%</div>
54	AO	241	<div>55%</div> <div>94%</div> <div>6%</div>
55	AE	196	<div>74%</div> <div>95%</div> <div>• •</div>
55	AP	196	<div>74%</div> <div>94%</div> <div>5% •</div>
56	AF	105	<div>38%</div> <div>95%</div> <div>• •</div>
56	AQ	105	<div>41%</div> <div>95%</div> <div>• •</div>
57	AG	75	<div>44%</div> <div>93%</div> <div>7%</div>
57	AR	75	<div>56%</div> <div>93%</div> <div>7%</div>
58	AH	67	<div>31%</div> <div>100%</div>
58	AS	67	<div>60%</div> <div>100%</div>
59	AI	57	<div>84%</div> <div>74%</div> <div>23% •</div>
59	AT	57	<div>89%</div> <div>74%</div> <div>23% •</div>
60	AJ	60	<div>63%</div> <div>97%</div> <div>•</div>
60	AU	60	<div>53%</div> <div>97%</div> <div>•</div>
61	AK	51	<div>73%</div> <div>96%</div> <div>•</div>
61	AV	51	<div>78%</div> <div>96%</div> <div>•</div>

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		

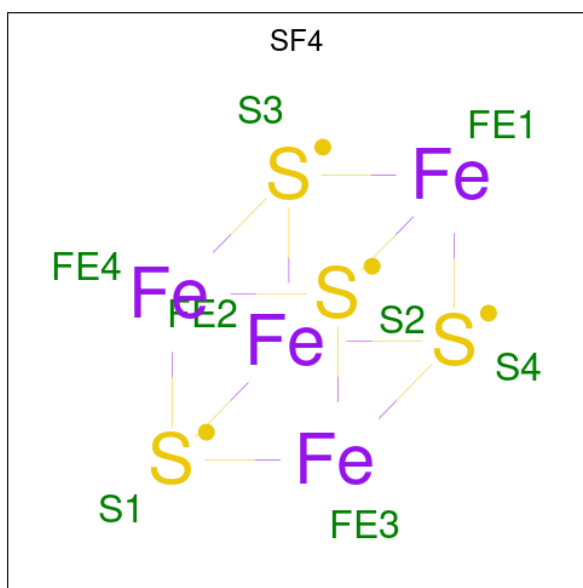
- Molecule 61 is a protein called COMPLEX III SUBUNIT 10 / 6.4KDA.

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:

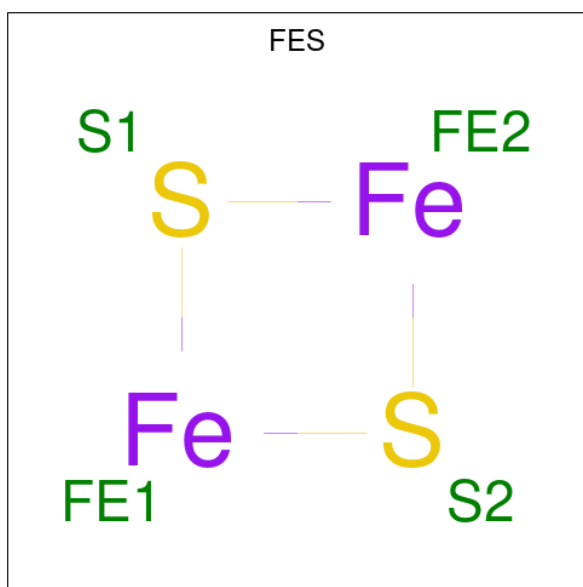
Chain	Residue	Modelled	Actual	Comment	Reference
AK	22	GLN	SER	conflict	UNP W5PSD1
AV	22	GLN	SER	conflict	UNP W5PSD1

- Molecule 62 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



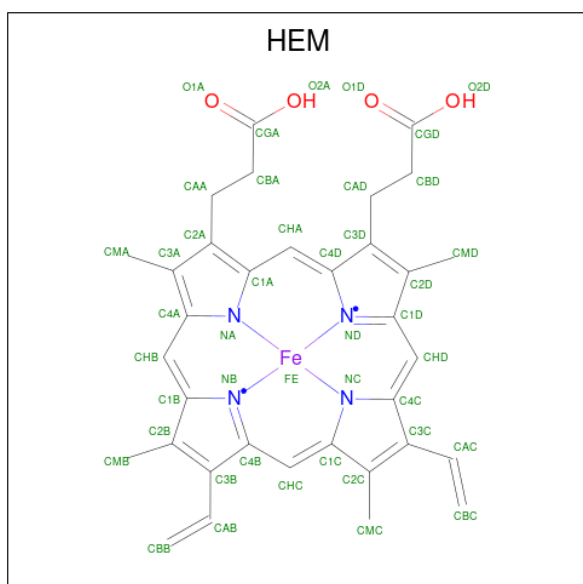
Mol	Chain	Residues	Atoms			AltConf
62	B	1	Total	Fe	S	0
			8	4	4	
62	F	1	Total	Fe	S	0
			8	4	4	
62	G	1	Total	Fe	S	0
			8	4	4	
62	G	1	Total	Fe	S	0
			8	4	4	
62	I	1	Total	Fe	S	0
			8	4	4	
62	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 63 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_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: $C_{34}H_{32}FeN_4O_4$).

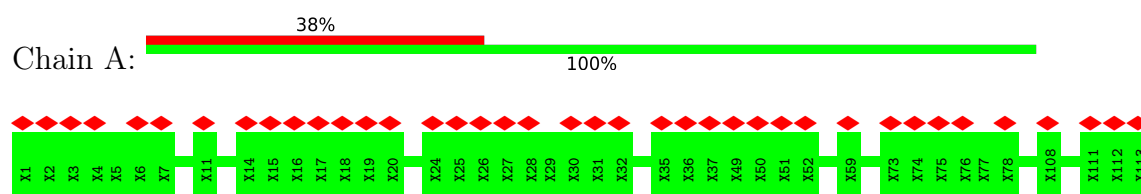


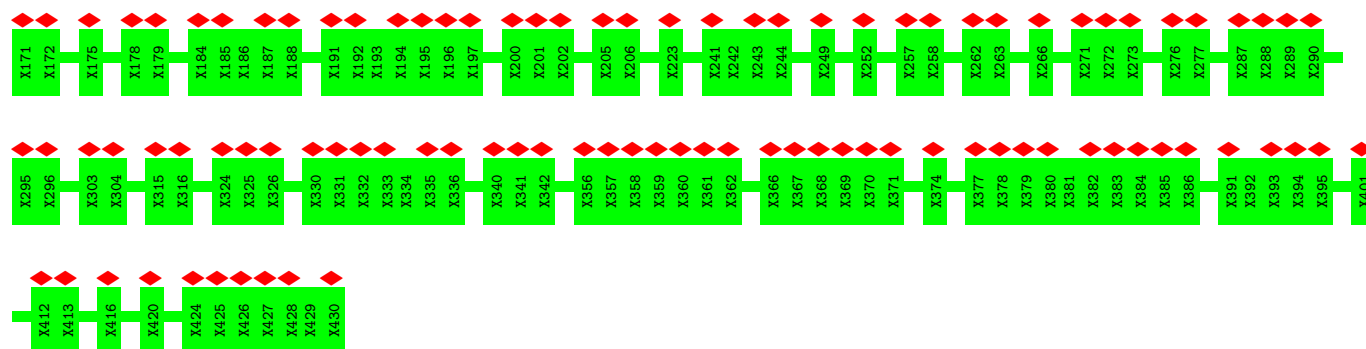
Mol	Chain	Residues	Atoms					AltConf
64	AC	1	Total 43	C 34	Fe 1	N 4	O 4	0
64	AC	1	Total 43	C 34	Fe 1	N 4	O 4	0
64	AD	1	Total 43	C 34	Fe 1	N 4	O 4	0
64	AN	1	Total 43	C 34	Fe 1	N 4	O 4	0
64	AN	1	Total 43	C 34	Fe 1	N 4	O 4	0
64	AO	1	Total 43	C 34	Fe 1	N 4	O 4	0

3 Residue-property plots [i](#)

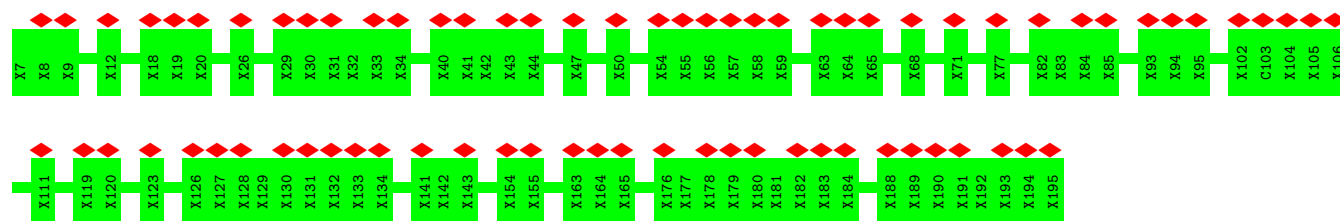
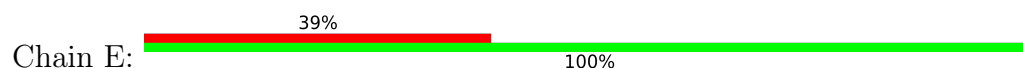
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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

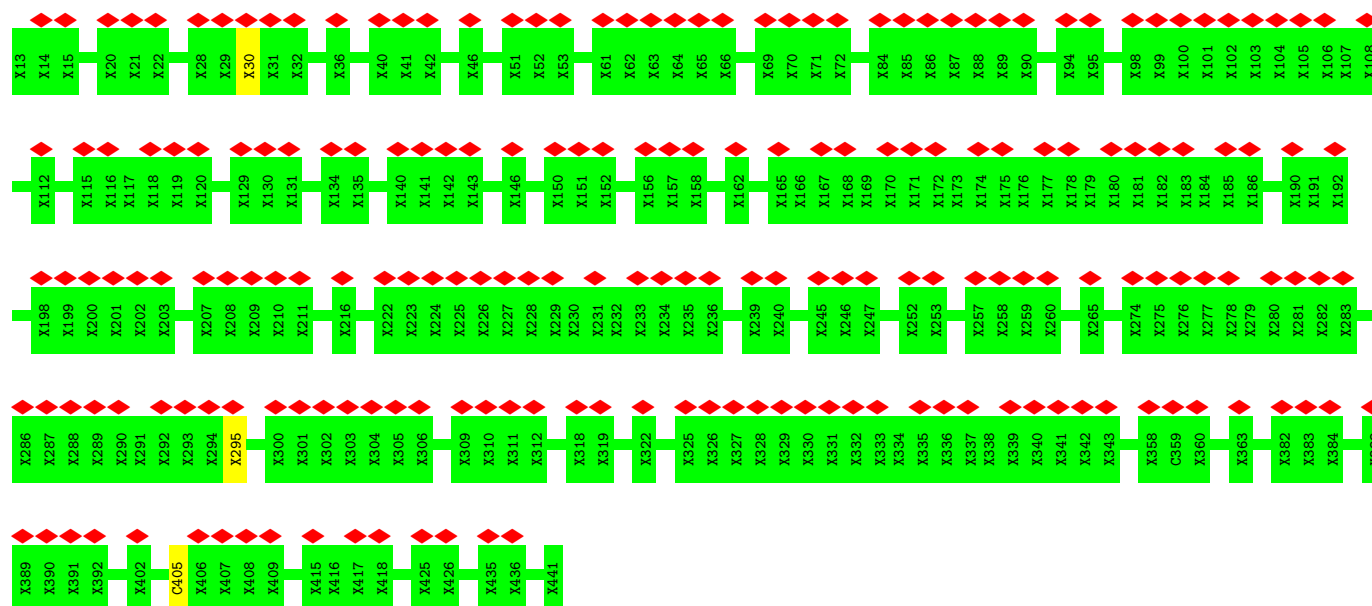




• Molecule 5: COMPLEX I 24KDA/NDUFV2

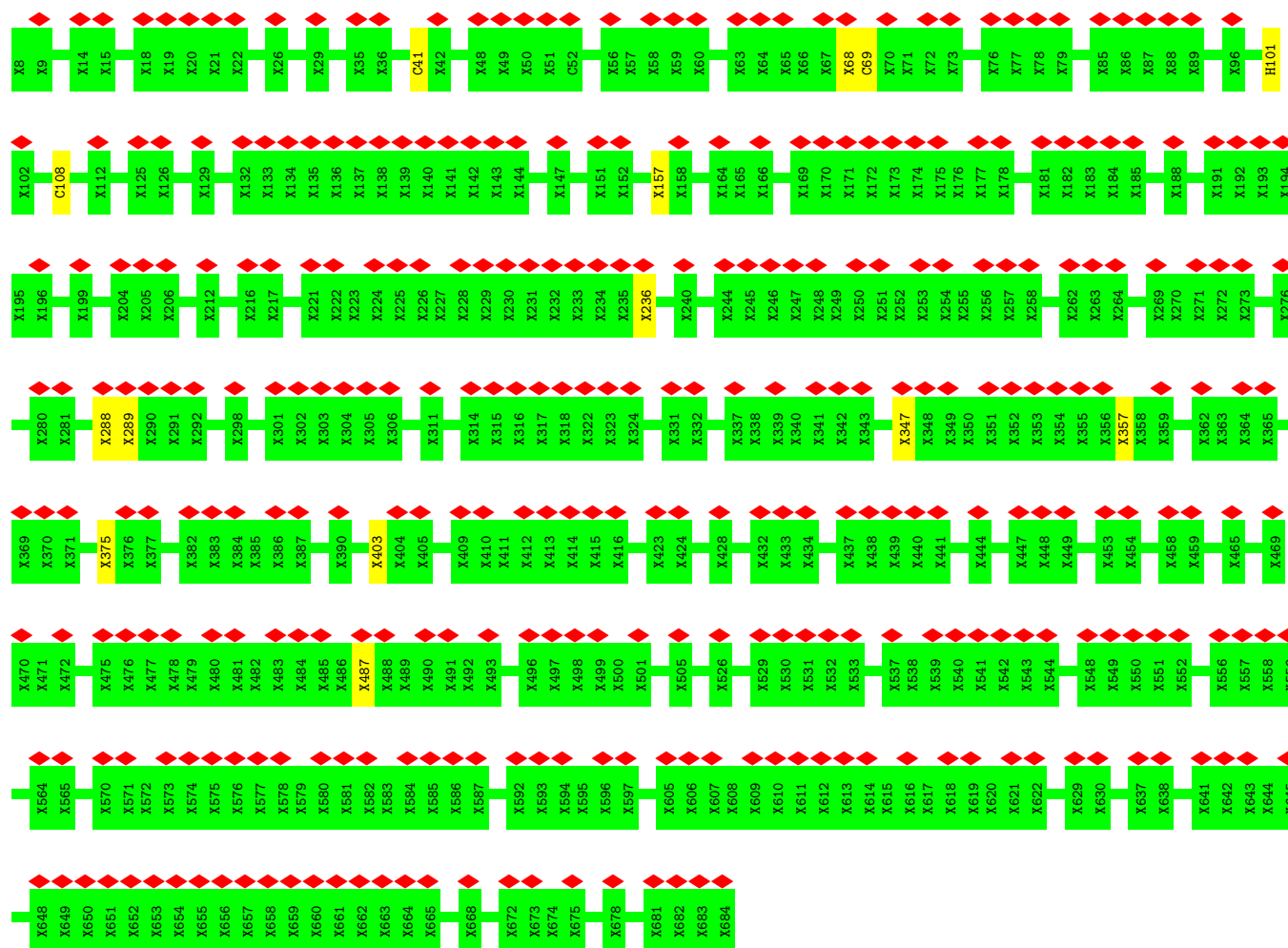


• Molecule 6: COMPLEX I 51KDA/NDUFV1

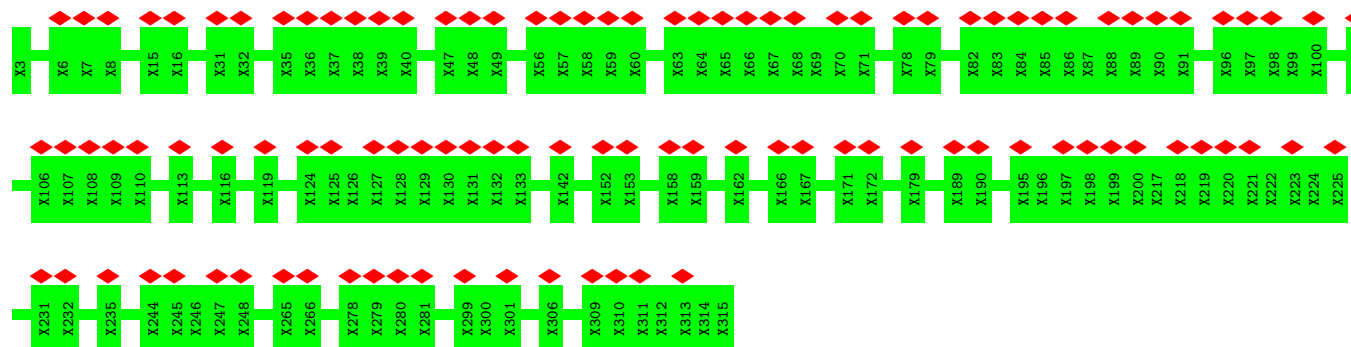


• Molecule 7: COMPLEX I 75KDA/NDUFS1



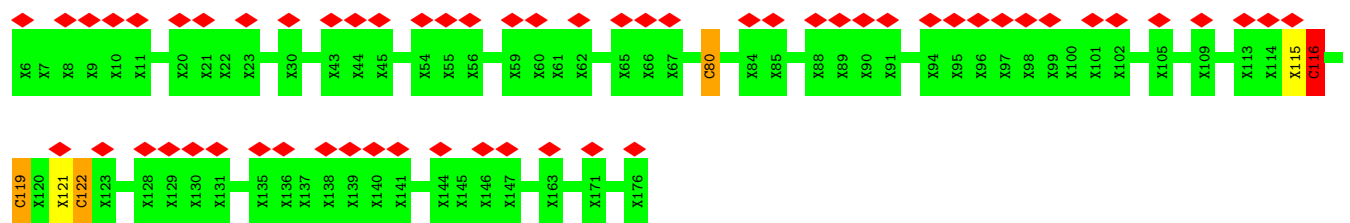


• Molecule 8: COMPLEX I ND1

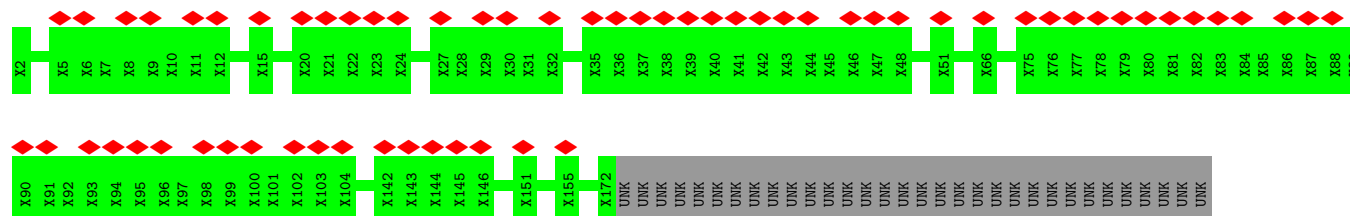
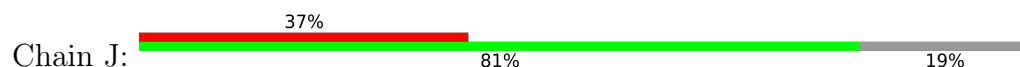


