



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 08:10 pm GMT

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

This is a wwPDB EM Validation Summary 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:

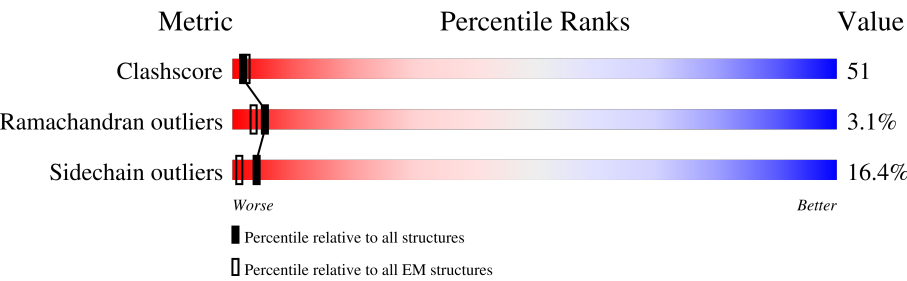
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 9.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
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	c	446	<div><div>15%</div><div>70%</div><div>26%</div><div>.</div></div>
1	l	446	<div><div>13%</div><div>70%</div><div>26%</div><div>.</div></div>
2	m	439	<div><div>13%</div><div>73%</div><div>20%</div><div>5%</div></div>
2	n	439	<div><div>9%</div><div>75%</div><div>19%</div><div>5%</div></div>
3	b	379	<div><div>28%</div><div>69%</div><div>28%</div><div>.</div></div>
3	o	379	<div><div>31%</div><div>74%</div><div>23%</div><div>.</div></div>
4	d	241	<div><div>21%</div><div>78%</div><div>18%</div><div>.</div></div>
4	p	241	<div><div>22%</div><div>76%</div><div>22%</div><div>.</div></div>






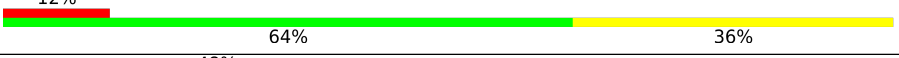
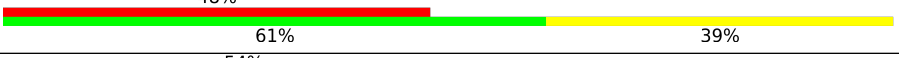
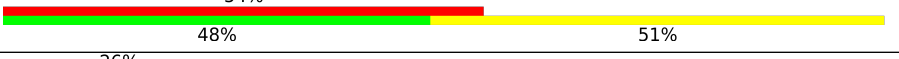
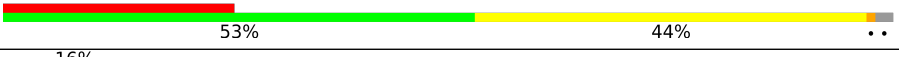


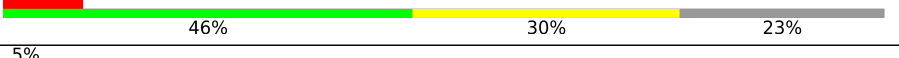





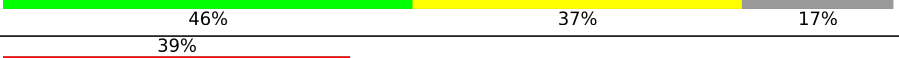


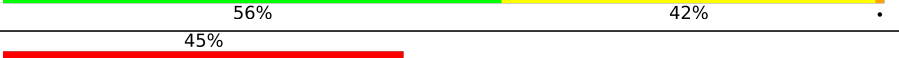
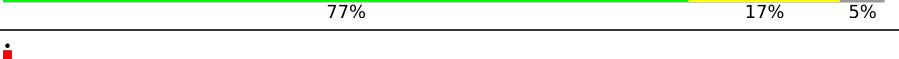

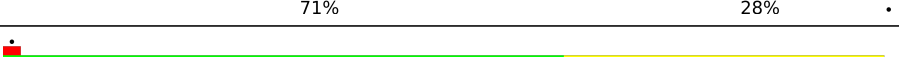

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Mol	Chain	Length	Quality of chain
5	e	196	
5	q	196	
6	f	110	
6	r	110	
7	g	81	
7	s	81	
8	h	78	
8	t	78	
9	i	78	
9	u	78	
10	j	62	
10	v	62	
11	k	56	
11	w	56	
12	x	514	
13	y	227	
14	z	261	
15	1	147	
16	2	109	
17	3	98	
18	4	84	
19	5	85	
20	6	73	
21	7	59	
22	8	56	

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Mol	Chain	Length	Quality of chain
23	9	47	
24	0	46	
25	A	111	
26	B	143	
27	C	154	
28	D	384	
29	E	159	
30	F	411	
31	G	538	
32	H	313	
33	I	162	
34	J	171	
35	K	84	
36	L	601	
37	M	453	
38	N	345	
39	O	220	
40	P	303	
41	Q	85	
42	R	47	
43	S	80	
44	T	75	