• Molecule 9: COMPLEX I TYKY/NDUFS8

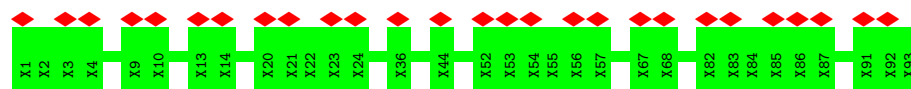




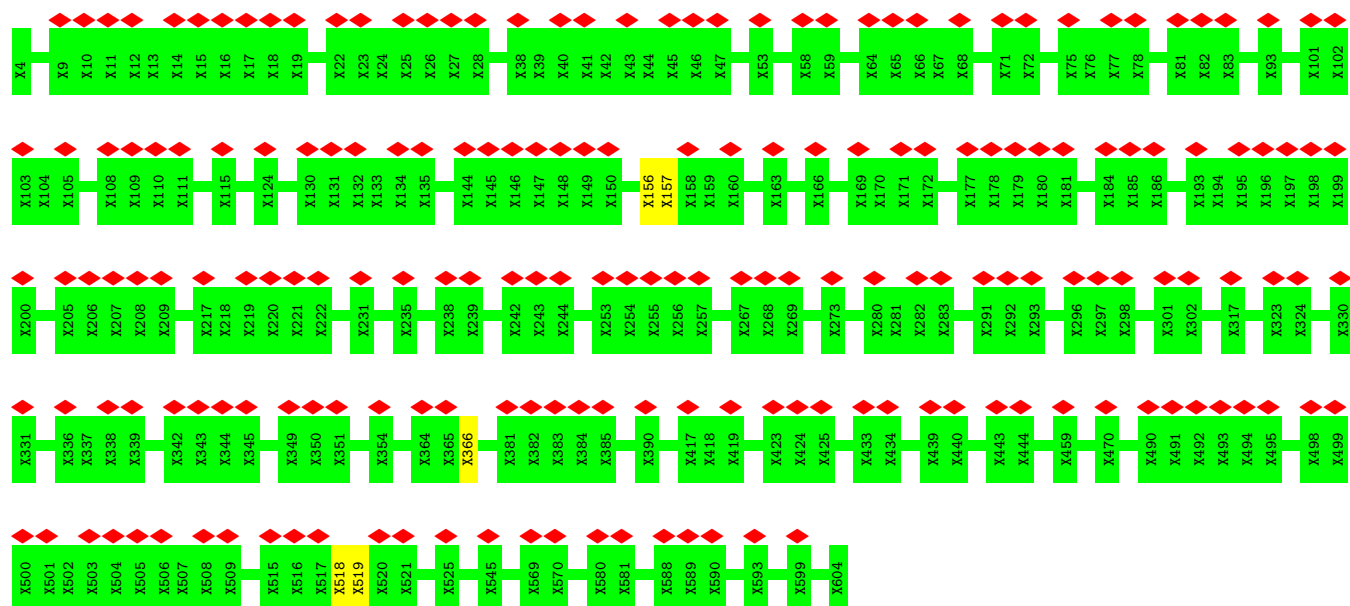
- Molecule 10: COMPLEX I ND6



- Molecule 11: COMPLEX I ND4L

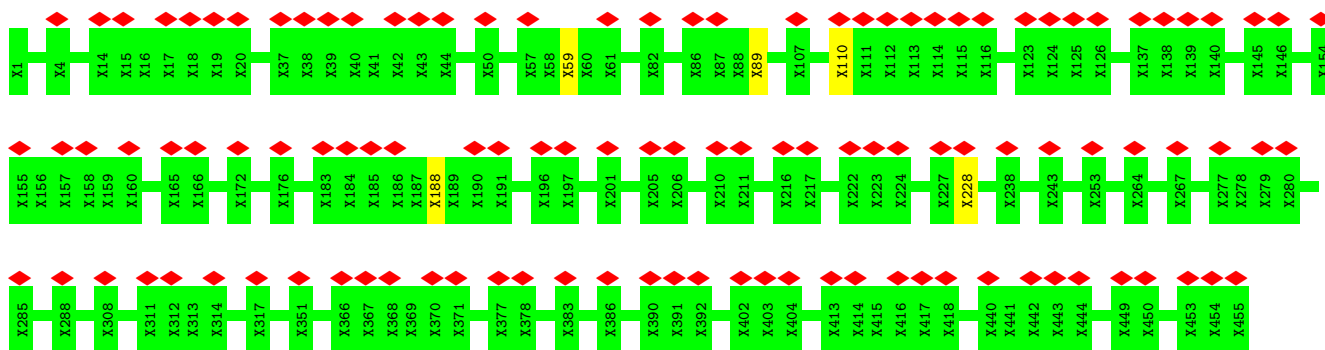


- Molecule 12: COMPLEX I ND5



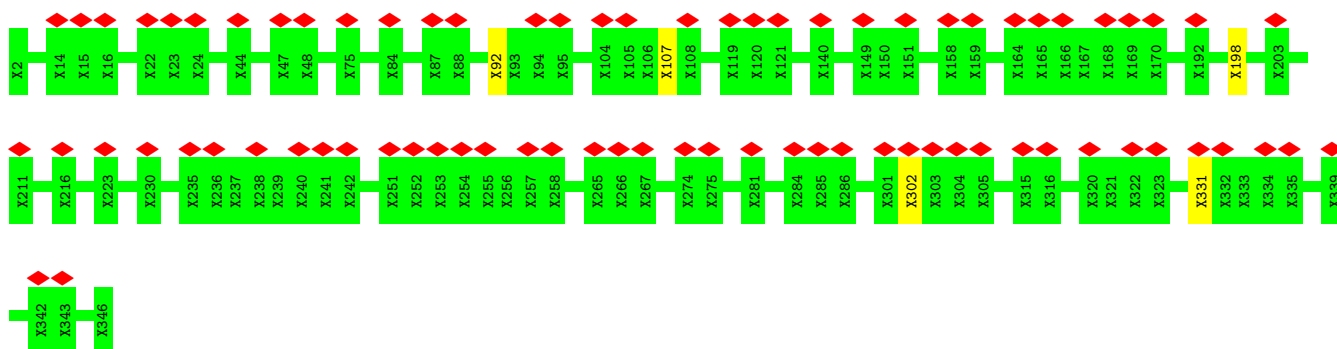
- Molecule 13: COMPLEX I ND4

Chain M:  25% 99%



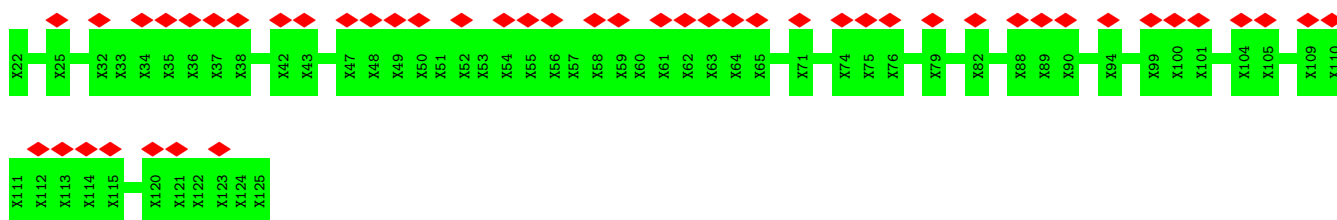
• Molecule 14: COMPLEX I ND2

Chain N:  22% 99%



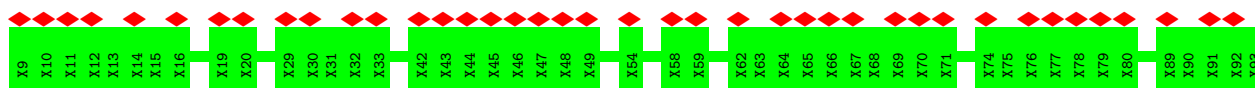
• Molecule 15: COMPLEX I 18KDA/NDUFS6

Chain O:  46% 100%



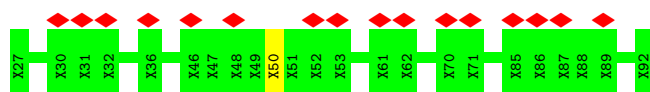
• Molecule 16: COMPLEX I 13KDA/NDUFS6

Chain P:  47% 100%

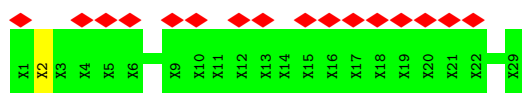


• Molecule 17: COMPLEX I 15KDA/NDUFS5

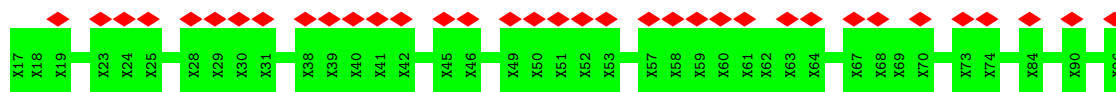
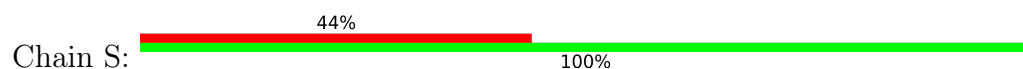
Chain Q:  24% 98%



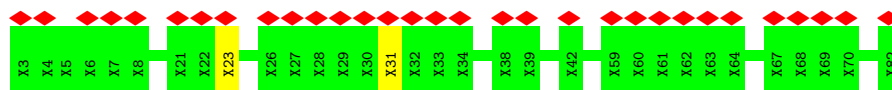
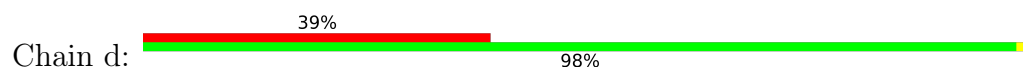
- Molecule 18: COMPLEX I MWFE/NDUFA1



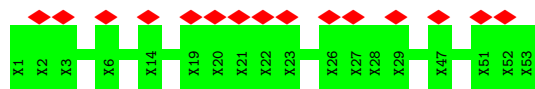
- Molecule 19: COMPLEX I B8/NDUFA2



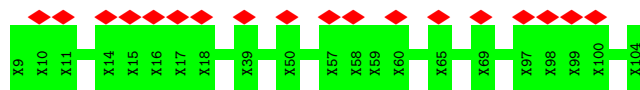
- Molecule 19: COMPLEX I B8/NDUFA2



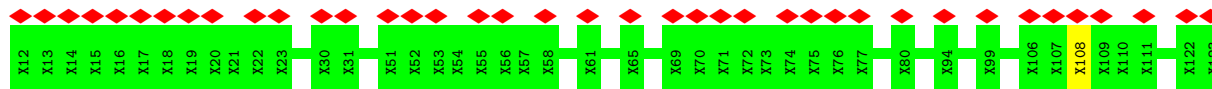
- Molecule 20: COMPLEX I B9/NDUFA3



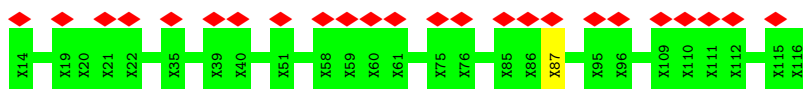
- Molecule 21: COMPLEX I B13/NDUFA5



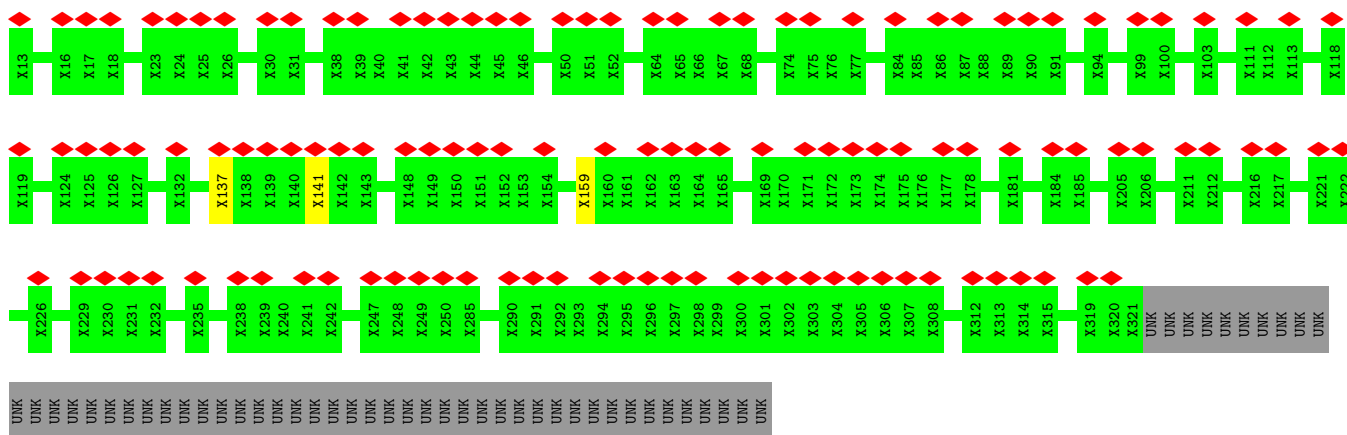
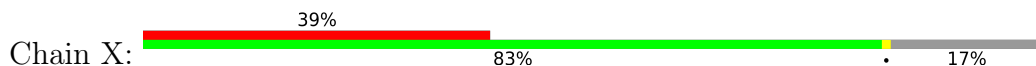
- Molecule 22: COMPLEX I B14/NDUFA6



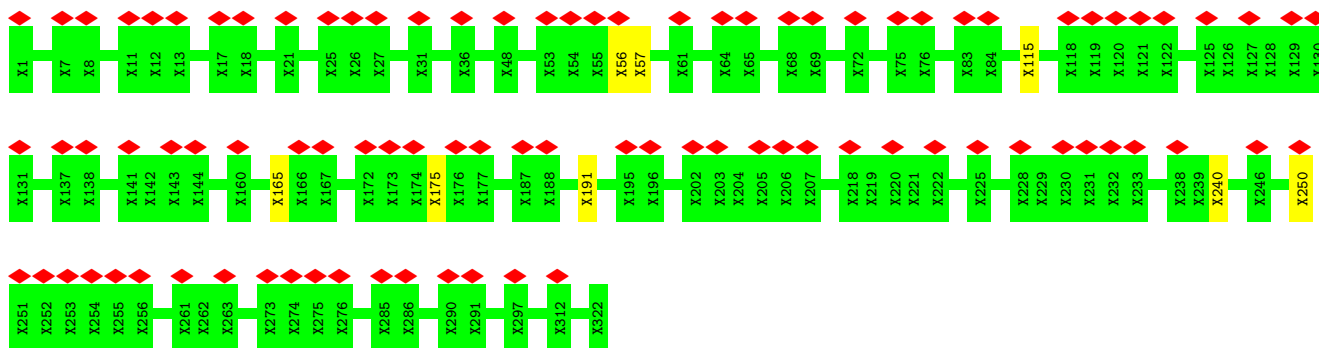
- Molecule 23: COMPLEX I PGIV/NDUFA8



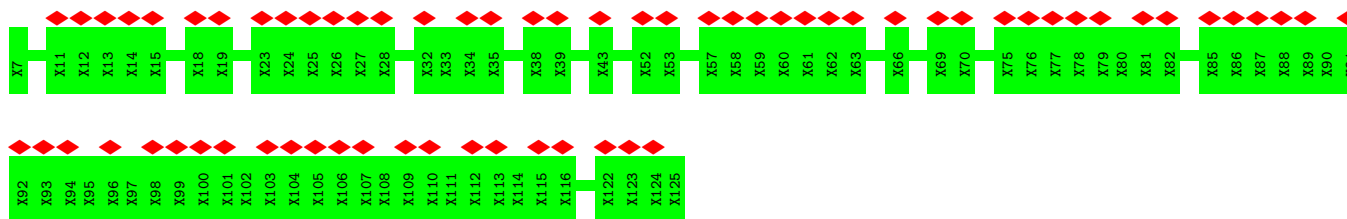
• Molecule 24: COMPLEX I 39KDA/NDUFA9



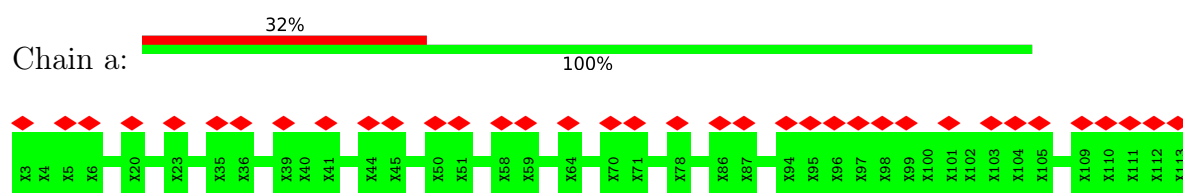
• Molecule 25: COMPLEX I 42KDA/NDUFA10



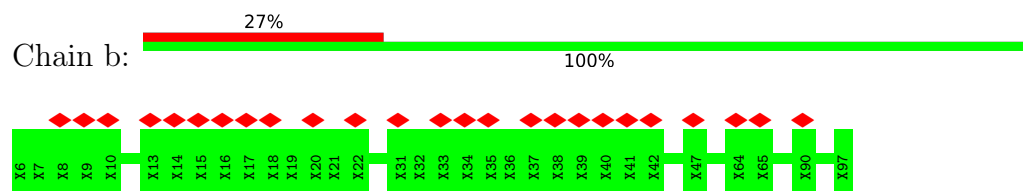
• Molecule 26: COMPLEX I B14.7/NDUFA11



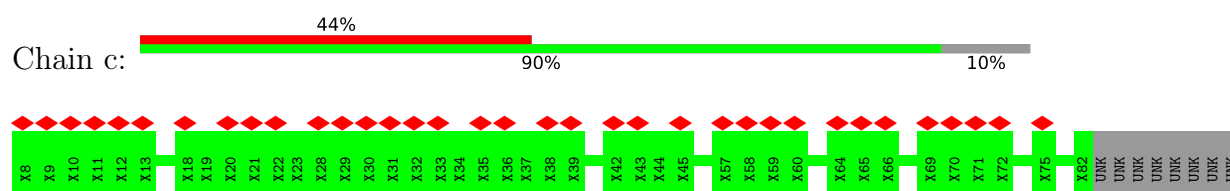
• Molecule 27: COMPLEX I B17.2/NDUFA12



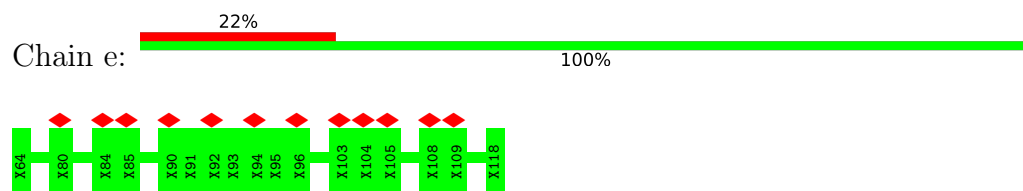
- Molecule 28: COMPLEX I B16.6/NDUFA13



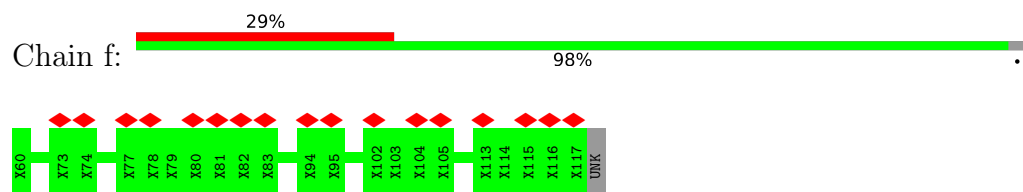
- Molecule 29: COMPLEX I SDAP/NDUFAB1



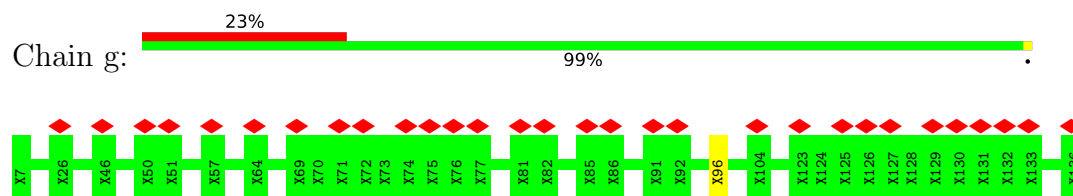
- Molecule 30: COMPLEX I B15/NDUFB4



- Molecule 31: COMPLEX I B18/NDUFB7

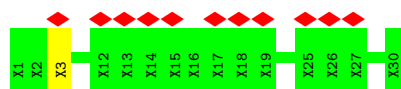


- Molecule 32: COMPLEX I B22/NDUFB9

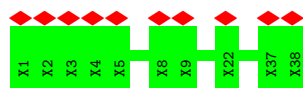


- Molecule 33: COMPLEX I PDSW/NDUFB10

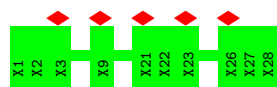




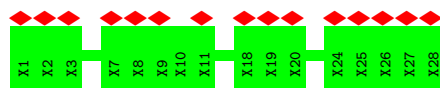
- Molecule 39: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 3



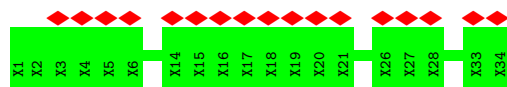
- Molecule 40: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 4



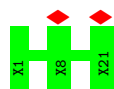
- Molecule 40: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 4



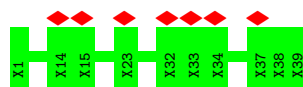
- Molecule 41: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 5



- Molecule 42: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 6

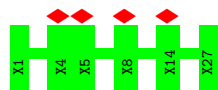


- Molecule 43: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 7



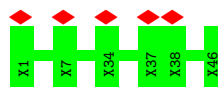
- Molecule 44: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 8

Chain 8:  15% 100%



- Molecule 45: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 11

Chain y:  11% 100%



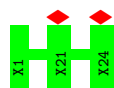
- Molecule 46: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 12

Chain x:  15% 100%



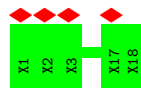
- Molecule 47: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 13

Chain w:  8% 100%



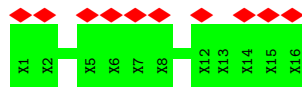
- Molecule 48: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 14

Chain v:  22% 100%



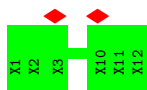
- Molecule 49: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 15

Chain u:  62% 100%

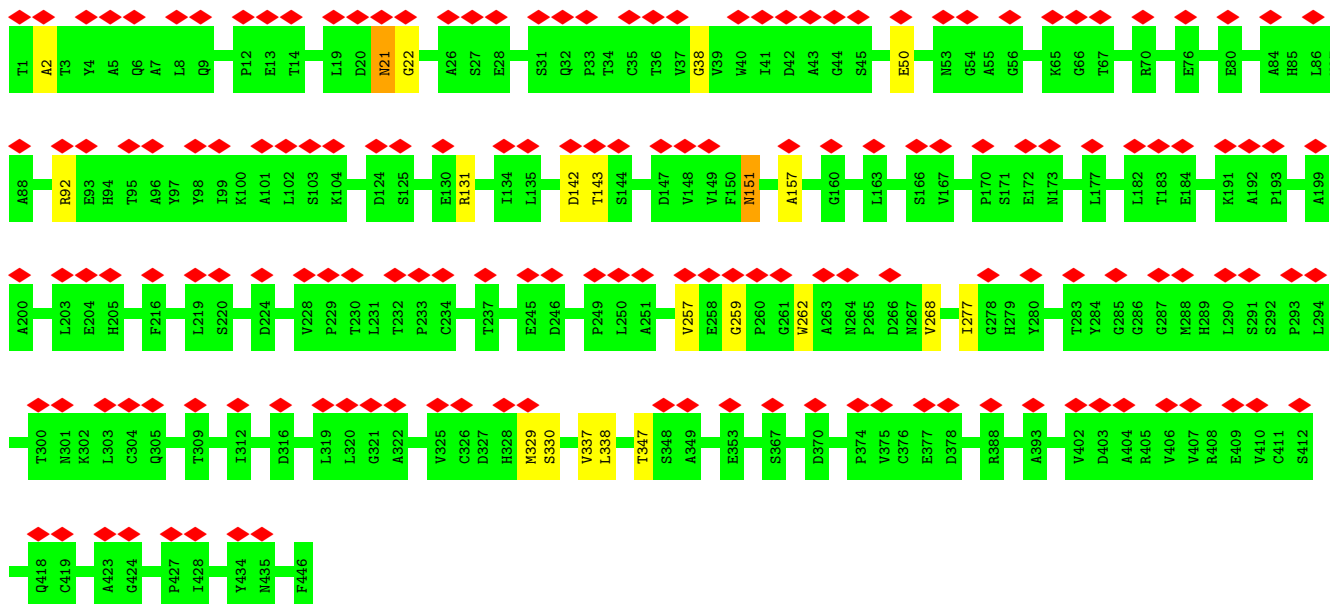
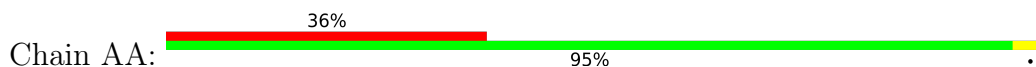


- Molecule 50: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 16

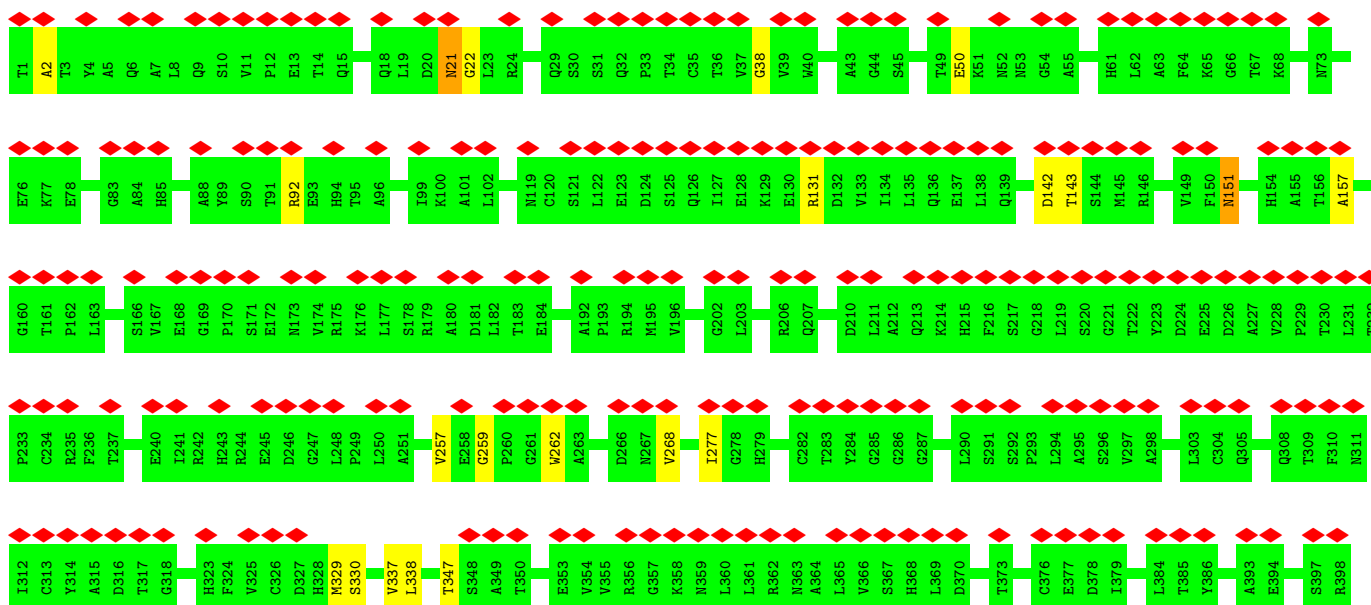
Chain t:  17% 100%

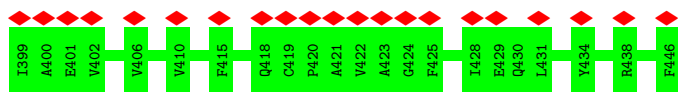


• Molecule 51: COMPLEX III SUBUNIT 1 / CORE 1



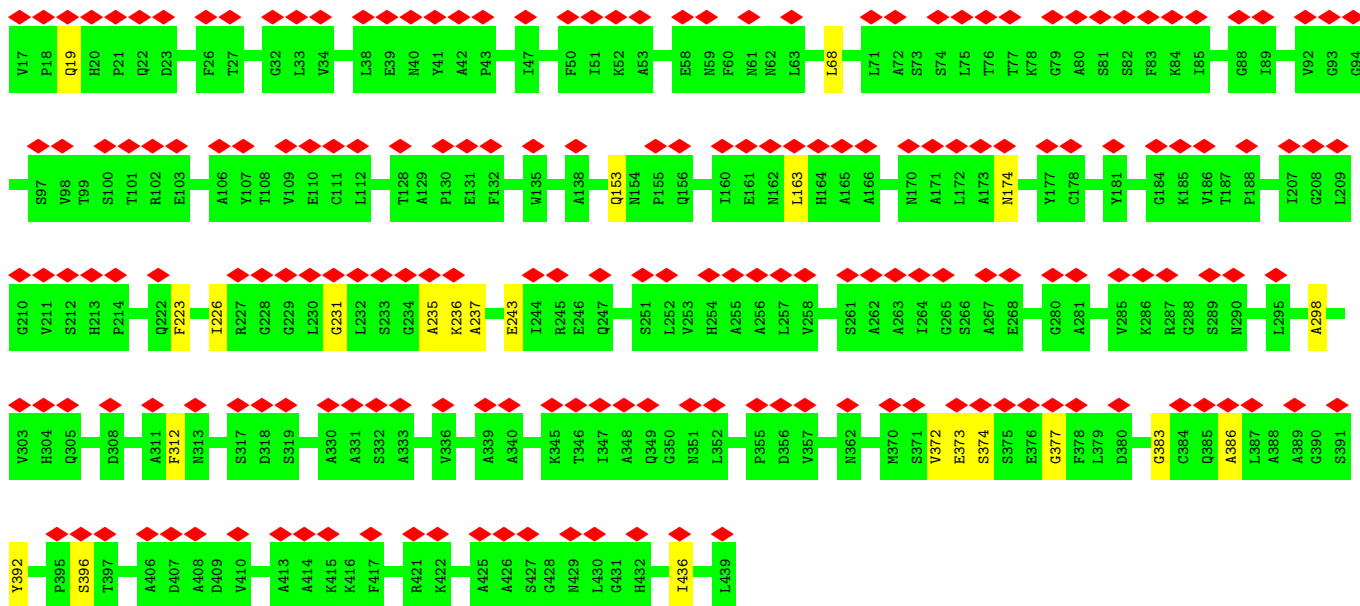
• Molecule 51: COMPLEX III SUBUNIT 1 / CORE 1





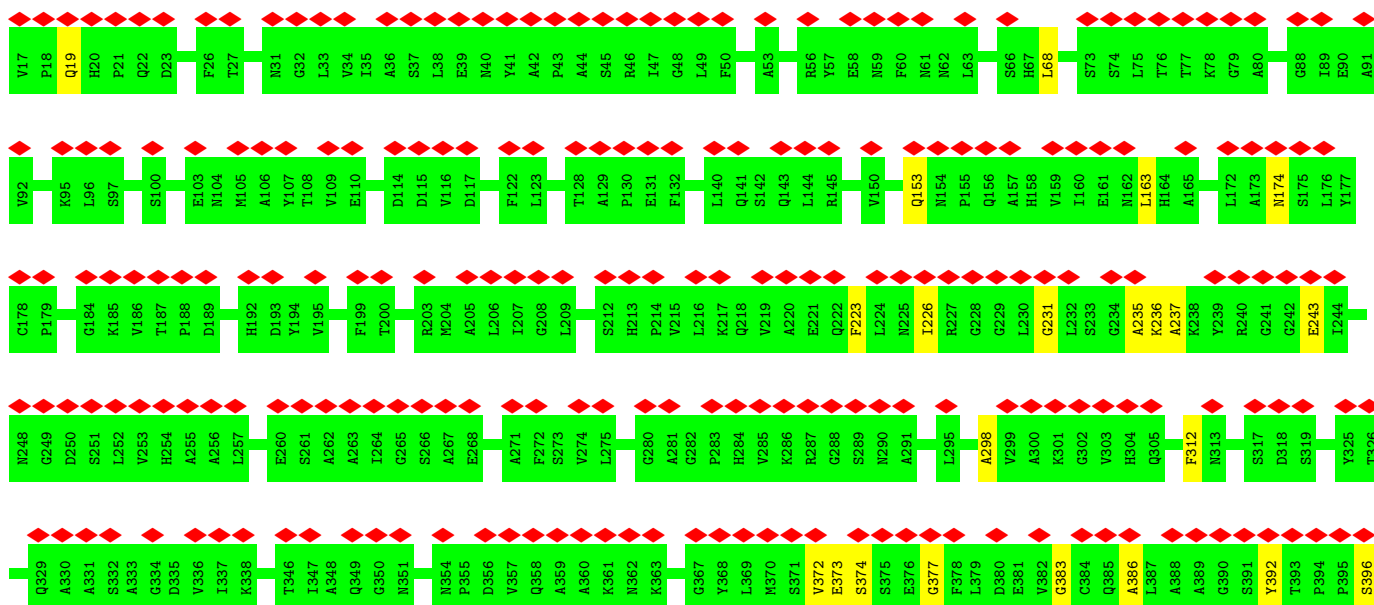
• Molecule 52: COMPLEX III SUBUNIT 2 / CORE 2

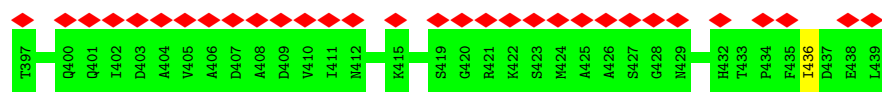
Chain AB: 45% 95% 5%



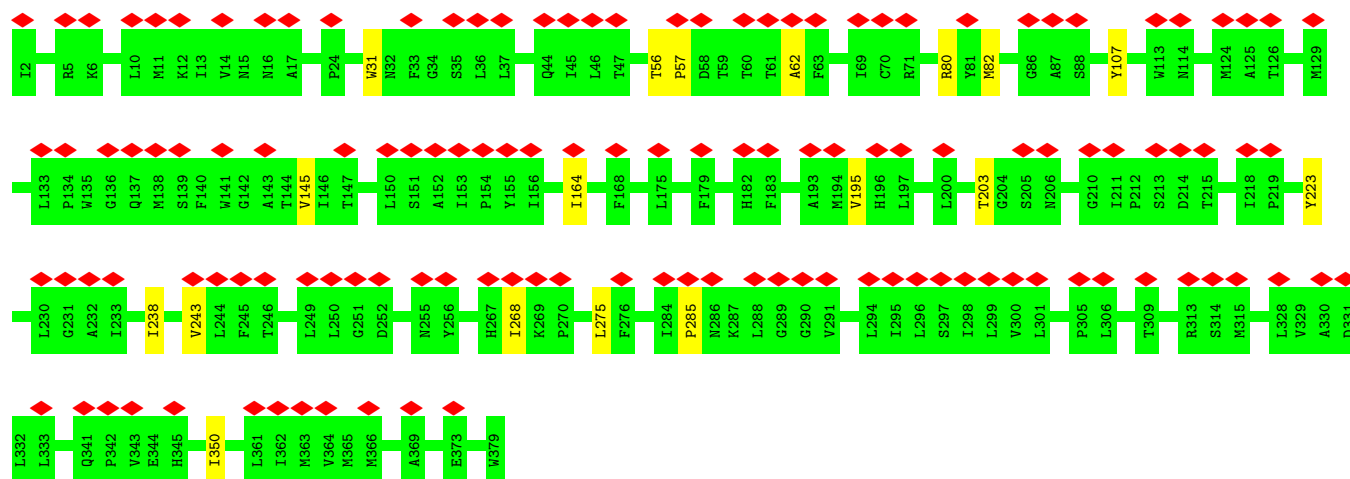
• Molecule 52: COMPLEX III SUBUNIT 2 / CORE 2

Chain AM: 62% 95% 5%

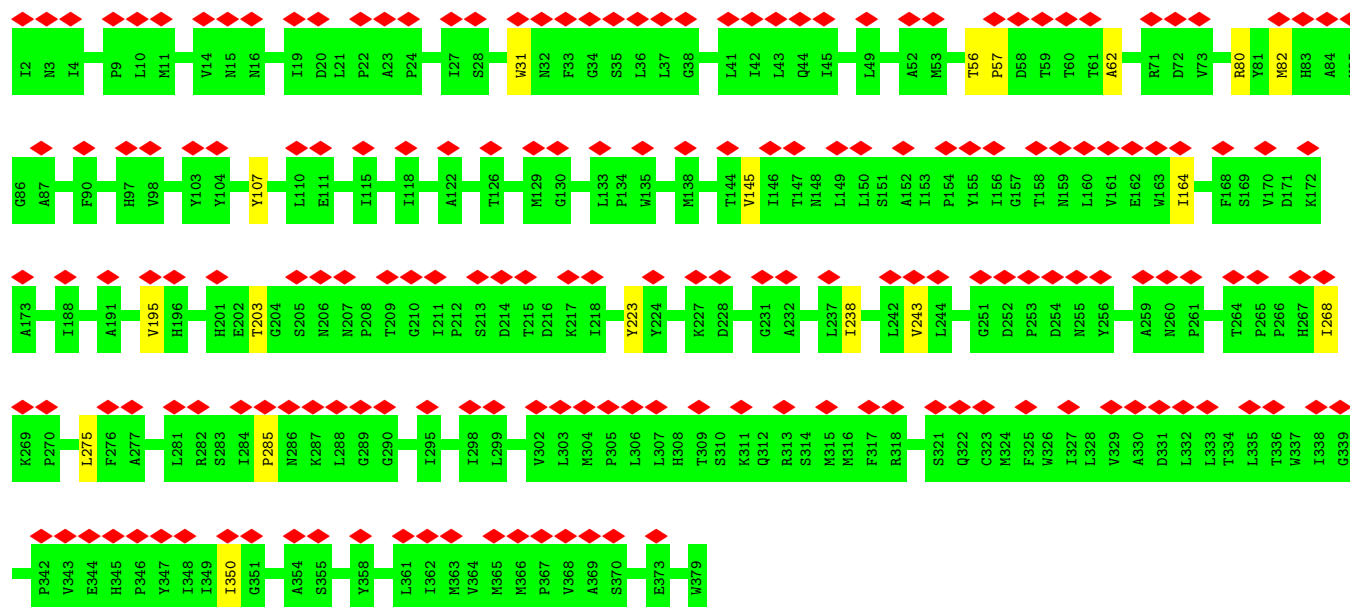




• Molecule 53: Cytochrome b

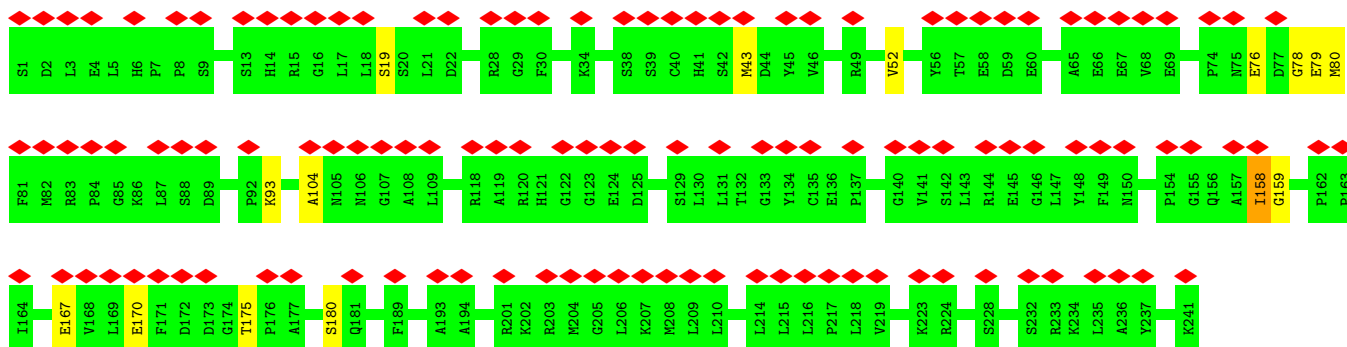


• Molecule 53: Cytochrome b

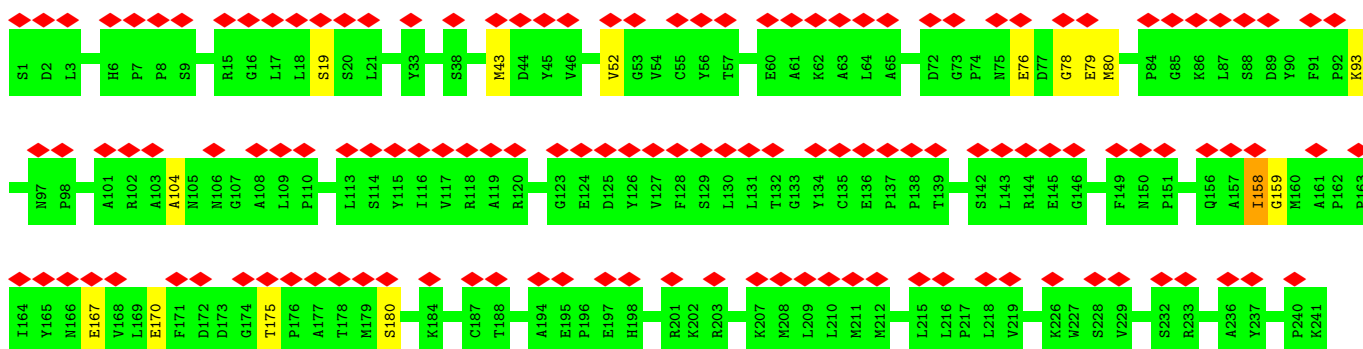


• Molecule 54: COMPLEX III SUBUNIT 4 / CYTOCHROME C1

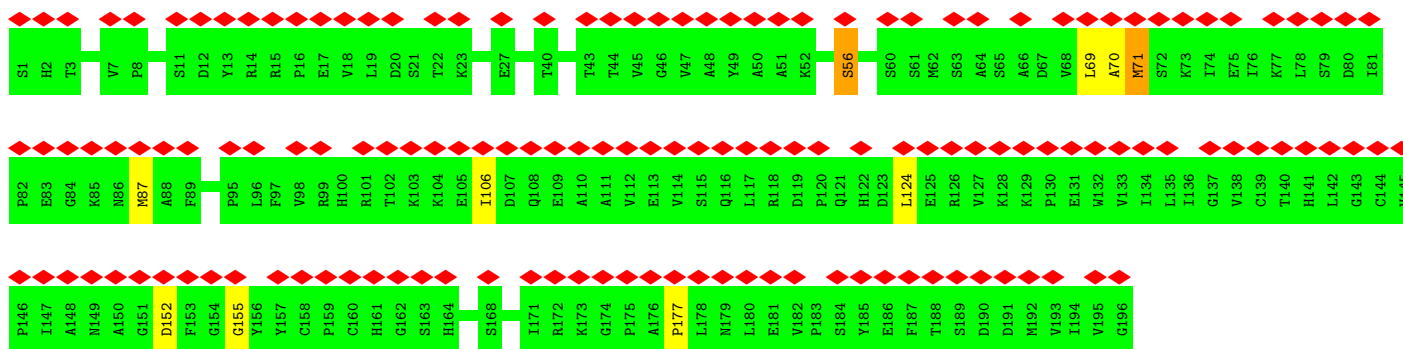
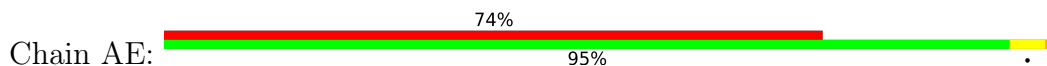




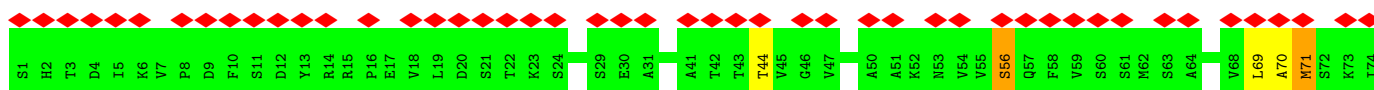
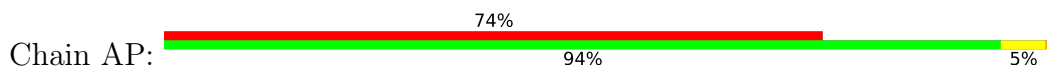
• Molecule 54: COMPLEX III SUBUNIT 4 / CYTOCHROME C1

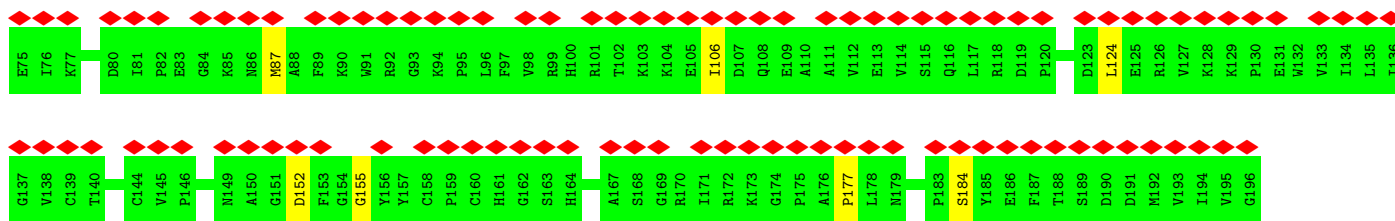


• Molecule 55: Cytochrome b-c1 complex subunit Rieske, mitochondrial

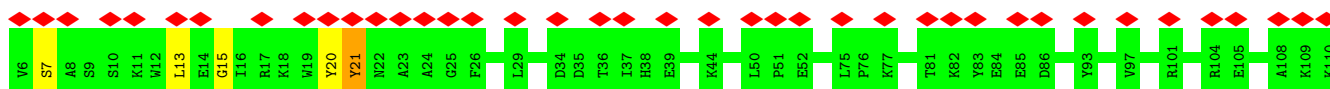


• Molecule 55: Cytochrome b-c1 complex subunit Rieske, mitochondrial

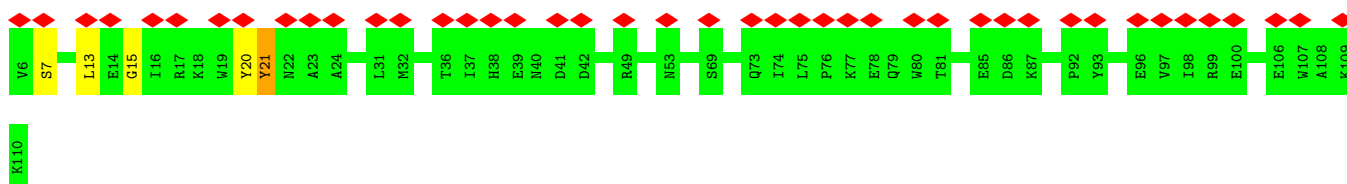
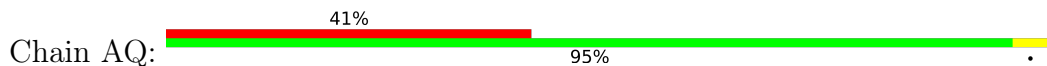




• Molecule 56: COMPLEX III SUBUNIT 7 / 14KDA



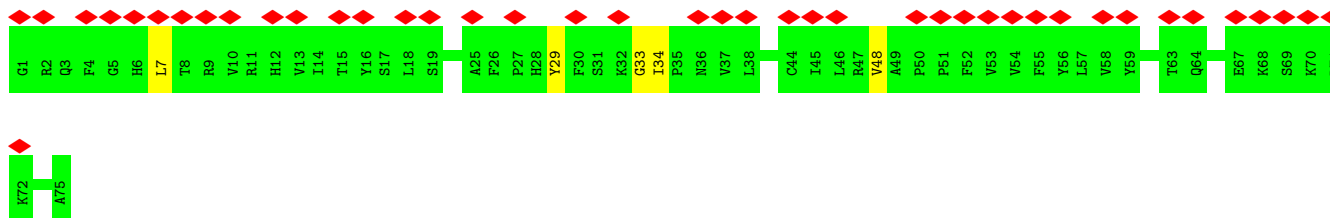
• Molecule 56: COMPLEX III SUBUNIT 7 / 14KDA



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

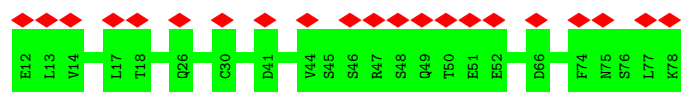


• Molecule 57: COMPLEX III SUBUNIT 8 / QP-C

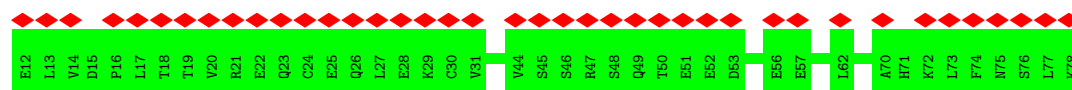


• Molecule 58: Cytochrome b-c1 complex subunit 6

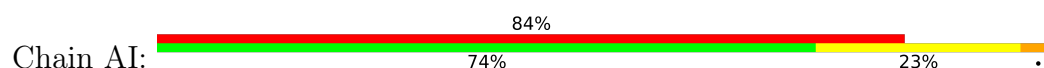




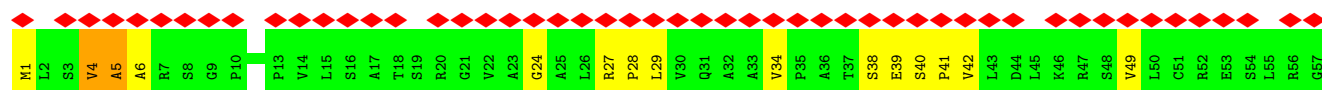
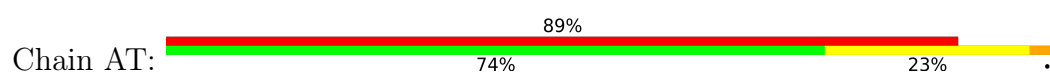
- Molecule 58: Cytochrome b-c1 complex subunit 6



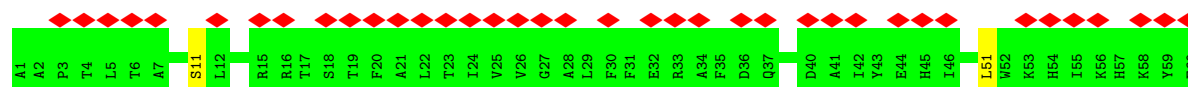
- Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial



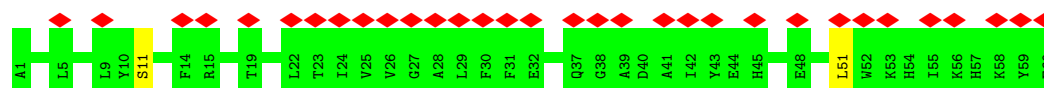
- Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial



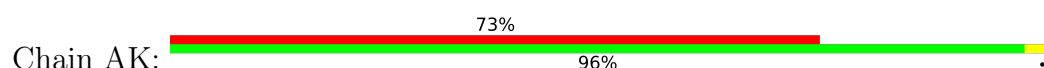
- Molecule 60: COMPLEX III SUBUNIT 9 / 7.2KDA



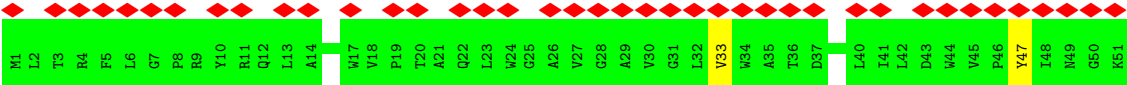
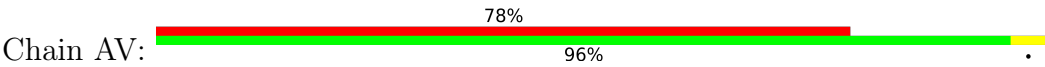
- Molecule 60: COMPLEX III SUBUNIT 9 / 7.2KDA



- Molecule 61: COMPLEX III SUBUNIT 10 / 6.4KDA



- Molecule 61: COMPLEX III SUBUNIT 10 / 6.4KDA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9844	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	34	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	81395	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.488	Depositor
Minimum map value	-0.233	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	853.12, 853.12, 853.12	wwPDB
Map dimensions	496, 496, 496	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.72, 1.72, 1.72	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	$\# Z > 5$	RMSZ	$\# Z > 5$
2	B	1.50	1/21 (4.8%)	0.85	0/23
5	E	0.76	0/20	0.79	0/20
6	F	1.42	0/20	1.21	0/20
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%)
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%)
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
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
2	B	0	2
3	C	0	5
4	D	0	1
6	F	0	3
7	G	0	10
9	I	0	5
12	L	0	5
13	M	0	5
14	N	0	5
17	Q	0	1
18	R	0	1
19	d	0	2
22	V	0	1
23	W	0	1
24	X	0	3
25	Y	0	8
32	g	0	1
33	h	0	1
33	z	0	1
34	i	0	1
38	l	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
60	AJ	0	1
60	AU	0	1
61	AK	0	1
61	AV	0	1

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

All (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
55	AE	56	SER	C-O	5.34	1.33	1.23
2	B	55	CYS	CB-SG	-5.31	1.73	1.81
9	I	80	CYS	CB-SG	-5.24	1.73	1.81

All (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
51	AL	21	ASN	N-CA-C	-7.76	90.04	111.00
51	AA	21	ASN	N-CA-C	-7.74	90.11	111.00
55	AP	44	THR	O-C-N	-7.54	110.64	122.70
59	AT	5	ALA	N-CA-C	6.58	128.78	111.00
59	AI	5	ALA	N-CA-C	6.53	128.62	111.00
59	AT	4	VAL	N-CA-C	6.07	127.38	111.00
59	AI	4	VAL	N-CA-C	6.00	127.20	111.00
59	AT	6	ALA	N-CA-C	5.94	127.04	111.00
59	AI	6	ALA	N-CA-C	5.90	126.93	111.00
56	AQ	21	TYR	C-N-CA	-5.84	107.10	121.70
56	AF	21	TYR	C-N-CA	-5.75	107.33	121.70
51	AL	22	GLY	N-CA-C	-5.64	99.01	113.10
51	AA	22	GLY	N-CA-C	-5.63	99.01	113.10
7	G	69	CYS	N-CA-C	-5.54	96.05	111.00
51	AL	151	ASN	C-N-CA	-5.50	107.96	121.70
51	AA	151	ASN	C-N-CA	-5.48	108.00	121.70
55	AE	56	SER	O-C-N	-5.31	114.20	122.70
55	AP	56	SER	O-C-N	-5.27	114.27	122.70
9	I	116	CYS	CA-CB-SG	-5.24	104.57	114.00
7	G	108	CYS	CA-CB-SG	-5.16	104.71	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	AT	39	GLU	C-N-CA	5.15	134.58	121.70
59	AI	39	GLU	C-N-CA	5.08	134.41	121.70
55	AE	56	SER	CB-CA-C	5.06	119.72	110.10
55	AP	56	SER	CB-CA-C	5.05	119.70	110.10

There are no chirality outliers.

All (180) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
38	1	3	UNK	Peptide
51	AA	131	ARG	Peptide
51	AA	142	ASP	Peptide
51	AA	151	ASN	Peptide
51	AA	157	ALA	Peptide
51	AA	2	ALA	Peptide
51	AA	21	ASN	Peptide
51	AA	257	VAL	Peptide
51	AA	259	GLY	Peptide
51	AA	262	TRP	Peptide
51	AA	329	MET	Peptide
51	AA	330	SER	Peptide
51	AA	347	THR	Peptide
51	AA	38	GLY	Peptide
52	AB	163	LEU	Peptide
52	AB	174	ASN	Peptide
52	AB	19	GLN	Peptide
52	AB	223	PHE	Peptide
52	AB	235	ALA	Peptide
52	AB	236	LYS	Peptide
52	AB	237	ALA	Peptide
52	AB	243	GLU	Peptide
52	AB	298	ALA	Peptide
52	AB	312	PHE	Peptide
52	AB	372	VAL	Peptide
52	AB	373	GLU	Peptide
52	AB	374	SER	Peptide
52	AB	377	GLY	Peptide
52	AB	383	GLY	Peptide
52	AB	386	ALA	Peptide
52	AB	392	TYR	Peptide
53	AC	203	THR	Peptide
53	AC	31	TRP	Peptide

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Mol	Chain	Res	Type	Group
54	AD	104	ALA	Peptide
54	AD	158	ILE	Peptide
54	AD	167	GLU	Peptide
54	AD	170	GLU	Peptide
54	AD	19	SER	Peptide
54	AD	43	MET	Peptide
54	AD	76	GLU	Peptide
54	AD	78	GLY	Peptide
55	AE	155	GLY	Mainchain
55	AE	56	SER	Mainchain
55	AE	71	MET	Mainchain
56	AF	13	LEU	Peptide
56	AF	15	GLY	Peptide
56	AF	20	TYR	Peptide
56	AF	21	TYR	Peptide
56	AF	7	SER	Peptide
57	AG	33	GLY	Peptide
57	AG	48	VAL	Peptide
59	AI	1	MET	Peptide
59	AI	24	GLY	Peptide
59	AI	34	VAL	Peptide
59	AI	38	SER	Peptide
59	AI	4	VAL	Peptide
59	AI	5	ALA	Peptide
60	AJ	51	LEU	Peptide
61	AK	47	TYR	Peptide
51	AL	131	ARG	Peptide
51	AL	142	ASP	Peptide
51	AL	151	ASN	Peptide
51	AL	157	ALA	Peptide
51	AL	2	ALA	Peptide
51	AL	21	ASN	Peptide
51	AL	257	VAL	Peptide
51	AL	259	GLY	Peptide
51	AL	262	TRP	Peptide
51	AL	329	MET	Peptide
51	AL	330	SER	Peptide
51	AL	347	THR	Peptide
51	AL	38	GLY	Peptide
52	AM	163	LEU	Peptide
52	AM	174	ASN	Peptide
52	AM	19	GLN	Peptide

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Mol	Chain	Res	Type	Group
52	AM	223	PHE	Peptide
52	AM	235	ALA	Peptide
52	AM	236	LYS	Peptide
52	AM	237	ALA	Peptide
52	AM	243	GLU	Peptide
52	AM	298	ALA	Peptide
52	AM	312	PHE	Peptide
52	AM	372	VAL	Peptide
52	AM	373	GLU	Peptide
52	AM	374	SER	Peptide
52	AM	377	GLY	Peptide
52	AM	383	GLY	Peptide
52	AM	386	ALA	Peptide
52	AM	392	TYR	Peptide
53	AN	203	THR	Peptide
53	AN	31	TRP	Peptide
54	AO	104	ALA	Peptide
54	AO	158	ILE	Peptide
54	AO	167	GLU	Peptide
54	AO	170	GLU	Peptide
54	AO	19	SER	Peptide
54	AO	43	MET	Peptide
54	AO	76	GLU	Peptide
54	AO	78	GLY	Peptide
55	AP	155	GLY	Mainchain
55	AP	184	SER	Mainchain
55	AP	56	SER	Mainchain
55	AP	71	MET	Mainchain
56	AQ	13	LEU	Peptide
56	AQ	15	GLY	Peptide
56	AQ	20	TYR	Peptide
56	AQ	21	TYR	Peptide
56	AQ	7	SER	Peptide
57	AR	33	GLY	Peptide
57	AR	48	VAL	Peptide
59	AT	1	MET	Peptide
59	AT	24	GLY	Peptide
59	AT	34	VAL	Peptide
59	AT	38	SER	Peptide
59	AT	4	VAL	Peptide
59	AT	5	ALA	Peptide
60	AU	51	LEU	Peptide

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Mol	Chain	Res	Type	Group
61	AV	47	TYR	Peptide
2	B	151	UNK	Peptide
2	B	54	CYS	Peptide
3	C	115	UNK	Peptide
3	C	150	UNK	Peptide
3	C	166	UNK	Peptide
3	C	168	UNK	Peptide
3	C	68	UNK	Peptide
4	D	60	UNK	Peptide
6	F	295	UNK	Peptide
6	F	30	UNK	Peptide
6	F	405	CYS	Peptide
7	G	157	UNK	Peptide
7	G	236	UNK	Peptide
7	G	288	UNK	Peptide
7	G	289	UNK	Peptide
7	G	347	UNK	Peptide
7	G	357	UNK	Peptide
7	G	375	UNK	Peptide
7	G	403	UNK	Peptide
7	G	487	UNK	Peptide
7	G	68	UNK	Peptide
9	I	115	UNK	Peptide
9	I	116	CYS	Peptide
9	I	119	CYS	Peptide
9	I	121	UNK	Peptide
9	I	122	CYS	Peptide
12	L	156	UNK	Peptide
12	L	157	UNK	Peptide
12	L	366	UNK	Peptide
12	L	518	UNK	Peptide
12	L	519	UNK	Peptide
13	M	110	UNK	Peptide
13	M	188	UNK	Peptide
13	M	228	UNK	Peptide
13	M	59	UNK	Peptide
13	M	89	UNK	Peptide
14	N	107	UNK	Peptide
14	N	198	UNK	Peptide
14	N	302	UNK	Peptide
14	N	331	UNK	Peptide
14	N	92	UNK	Peptide

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Mol	Chain	Res	Type	Group
17	Q	50	UNK	Peptide
18	R	2	UNK	Peptide
22	V	108	UNK	Peptide
23	W	87	UNK	Peptide
24	X	137	UNK	Peptide
24	X	141	UNK	Peptide
24	X	159	UNK	Peptide
25	Y	115	UNK	Peptide
25	Y	165	UNK	Peptide
25	Y	175	UNK	Peptide
25	Y	191	UNK	Peptide
25	Y	240	UNK	Peptide
25	Y	250	UNK	Peptide
25	Y	56	UNK	Peptide
25	Y	57	UNK	Peptide
19	d	23	UNK	Peptide
19	d	31	UNK	Peptide
32	g	96	UNK	Peptide
33	h	117	UNK	Peptide
34	i	59	UNK	Peptide
33	z	12	UNK	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	4/154 (3%)	4 (100%)	0	0	100	100
5	E	4/189 (2%)	2 (50%)	2 (50%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	4/429 (1%)	4 (100%)	0	0	100	100
7	G	12/652 (2%)	6 (50%)	4 (33%)	2 (17%)	0	2
9	I	8/171 (5%)	4 (50%)	3 (38%)	1 (12%)	0	4
51	AA	444/446 (100%)	369 (83%)	68 (15%)	7 (2%)	8	38
51	AL	444/446 (100%)	370 (83%)	67 (15%)	7 (2%)	8	38
52	AB	421/423 (100%)	370 (88%)	46 (11%)	5 (1%)	11	44
52	AM	421/423 (100%)	369 (88%)	47 (11%)	5 (1%)	11	44
53	AC	376/378 (100%)	288 (77%)	73 (19%)	15 (4%)	2	18
53	AN	376/378 (100%)	287 (76%)	74 (20%)	15 (4%)	2	18
54	AD	239/241 (99%)	180 (75%)	52 (22%)	7 (3%)	3	23
54	AO	239/241 (99%)	180 (75%)	52 (22%)	7 (3%)	3	23
55	AE	192/196 (98%)	148 (77%)	36 (19%)	8 (4%)	2	17
55	AP	194/196 (99%)	151 (78%)	35 (18%)	8 (4%)	2	18
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%)	2	18
57	AR	73/75 (97%)	59 (81%)	11 (15%)	3 (4%)	2	18
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	4
59	AT	55/57 (96%)	31 (56%)	17 (31%)	7 (13%)	0	4
60	AJ	58/60 (97%)	47 (81%)	10 (17%)	1 (2%)	7	37
60	AU	58/60 (97%)	47 (81%)	10 (17%)	1 (2%)	7	37
61	AK	49/51 (96%)	44 (90%)	4 (8%)	1 (2%)	6	32
61	AV	49/51 (96%)	44 (90%)	4 (8%)	1 (2%)	6	32
All	All	4184/5793 (72%)	3372 (81%)	701 (17%)	111 (3%)	6	25

All (111) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
51	AA	143	THR
52	AB	436	ILE
54	AD	79	GLU

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Mol	Chain	Res	Type
55	AE	70	ALA
55	AE	177	PRO
59	AI	29	LEU
59	AI	49	VAL
51	AL	143	THR
52	AM	436	ILE
54	AO	79	GLU
55	AP	70	ALA
55	AP	177	PRO
59	AT	29	LEU
59	AT	49	VAL
7	G	101	HIS
54	AD	158	ILE
55	AE	71	MET
55	AE	87	MET
55	AE	124	LEU
59	AI	42	VAL
54	AO	158	ILE
55	AP	71	MET
55	AP	87	MET
55	AP	124	LEU
59	AT	42	VAL
54	AD	80	MET
55	AE	69	LEU
55	AP	69	LEU
9	I	80	CYS
51	AA	337	VAL
52	AB	153	GLN
53	AC	62	ALA
53	AC	80	ARG
53	AC	82	MET
53	AC	107	TYR
59	AI	28	PRO
51	AL	337	VAL
52	AM	153	GLN
53	AN	62	ALA
53	AN	80	ARG
53	AN	82	MET
53	AN	107	TYR
54	AO	80	MET
59	AT	28	PRO
7	G	41	CYS

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Mol	Chain	Res	Type
51	AA	50	GLU
51	AA	92	ARG
51	AA	277	ILE
51	AA	338	LEU
52	AB	68	LEU
52	AB	396	SER
53	AC	275	LEU
54	AD	180	SER
55	AE	152	ASP
60	AJ	11	SER
51	AL	50	GLU
51	AL	92	ARG
51	AL	277	ILE
51	AL	338	LEU
52	AM	68	LEU
52	AM	396	SER
53	AN	223	TYR
53	AN	275	LEU
54	AO	180	SER
55	AP	152	ASP
60	AU	11	SER
53	AC	223	TYR
55	AE	106	ILE
57	AG	7	LEU
57	AG	29	TYR
59	AI	27	ARG
59	AI	41	PRO
55	AP	106	ILE
57	AR	7	LEU
57	AR	29	TYR
59	AT	41	PRO
51	AA	268	VAL
53	AC	57	PRO
51	AL	268	VAL
53	AN	57	PRO
59	AT	27	ARG
52	AB	226	ILE
53	AC	145	VAL
53	AC	238	ILE
54	AD	175	THR
61	AK	33	VAL
52	AM	226	ILE

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Mol	Chain	Res	Type
53	AN	145	VAL
53	AN	164	ILE
53	AN	238	ILE
54	AO	175	THR
61	AV	33	VAL
53	AC	164	ILE
53	AC	195	VAL
53	AC	243	VAL
53	AC	350	ILE
54	AD	52	VAL
53	AN	195	VAL
53	AN	243	VAL
53	AN	350	ILE
54	AO	52	VAL
53	AC	268	ILE
53	AC	285	PRO
54	AD	93	LYS
59	AI	40	SER
53	AN	268	ILE
54	AO	93	LYS
59	AT	40	SER
57	AG	34	ILE
53	AN	285	PRO
57	AR	34	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	0	3
All	All	32/32 (100%)	30 (94%)	2 (6%)	17	36

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

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

Sometimes 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 oligosaccharides 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	$\# Z > 2$
62	SF4	G	801	7	0,12,12	-	-	-		
64	HEM	AC	402	-	41,50,50	2.90	19 (46%)	45,82,82	2.47	16 (35%)
64	HEM	AD	301	-	41,50,50	3.03	19 (46%)	45,82,82	2.66	19 (42%)
62	SF4	I	202	9	0,12,12	-	-	-		
64	HEM	AN	402	-	41,50,50	2.90	19 (46%)	45,82,82	2.48	16 (35%)
64	HEM	AO	301	-	41,50,50	3.03	19 (46%)	45,82,82	2.66	20 (44%)
62	SF4	G	802	7	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
62	SF4	F	500	6	0,12,12	-	-	-		
63	FES	E	201	5	0,4,4	-	-	-		
63	FES	AP	201	-	0,4,4	-	-	-		
62	SF4	I	201	9	0,12,12	-	-	-		
64	HEM	AC	401	-	41,50,50	3.05	20 (48%)	45,82,82	2.91	14 (31%)
64	HEM	AN	401	-	41,50,50	3.05	19 (46%)	45,82,82	2.91	14 (31%)
63	FES	AE	201	-	0,4,4	-	-	-		
62	SF4	B	201	2	0,12,12	-	-	-		
63	FES	G	803	7	0,4,4	-	-	-		

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
62	SF4	G	801	7	-	-	0/6/5/5
64	HEM	AC	402	-	-	7/12/54/54	-
64	HEM	AD	301	-	-	2/12/54/54	-
62	SF4	I	202	9	-	-	0/6/5/5
64	HEM	AN	402	-	-	8/12/54/54	-
64	HEM	AO	301	-	-	2/12/54/54	-
62	SF4	G	802	7	-	-	0/6/5/5
62	SF4	F	500	6	-	-	0/6/5/5
63	FES	E	201	5	-	-	0/1/1/1
63	FES	AP	201	-	-	-	0/1/1/1
62	SF4	I	201	9	-	-	0/6/5/5
64	HEM	AC	401	-	-	6/12/54/54	-
64	HEM	AN	401	-	-	6/12/54/54	-
63	FES	AE	201	-	-	-	0/1/1/1
62	SF4	B	201	2	-	-	0/6/5/5
63	FES	G	803	7	-	-	0/1/1/1

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	AN	401	HEM	C4D-C3D	-7.63	1.31	1.45
64	AC	401	HEM	C4D-C3D	-7.61	1.31	1.45
64	AD	301	HEM	C4D-C3D	-6.80	1.33	1.45
64	AO	301	HEM	C4D-C3D	-6.79	1.33	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	AO	301	HEM	C1B-C2B	-6.64	1.31	1.44
64	AD	301	HEM	C1B-C2B	-6.63	1.31	1.44
64	AC	401	HEM	C3C-C2C	-6.60	1.31	1.40
64	AN	401	HEM	C3C-C2C	-6.59	1.31	1.40
64	AC	402	HEM	C1B-C2B	-6.17	1.32	1.44
64	AN	402	HEM	C1B-C2B	-6.15	1.32	1.44
64	AC	402	HEM	C4D-C3D	-5.99	1.34	1.45
64	AN	402	HEM	C4D-C3D	-5.95	1.34	1.45
64	AC	402	HEM	CHA-C4D	5.88	1.50	1.35
64	AN	402	HEM	CHA-C4D	5.85	1.50	1.35
64	AC	402	HEM	C1D-C2D	-5.84	1.33	1.44
64	AN	402	HEM	C1D-C2D	-5.82	1.33	1.44
64	AC	402	HEM	C3B-C4B	-5.74	1.33	1.44
64	AN	402	HEM	C3B-C4B	-5.74	1.33	1.44
64	AO	301	HEM	C3C-C2C	-5.63	1.32	1.40
64	AD	301	HEM	C1D-C2D	-5.60	1.33	1.44
64	AO	301	HEM	C3B-C4B	-5.57	1.33	1.44
64	AD	301	HEM	C3B-C4B	-5.56	1.33	1.44
64	AD	301	HEM	C3C-C2C	-5.55	1.32	1.40
64	AO	301	HEM	C1D-C2D	-5.53	1.33	1.44
64	AN	401	HEM	C3B-C4B	-5.40	1.34	1.44
64	AC	401	HEM	C3B-C4B	-5.36	1.34	1.44
64	AN	401	HEM	C1D-C2D	-5.35	1.34	1.44
64	AN	401	HEM	CHA-C4D	5.34	1.48	1.35
64	AC	401	HEM	CHA-C4D	5.33	1.48	1.35
64	AC	401	HEM	C1D-C2D	-5.31	1.34	1.44
64	AN	401	HEM	CHB-C1B	5.19	1.48	1.35
64	AC	401	HEM	CHB-C1B	5.17	1.48	1.35
64	AD	301	HEM	CHB-C1B	5.13	1.48	1.35
64	AO	301	HEM	CHB-C1B	5.12	1.48	1.35
64	AC	401	HEM	C1B-C2B	-5.12	1.34	1.44
64	AN	401	HEM	C1B-C2B	-5.09	1.34	1.44
64	AD	301	HEM	CHA-C4D	4.94	1.47	1.35
64	AO	301	HEM	CHA-C4D	4.91	1.47	1.35
64	AC	402	HEM	CHB-C1B	4.82	1.47	1.35
64	AN	402	HEM	CHB-C1B	4.79	1.47	1.35
64	AD	301	HEM	CBB-CAB	4.67	1.53	1.30
64	AO	301	HEM	CBB-CAB	4.65	1.53	1.30
64	AN	402	HEM	CBB-CAB	4.61	1.53	1.30
64	AC	402	HEM	CBB-CAB	4.60	1.53	1.30
64	AN	402	HEM	C3C-C2C	-4.51	1.34	1.40
64	AC	402	HEM	C3C-C2C	-4.49	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	AC	401	HEM	CBB-CAB	4.47	1.52	1.30
64	AN	401	HEM	CBB-CAB	4.46	1.52	1.30
64	AN	401	HEM	C2C-C1C	-4.33	1.32	1.42
64	AC	401	HEM	C2C-C1C	-4.33	1.32	1.42
64	AO	301	HEM	C2C-C1C	-4.31	1.32	1.42
64	AD	301	HEM	C2C-C1C	-4.30	1.32	1.42
64	AC	402	HEM	C2C-C1C	-4.21	1.33	1.42
64	AN	402	HEM	C2C-C1C	-4.18	1.33	1.42
64	AO	301	HEM	CBC-CAC	3.75	1.54	1.29
64	AD	301	HEM	CBC-CAC	3.74	1.54	1.29
64	AC	401	HEM	CBC-CAC	3.49	1.52	1.29
64	AN	401	HEM	CBC-CAC	3.48	1.52	1.29
64	AC	402	HEM	CBC-CAC	3.42	1.52	1.29
64	AN	402	HEM	CBC-CAC	3.40	1.51	1.29
64	AN	401	HEM	CHC-C4B	3.24	1.50	1.41
64	AC	402	HEM	C4A-CHB	3.23	1.50	1.41
64	AN	402	HEM	C4A-CHB	3.22	1.50	1.41
64	AC	401	HEM	CHC-C4B	3.22	1.50	1.41
64	AO	301	HEM	C2A-C3A	3.21	1.47	1.37
64	AD	301	HEM	C2A-C3A	3.17	1.47	1.37
64	AN	402	HEM	C1A-CHA	3.08	1.49	1.41
64	AC	401	HEM	C2A-C3A	3.06	1.46	1.37
64	AC	402	HEM	C1A-CHA	3.05	1.49	1.41
64	AN	401	HEM	C2A-C3A	3.04	1.46	1.37
64	AD	301	HEM	CHC-C4B	3.03	1.49	1.41
64	AO	301	HEM	CHC-C4B	2.99	1.49	1.41
64	AN	402	HEM	O2A-CGA	-2.94	1.20	1.30
64	AC	402	HEM	O2A-CGA	-2.94	1.20	1.30
64	AO	301	HEM	C4A-CHB	2.93	1.49	1.41
64	AC	402	HEM	CHD-C1D	2.93	1.49	1.41
64	AN	402	HEM	CHD-C1D	2.91	1.49	1.41
64	AD	301	HEM	C4A-CHB	2.90	1.49	1.41
64	AN	402	HEM	C2A-C3A	2.89	1.46	1.37
64	AC	401	HEM	C1A-CHA	2.88	1.49	1.41
64	AD	301	HEM	CHD-C1D	2.86	1.49	1.41
64	AC	402	HEM	C2A-C3A	2.86	1.46	1.37
64	AO	301	HEM	CHD-C1D	2.86	1.49	1.41
64	AN	401	HEM	C1A-CHA	2.83	1.48	1.41
64	AN	401	HEM	CHD-C1D	2.78	1.49	1.41
64	AC	401	HEM	CHD-C1D	2.77	1.49	1.41
64	AC	401	HEM	C3B-C2B	-2.69	1.31	1.37
64	AO	301	HEM	O2D-CGD	-2.68	1.21	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	AN	401	HEM	C3B-C2B	-2.66	1.31	1.37
64	AD	301	HEM	O2D-CGD	-2.66	1.21	1.30
64	AC	401	HEM	C4A-CHB	2.64	1.48	1.41
64	AN	401	HEM	C4A-CHB	2.62	1.48	1.41
64	AO	301	HEM	O2A-CGA	-2.61	1.22	1.30
64	AD	301	HEM	O2A-CGA	-2.59	1.22	1.30
64	AD	301	HEM	C1A-CHA	2.59	1.48	1.41
64	AO	301	HEM	C1A-CHA	2.57	1.48	1.41
64	AN	401	HEM	C4B-NB	2.53	1.44	1.38
64	AC	401	HEM	C4B-NB	2.53	1.44	1.38
64	AC	401	HEM	O2A-CGA	-2.50	1.22	1.30
64	AD	301	HEM	C3C-CAC	2.50	1.52	1.47
64	AN	401	HEM	O2A-CGA	-2.49	1.22	1.30
64	AO	301	HEM	C3C-CAC	2.49	1.52	1.47
64	AD	301	HEM	C3D-C2D	-2.44	1.31	1.36
64	AN	402	HEM	CHC-C4B	2.44	1.48	1.41
64	AC	402	HEM	CHC-C4B	2.43	1.48	1.41
64	AO	301	HEM	C3D-C2D	-2.42	1.31	1.36
64	AC	402	HEM	O2D-CGD	-2.33	1.22	1.30
64	AN	402	HEM	O2D-CGD	-2.32	1.22	1.30
64	AN	401	HEM	O2D-CGD	-2.27	1.23	1.30
64	AC	401	HEM	O2D-CGD	-2.24	1.23	1.30
64	AN	402	HEM	C3C-CAC	2.15	1.52	1.47
64	AC	402	HEM	C3C-CAC	2.11	1.52	1.47
64	AC	402	HEM	C3B-C2B	-2.03	1.33	1.37
64	AC	401	HEM	C3D-C2D	-2.01	1.32	1.36
64	AN	402	HEM	C3B-C2B	-2.00	1.33	1.37

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	AC	402	HEM	C4C-CHD-C1D	-8.88	110.83	122.56
64	AN	402	HEM	C4C-CHD-C1D	-8.87	110.85	122.56
64	AC	401	HEM	C4B-CHC-C1C	-8.53	111.31	122.56
64	AN	401	HEM	C4B-CHC-C1C	-8.50	111.33	122.56
64	AO	301	HEM	C4B-CHC-C1C	-7.92	112.10	122.56
64	AD	301	HEM	C4B-CHC-C1C	-7.92	112.11	122.56
64	AC	401	HEM	C4C-CHD-C1D	-7.55	112.59	122.56
64	AN	401	HEM	C4C-CHD-C1D	-7.53	112.62	122.56
64	AN	402	HEM	C4B-CHC-C1C	-7.26	112.98	122.56
64	AO	301	HEM	C4C-CHD-C1D	-7.22	113.02	122.56
64	AD	301	HEM	C4C-CHD-C1D	-7.22	113.03	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	AC	402	HEM	C4B-CHC-C1C	-7.21	113.05	122.56
64	AN	401	HEM	C4D-ND-C1D	-6.27	98.59	105.07
64	AC	401	HEM	C4D-ND-C1D	-6.24	98.63	105.07
64	AN	401	HEM	C1B-NB-C4B	-5.22	99.68	105.07
64	AC	401	HEM	C1B-NB-C4B	-5.18	99.72	105.07
64	AD	301	HEM	C4D-ND-C1D	-4.84	100.07	105.07
64	AO	301	HEM	C4D-ND-C1D	-4.83	100.08	105.07
64	AC	401	HEM	C2C-C3C-C4C	4.75	110.21	106.90
64	AC	401	HEM	CHC-C4B-NB	4.69	129.53	124.43
64	AN	401	HEM	C2C-C3C-C4C	4.69	110.17	106.90
64	AD	301	HEM	CHB-C1B-NB	4.67	130.15	124.38
64	AO	301	HEM	CHB-C1B-NB	4.65	130.12	124.38
64	AN	401	HEM	CHC-C4B-NB	4.65	129.48	124.43
64	AD	301	HEM	C1B-NB-C4B	-4.48	100.44	105.07
64	AO	301	HEM	C1B-NB-C4B	-4.45	100.47	105.07
64	AN	401	HEM	C4B-C3B-C2B	4.32	110.55	107.11
64	AC	401	HEM	C4B-C3B-C2B	4.31	110.53	107.11
64	AC	401	HEM	CBB-CAB-C3B	-3.93	108.06	127.62
64	AN	401	HEM	CBB-CAB-C3B	-3.92	108.09	127.62
64	AN	401	HEM	CHA-C4D-C3D	-3.83	118.13	125.33
64	AN	401	HEM	CHA-C4D-ND	3.83	129.11	124.38
64	AC	401	HEM	CHA-C4D-ND	3.82	129.10	124.38
64	AC	401	HEM	CHA-C4D-C3D	-3.81	118.17	125.33
64	AN	402	HEM	CHC-C4B-NB	3.48	128.21	124.43
64	AN	402	HEM	CHB-C1B-NB	3.42	128.60	124.38
64	AC	402	HEM	CHB-C1B-NB	3.41	128.59	124.38
64	AO	301	HEM	CHC-C4B-NB	3.40	128.12	124.43
64	AC	402	HEM	CHC-C4B-NB	3.39	128.12	124.43
64	AC	402	HEM	C1B-NB-C4B	-3.35	101.61	105.07
64	AC	402	HEM	CHD-C1D-ND	3.30	128.01	124.43
64	AD	301	HEM	CHC-C4B-NB	3.29	128.00	124.43
64	AN	402	HEM	CHD-C1D-ND	3.29	128.00	124.43
64	AN	402	HEM	C1B-NB-C4B	-3.27	101.69	105.07
64	AD	301	HEM	C3B-C2B-C1B	3.24	108.89	106.49
64	AN	401	HEM	CHB-C1B-NB	3.23	128.37	124.38
64	AO	301	HEM	C3B-C2B-C1B	3.21	108.87	106.49
64	AC	401	HEM	CHB-C1B-NB	3.21	128.34	124.38
64	AD	301	HEM	CHA-C4D-ND	3.10	128.21	124.38
64	AO	301	HEM	CHA-C4D-ND	3.08	128.18	124.38
64	AD	301	HEM	CHB-C1B-C2B	-3.03	118.34	126.72
64	AO	301	HEM	CHB-C1B-C2B	-3.02	118.36	126.72
64	AO	301	HEM	C2C-C3C-C4C	2.93	108.94	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	AN	402	HEM	C4B-C3B-C2B	2.90	109.41	107.11
64	AC	402	HEM	C4B-C3B-C2B	2.88	109.41	107.11
64	AC	402	HEM	CBB-CAB-C3B	-2.87	113.35	127.62
64	AN	402	HEM	CBB-CAB-C3B	-2.87	113.35	127.62
64	AC	401	HEM	CHC-C4B-C3B	-2.85	120.20	124.57
64	AN	401	HEM	CHC-C4B-C3B	-2.85	120.20	124.57
64	AD	301	HEM	C2C-C3C-C4C	2.84	108.88	106.90
64	AO	301	HEM	CHA-C4D-C3D	-2.81	120.05	125.33
64	AD	301	HEM	CHA-C4D-C3D	-2.81	120.06	125.33
64	AO	301	HEM	CHD-C1D-ND	2.78	127.45	124.43
64	AD	301	HEM	CHD-C1D-ND	2.72	127.38	124.43
64	AN	402	HEM	C1D-C2D-C3D	2.65	109.74	106.96
64	AD	301	HEM	C1D-C2D-C3D	2.61	109.70	106.96
64	AC	402	HEM	C1D-C2D-C3D	2.59	109.68	106.96
64	AN	401	HEM	CHB-C1B-C2B	-2.56	119.63	126.72
64	AC	401	HEM	CHB-C1B-C2B	-2.55	119.68	126.72
64	AO	301	HEM	C1D-C2D-C3D	2.52	109.61	106.96
64	AN	402	HEM	O2A-CGA-CBA	2.50	122.08	114.03
64	AC	402	HEM	O2A-CGA-CBA	2.50	122.06	114.03
64	AN	402	HEM	C3B-C2B-C1B	2.46	108.31	106.49
64	AC	402	HEM	C3B-C2B-C1B	2.46	108.31	106.49
64	AC	402	HEM	CMC-C2C-C3C	2.38	129.13	124.68
64	AN	402	HEM	CMC-C2C-C3C	2.37	129.12	124.68
64	AO	301	HEM	C4A-C3A-C2A	-2.35	105.36	107.00
64	AD	301	HEM	C4A-C3A-C2A	-2.35	105.36	107.00
64	AO	301	HEM	C4B-C3B-C2B	2.30	108.94	107.11
64	AO	301	HEM	CAD-CBD-CGD	-2.28	108.70	113.60
64	AC	402	HEM	CHB-C1B-C2B	-2.27	120.44	126.72
64	AD	301	HEM	CBB-CAB-C3B	-2.27	116.35	127.62
64	AD	301	HEM	CAD-CBD-CGD	-2.26	108.73	113.60
64	AN	402	HEM	CHB-C1B-C2B	-2.25	120.49	126.72
64	AO	301	HEM	CBB-CAB-C3B	-2.25	116.43	127.62
64	AD	301	HEM	C4B-C3B-C2B	2.23	108.88	107.11
64	AO	301	HEM	CAA-CBA-CGA	-2.16	107.72	113.76
64	AD	301	HEM	CAA-CBA-CGA	-2.12	107.81	113.76
64	AO	301	HEM	CMB-C2B-C1B	-2.12	121.81	125.04
64	AC	402	HEM	C4D-ND-C1D	-2.12	102.89	105.07
64	AN	402	HEM	C4D-ND-C1D	-2.12	102.89	105.07
64	AN	402	HEM	C2C-C3C-C4C	2.11	108.37	106.90
64	AD	301	HEM	CMB-C2B-C1B	-2.09	121.86	125.04
64	AC	401	HEM	CHD-C1D-C2D	-2.08	121.74	124.98
64	AC	402	HEM	C2C-C3C-C4C	2.07	108.34	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	AC	402	HEM	CBA-CAA-C2A	2.06	116.14	112.62
64	AN	402	HEM	CBA-CAA-C2A	2.05	116.12	112.62
64	AN	401	HEM	CHD-C1D-C2D	-2.04	121.80	124.98
64	AO	301	HEM	CHD-C1D-C2D	-2.03	121.81	124.98

There are no chirality outliers.

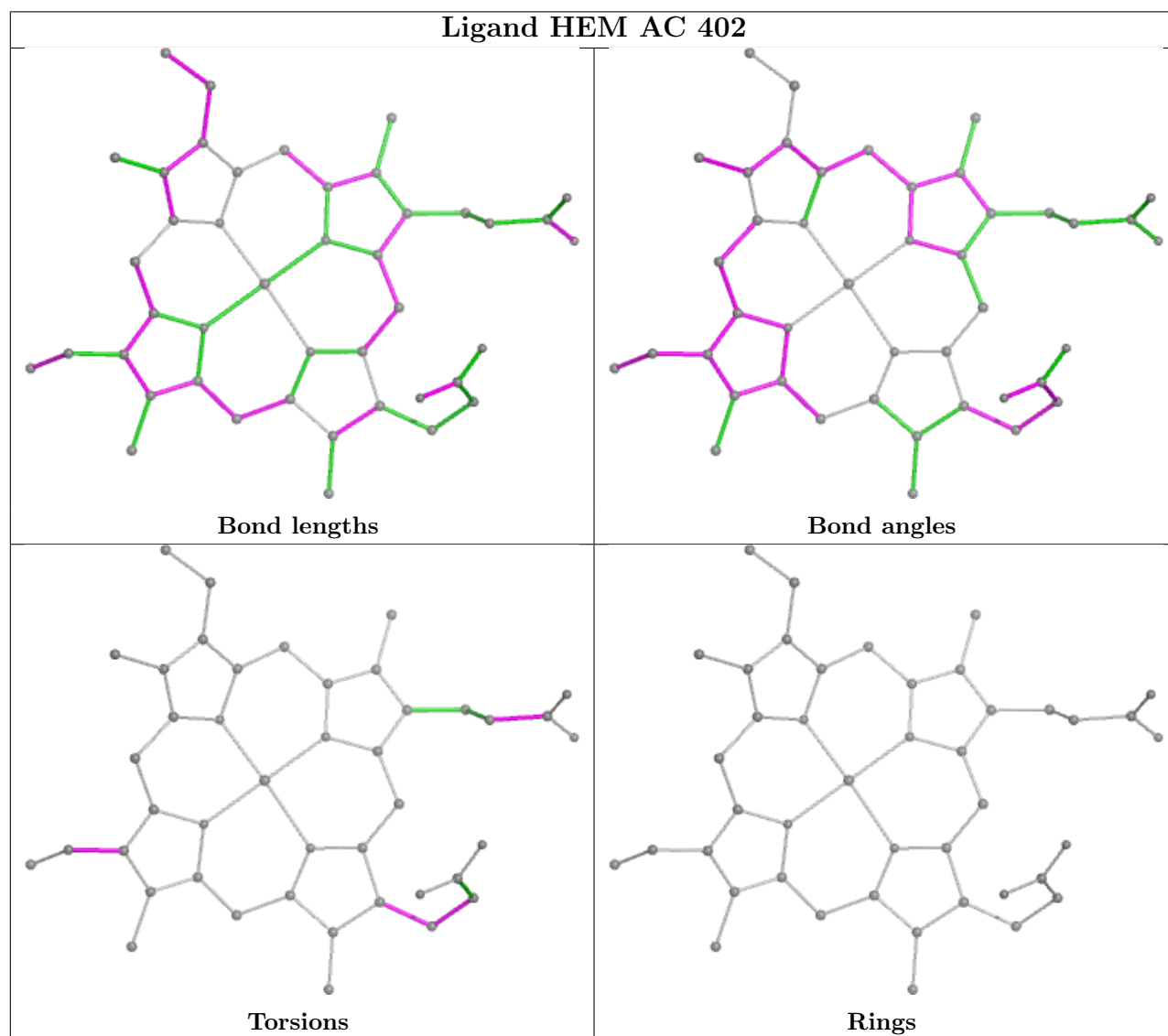
All (31) torsion outliers are listed below:

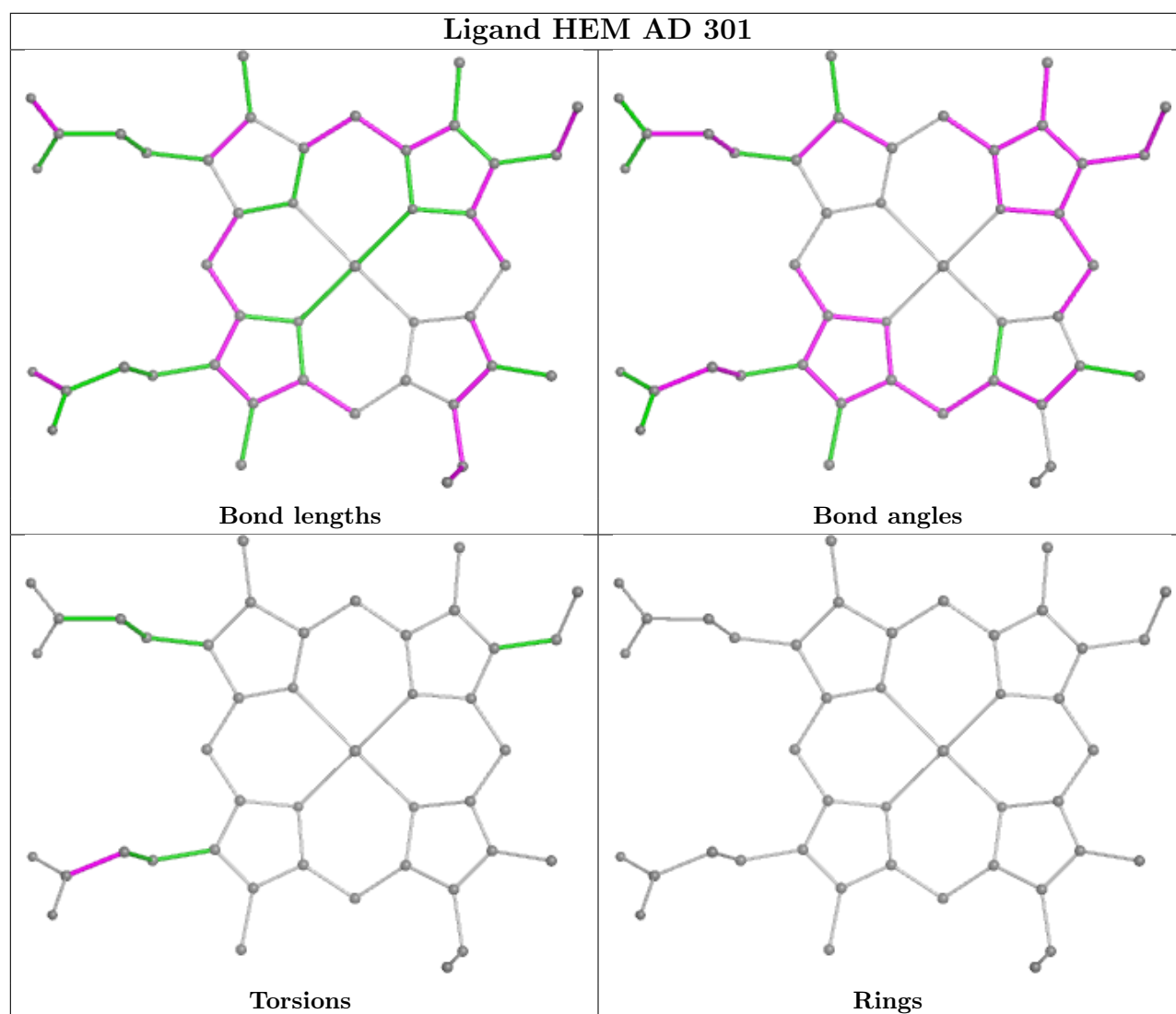
Mol	Chain	Res	Type	Atoms
64	AC	401	HEM	C2B-C3B-CAB-CBB
64	AC	401	HEM	C4B-C3B-CAB-CBB
64	AC	402	HEM	C1A-C2A-CAA-CBA
64	AC	402	HEM	C3A-C2A-CAA-CBA
64	AC	402	HEM	C2B-C3B-CAB-CBB
64	AN	401	HEM	C2B-C3B-CAB-CBB
64	AN	401	HEM	C4B-C3B-CAB-CBB
64	AN	402	HEM	C1A-C2A-CAA-CBA
64	AN	402	HEM	C3A-C2A-CAA-CBA
64	AN	402	HEM	C2B-C3B-CAB-CBB
64	AC	402	HEM	C4B-C3B-CAB-CBB
64	AN	402	HEM	C4B-C3B-CAB-CBB
64	AC	402	HEM	C2A-CAA-CBA-CGA
64	AN	402	HEM	C2A-CAA-CBA-CGA
64	AC	401	HEM	C3D-CAD-CBD-CGD
64	AN	401	HEM	C3D-CAD-CBD-CGD
64	AN	401	HEM	CAD-CBD-CGD-O1D
64	AC	401	HEM	CAD-CBD-CGD-O1D
64	AC	401	HEM	CAD-CBD-CGD-O2D
64	AD	301	HEM	CAD-CBD-CGD-O1D
64	AN	401	HEM	CAD-CBD-CGD-O2D
64	AN	402	HEM	CAD-CBD-CGD-O2D
64	AO	301	HEM	CAD-CBD-CGD-O1D
64	AC	402	HEM	CAD-CBD-CGD-O2D
64	AO	301	HEM	CAD-CBD-CGD-O2D
64	AD	301	HEM	CAD-CBD-CGD-O2D
64	AC	402	HEM	CAD-CBD-CGD-O1D
64	AN	402	HEM	CAD-CBD-CGD-O1D
64	AC	401	HEM	C2A-CAA-CBA-CGA
64	AN	401	HEM	C2A-CAA-CBA-CGA
64	AN	402	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

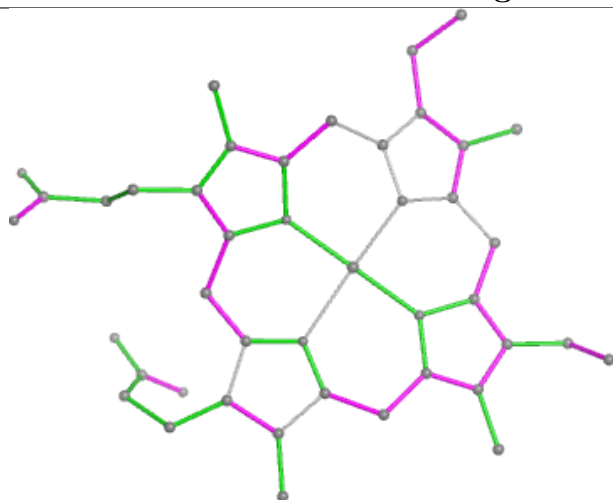
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

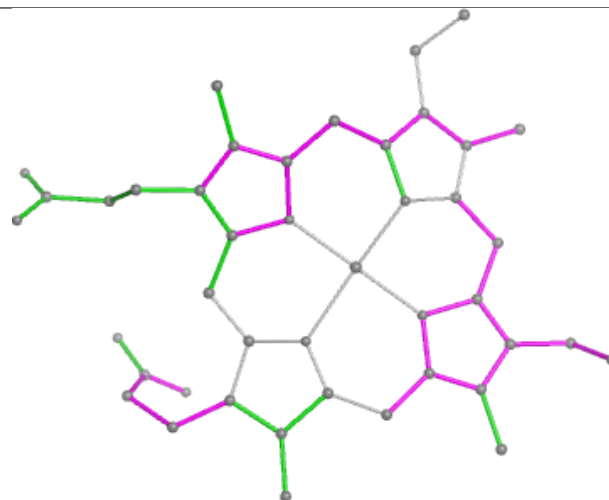




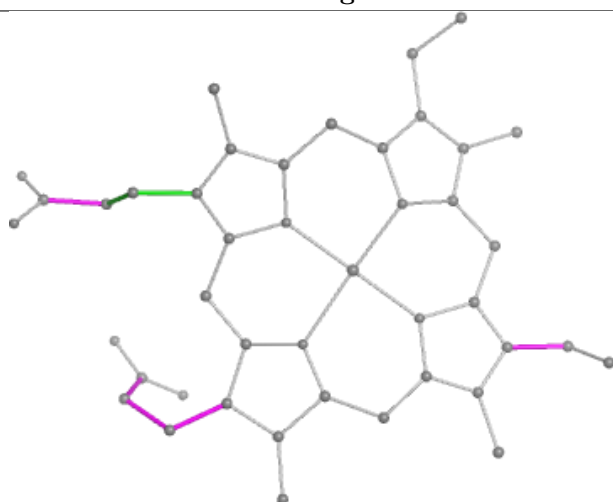
Ligand HEM AN 402



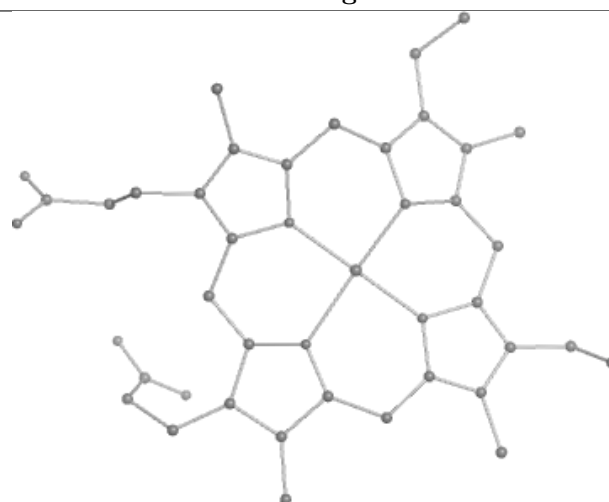
Bond lengths



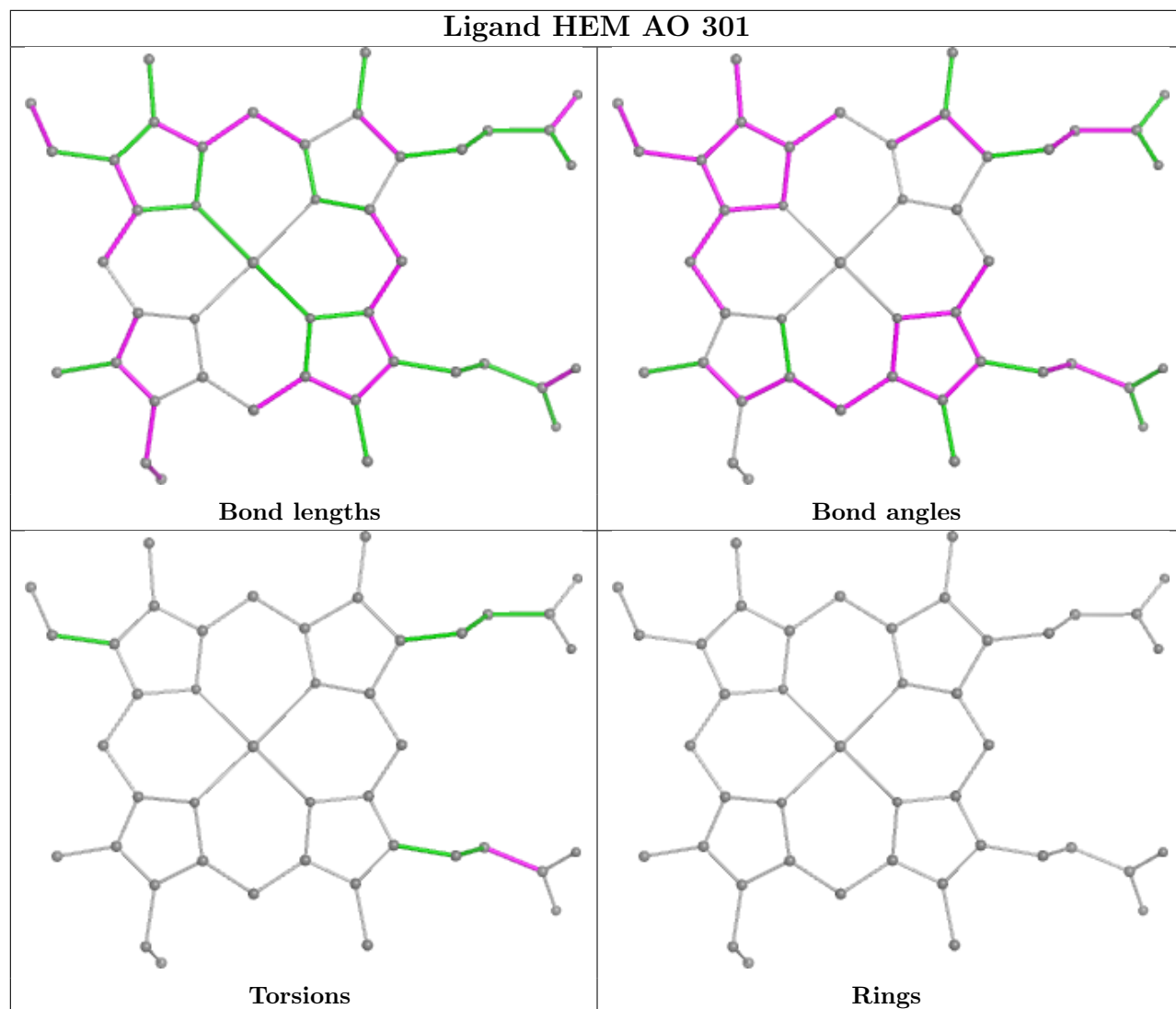
Bond angles



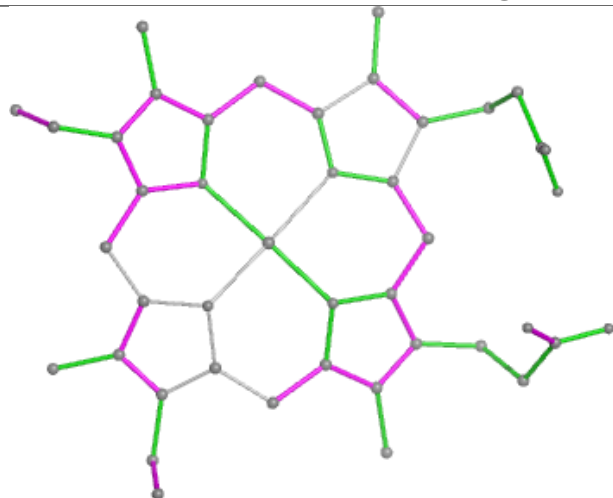
Torsions



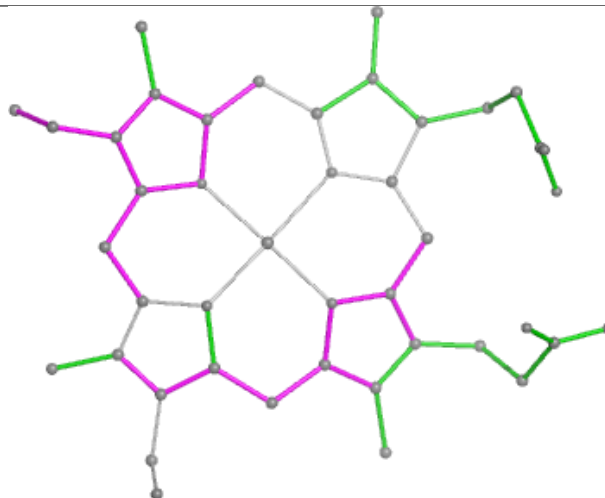
Rings



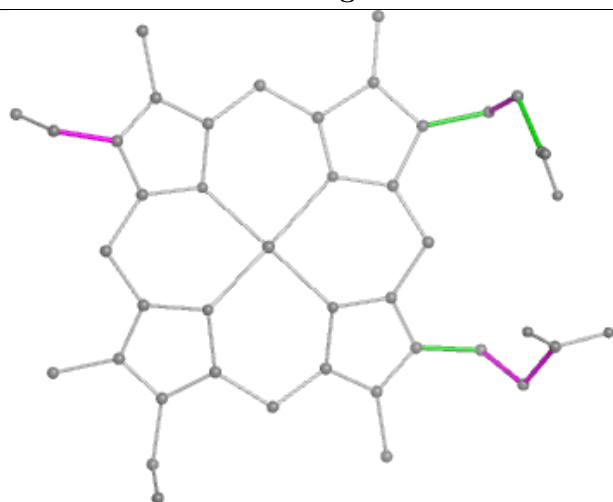
Ligand HEM AC 401



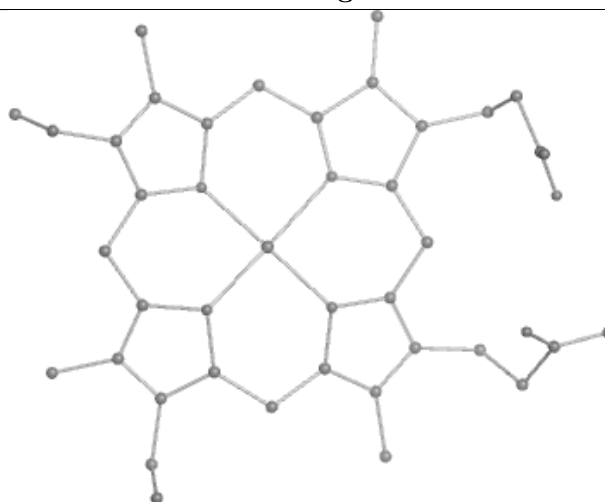
Bond lengths



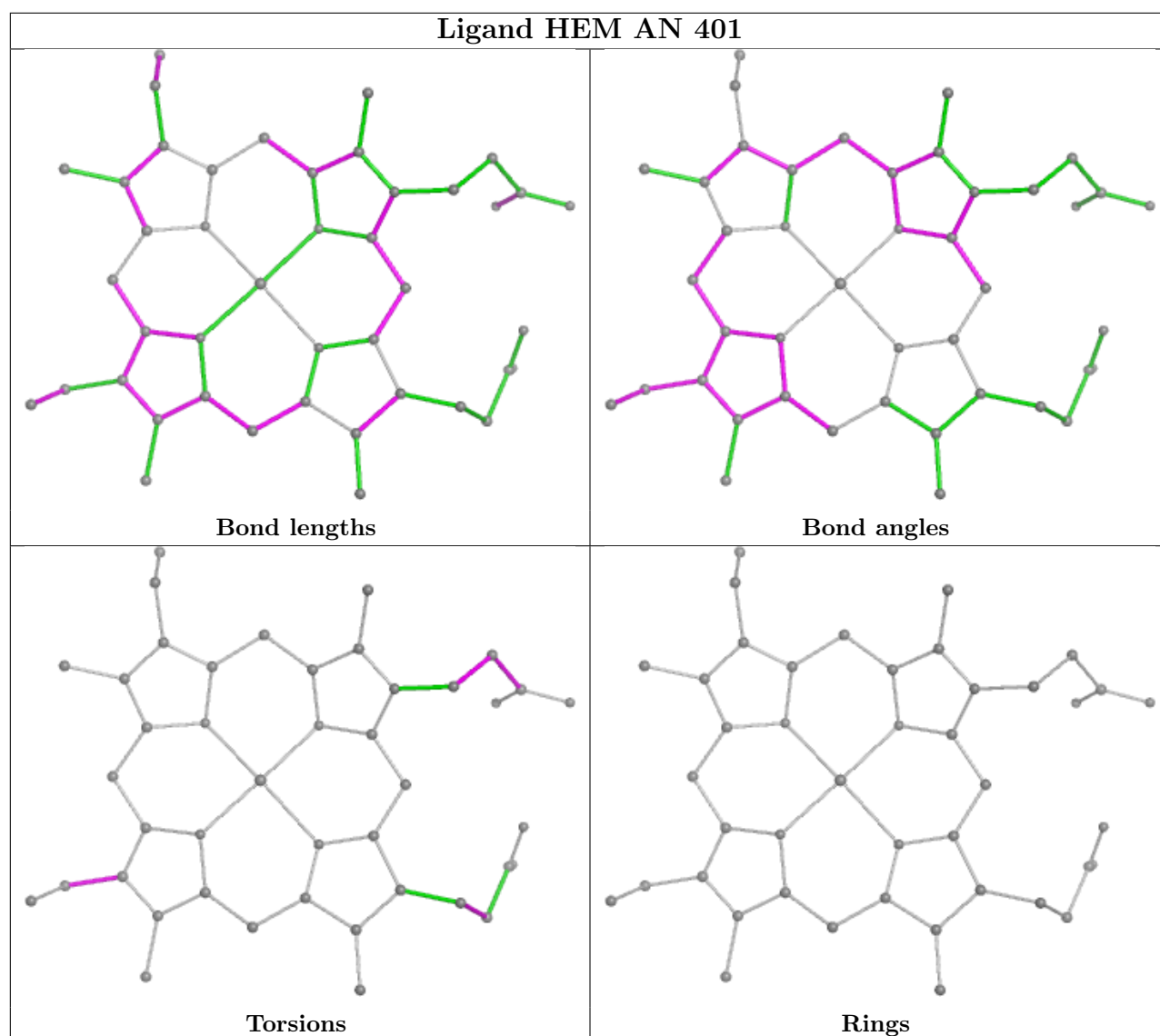
Bond angles



Torsions



Rings



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
10	J	1
1	A	1

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Mol	Chain	Number of breaks
36	k	1
8	H	1
29	c	1
55	AE	1
55	AP	1
53	AC	1
53	AN	1

All 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
1	L	471:UNK	C	487:UNK	N	16.85
1	G	506:UNK	C	525:UNK	N	14.31
1	k	50:UNK	C	54:UNK	N	13.65
1	L	400:UNK	C	408:UNK	N	13.52
1	H	200:UNK	C	217:UNK	N	12.06
1	c	23:UNK	C	28:UNK	N	9.19
1	G	318:UNK	C	322:UNK	N	8.89
1	L	358:UNK	C	363:UNK	N	7.00
1	AE	43:THR	C	44:THR	N	2.11
1	AP	44:THR	C	45:VAL	N	1.09
1	AC	56:THR	C	57:PRO	N	0.83
1	AN	56:THR	C	57:PRO	N	0.83

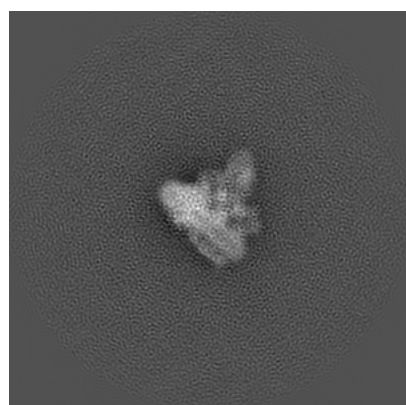
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8129. These allow visual inspection of the internal detail of the map and identification of artifacts.

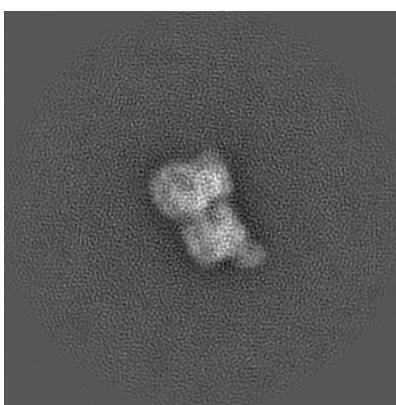
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

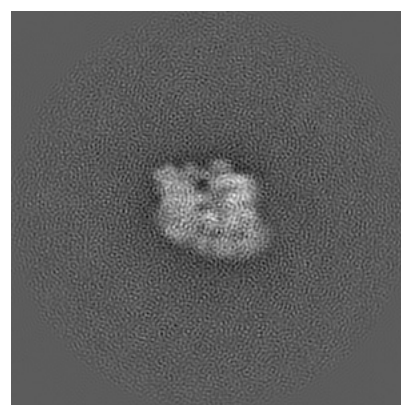
6.1.1 Primary map



X



Y

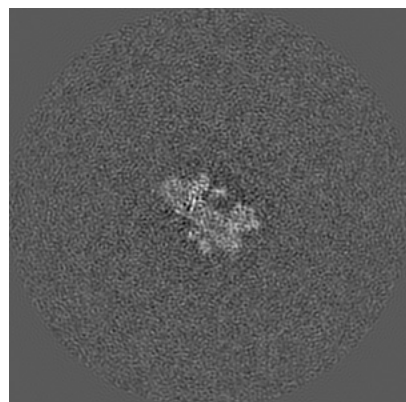


Z

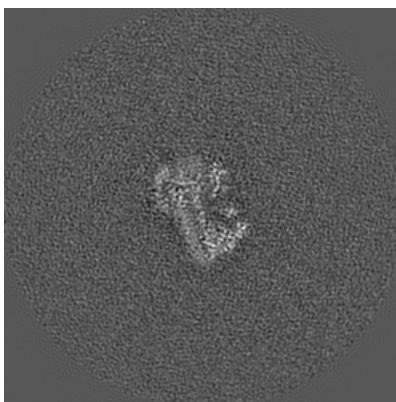
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

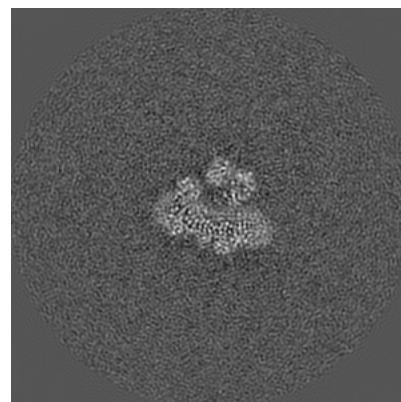
6.2.1 Primary map



X Index: 248



Y Index: 248

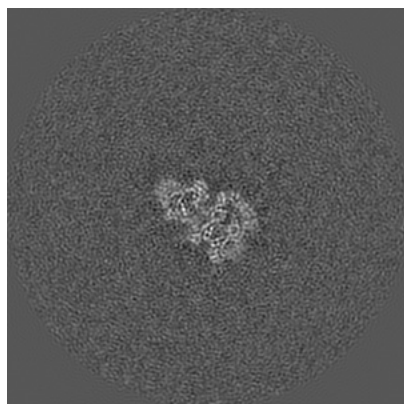


Z Index: 248

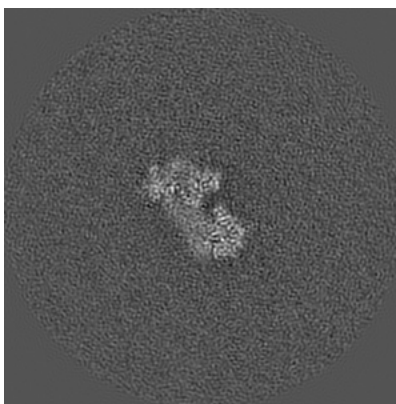
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

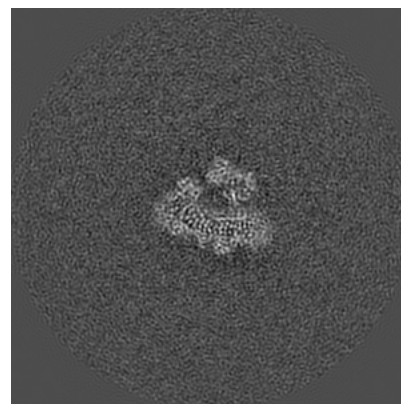
6.3.1 Primary map



X Index: 270



Y Index: 260

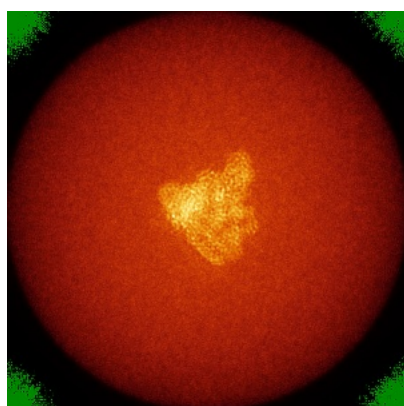


Z Index: 249

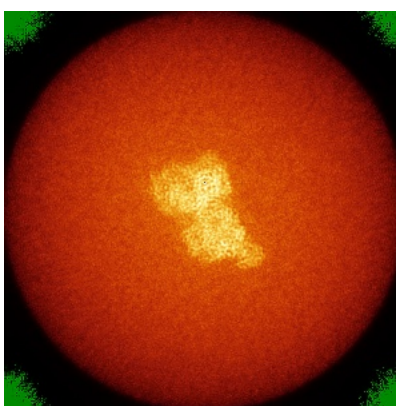
The images above show the largest variance slices of the map in three orthogonal directions.

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

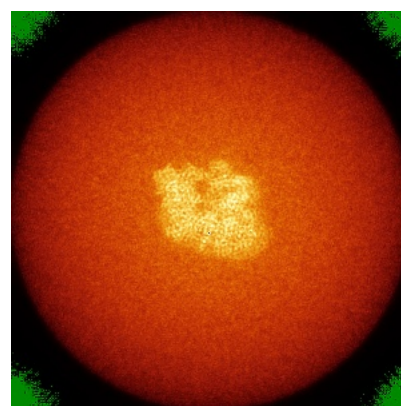
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

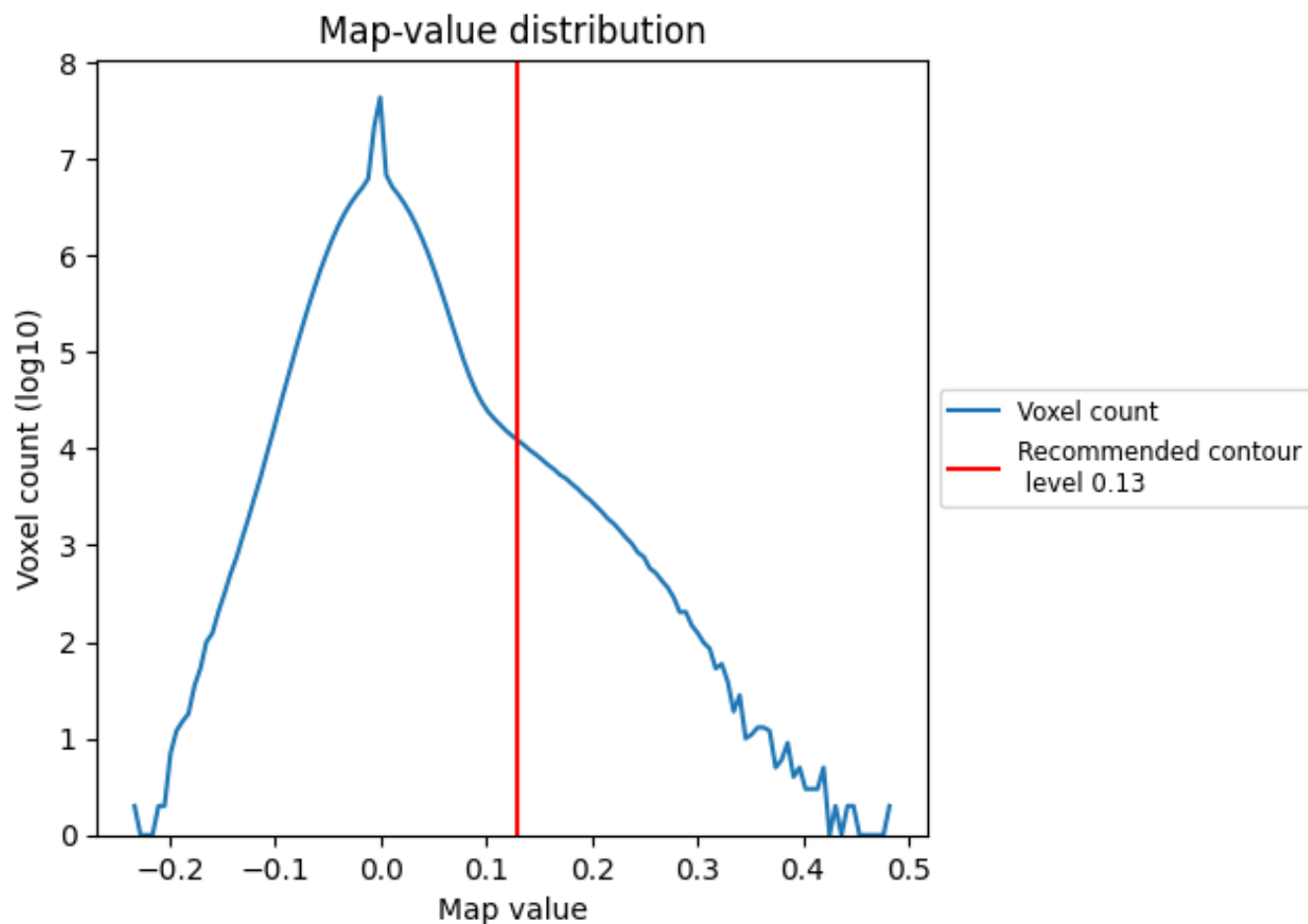
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

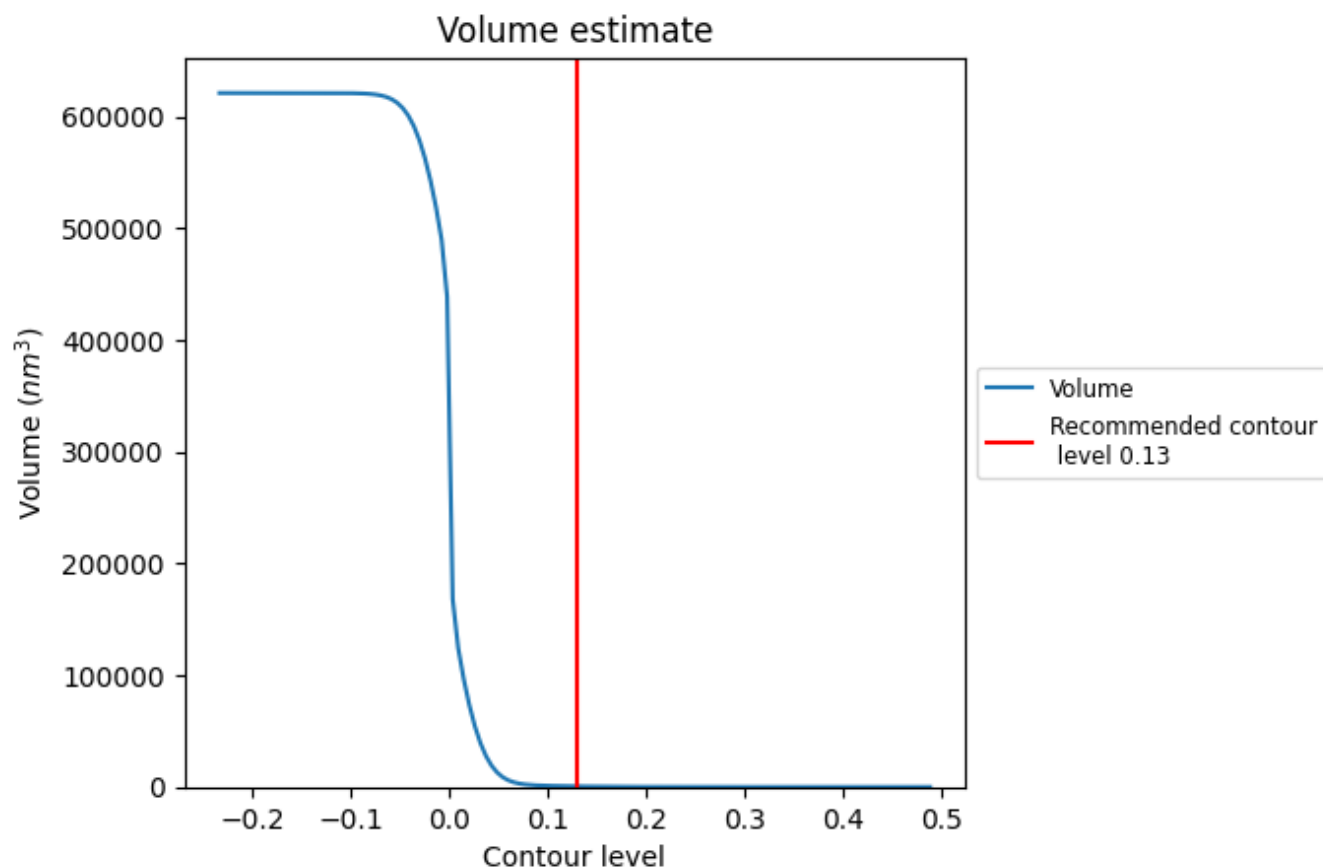
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

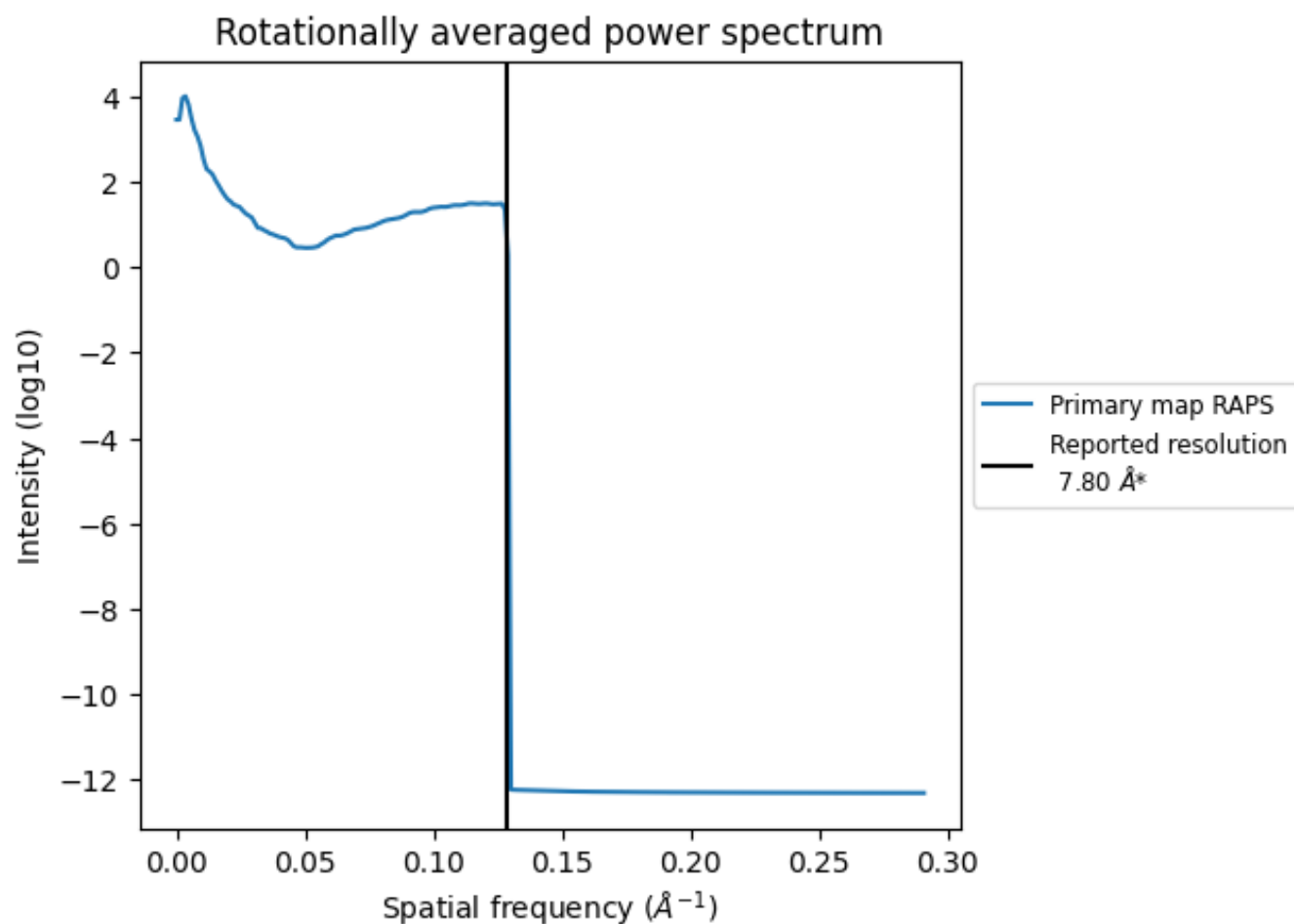
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 528 nm³; this corresponds to an approximate mass of 477 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

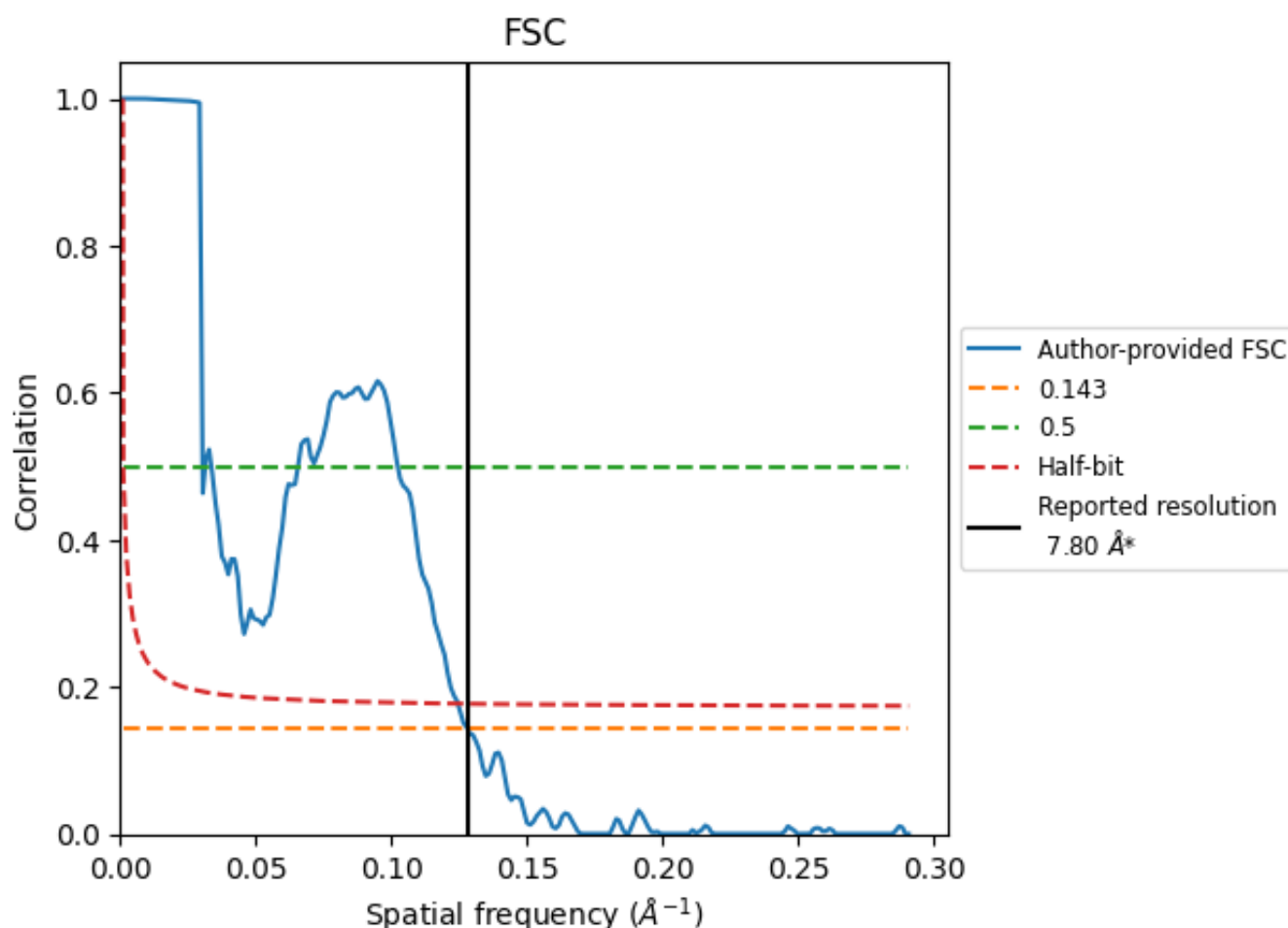


*Reported resolution corresponds to spatial frequency of 0.128 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.128 \AA^{-1}

8.2 Resolution estimates [i](#)

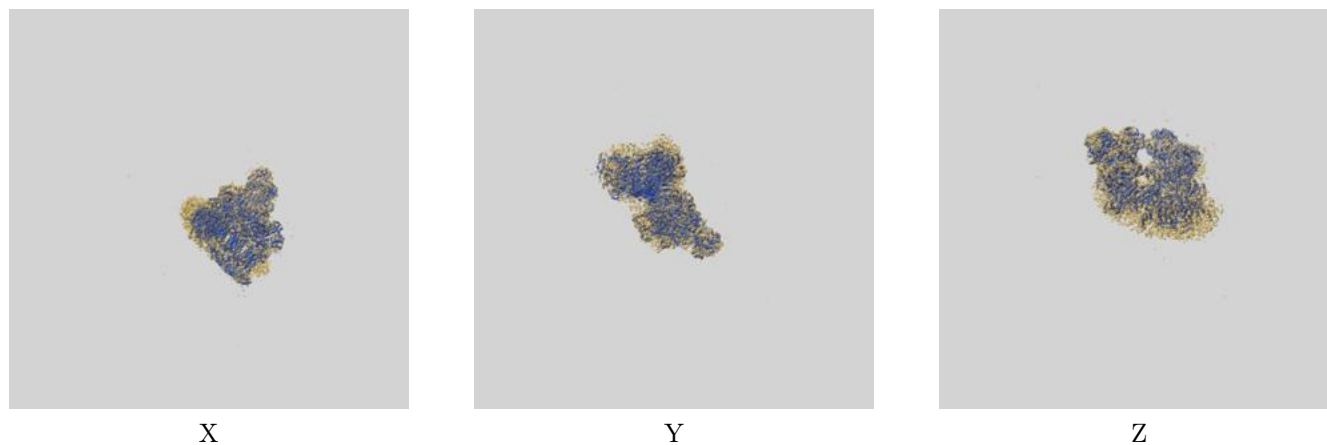
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.80	-	-
Author-provided FSC curve	7.81	32.89	8.03
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

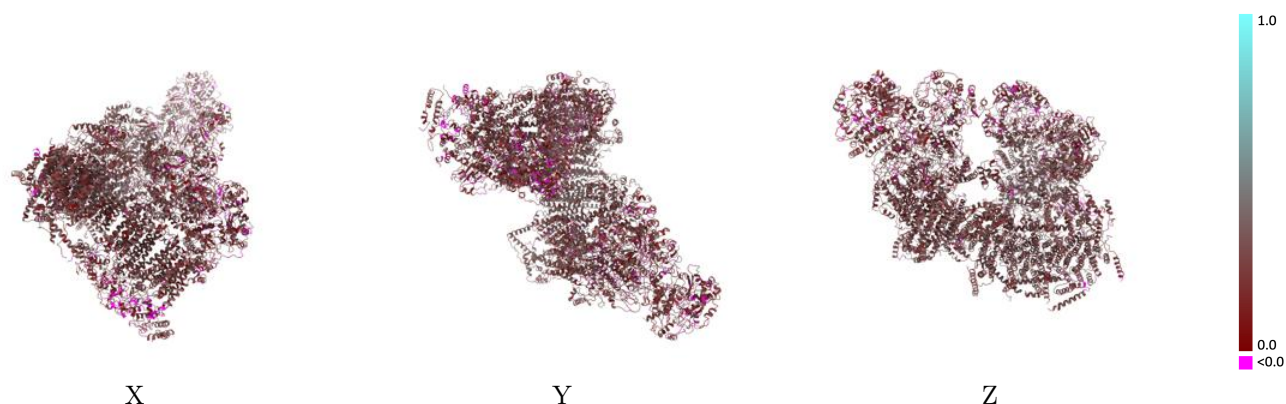
This section contains information regarding the fit between EMDB map EMD-8129 and PDB model 5J8K. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



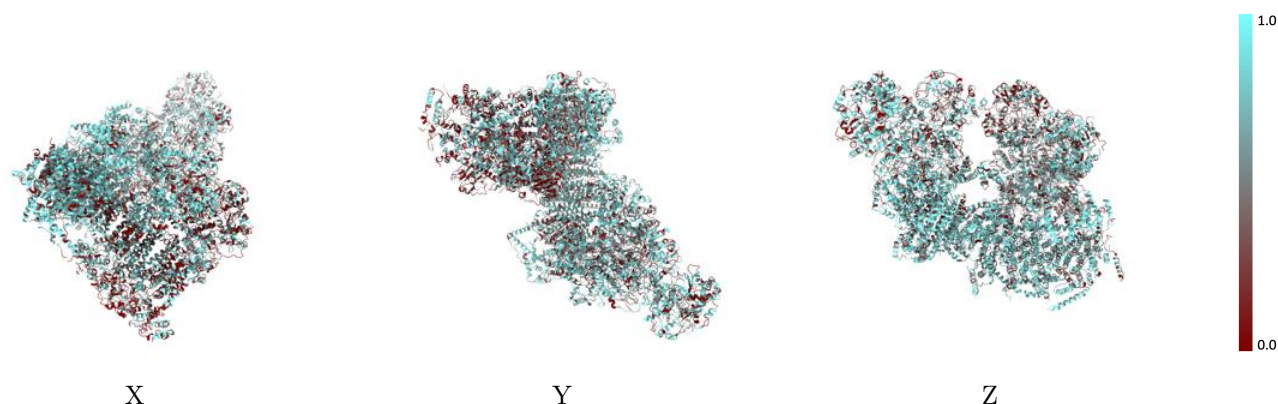
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



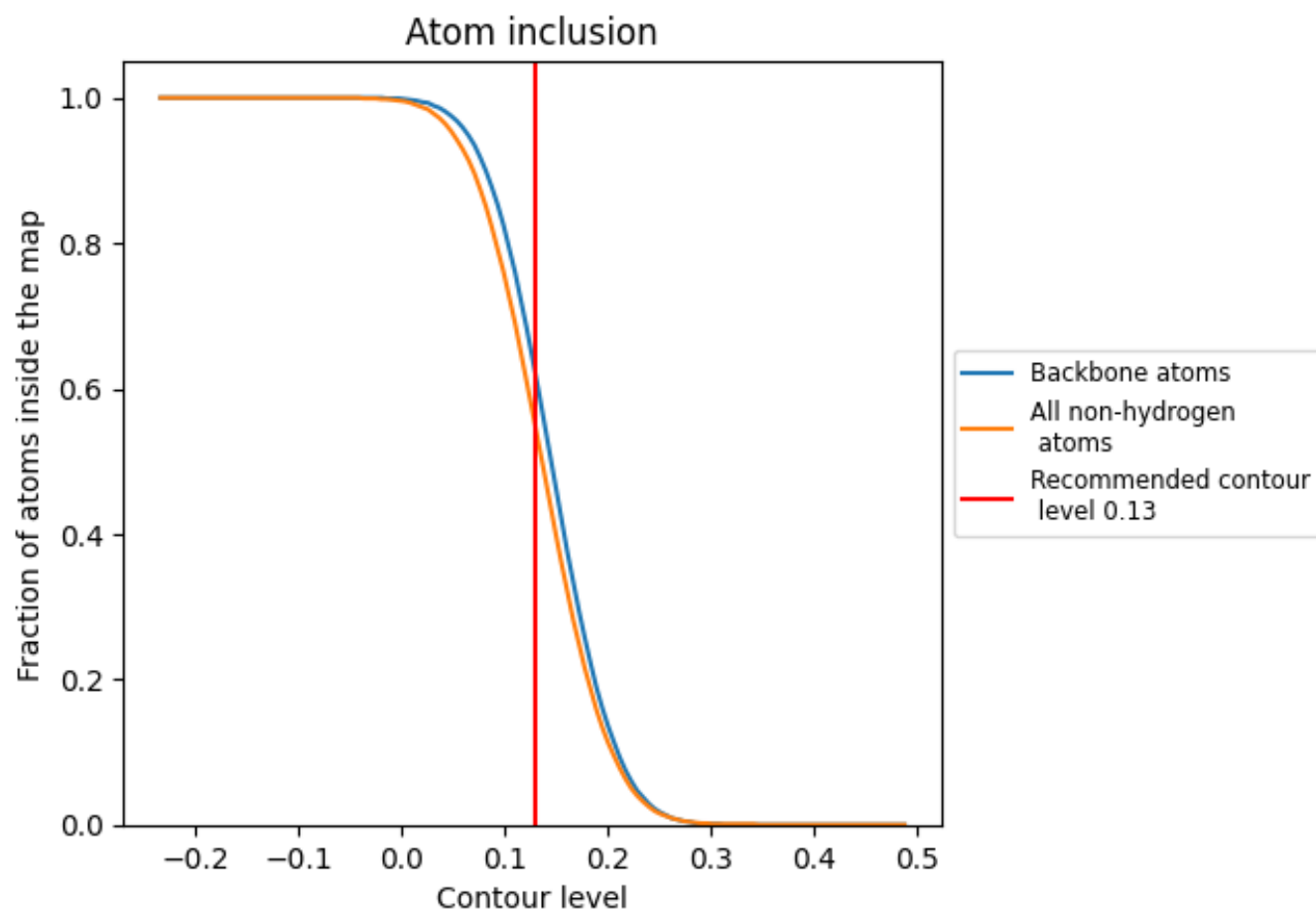
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5470	 0.2420
0	 0.5170	 0.2460
1	 0.6200	 0.2760
2	 0.6840	 0.2160
3	 0.7430	 0.2660
4	 0.4140	 0.2050
5	 0.4760	 0.2600
6	 0.8190	 0.2780
7	 0.7230	 0.2970
8	 0.7480	 0.2760
9	 0.6540	 0.2670
A	 0.5490	 0.2600
AA	 0.5910	 0.2550
AB	 0.5380	 0.2360
AC	 0.5890	 0.2740
AD	 0.4830	 0.2140
AE	 0.2810	 0.1470
AF	 0.5900	 0.2480
AG	 0.5530	 0.2690
AH	 0.6030	 0.2610
AI	 0.1740	 0.1330
AJ	 0.3810	 0.2570
AK	 0.2880	 0.2360
AL	 0.4280	 0.2150
AM	 0.3930	 0.1890
AN	 0.4880	 0.2530
AO	 0.4300	 0.1850
AP	 0.2870	 0.1680
AQ	 0.5670	 0.2370
AR	 0.4260	 0.2210
AS	 0.4240	 0.2530
AT	 0.1250	 0.1240
AU	 0.4240	 0.2270
AV	 0.2560	 0.2200
B	 0.5690	 0.2390



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Chain	Atom inclusion	Q-score
C	 0.6010	 0.2530
D	 0.5940	 0.2520
E	 0.5920	 0.2230
F	 0.5120	 0.1900
G	 0.4870	 0.2100
H	 0.5810	 0.2650
I	 0.6120	 0.2330
J	 0.5210	 0.2570
K	 0.6390	 0.2830
L	 0.6100	 0.2670
M	 0.6630	 0.2800
N	 0.6740	 0.2800
O	 0.5230	 0.2350
P	 0.4800	 0.2260
Q	 0.7090	 0.2750
R	 0.4620	 0.2410
S	 0.5620	 0.2060
T	 0.6570	 0.2880
U	 0.7270	 0.2960
V	 0.6130	 0.2690
W	 0.6820	 0.2590
X	 0.5050	 0.2420
Y	 0.6420	 0.2690
Z	 0.4970	 0.2590
a	 0.6110	 0.2610
b	 0.6520	 0.2770
c	 0.5270	 0.2570
d	 0.5830	 0.2360
e	 0.6760	 0.2890
f	 0.6830	 0.2660
g	 0.7030	 0.2950
h	 0.7900	 0.2850
i	 0.6860	 0.2900
j	 0.6540	 0.2710
k	 0.6650	 0.2850
t	 0.8000	 0.2960
u	 0.3500	 0.1910
v	 0.7110	 0.2730
w	 0.8000	 0.3110
x	 0.7230	 0.3050
y	 0.8170	 0.2990
z	 0.6000	 0.2550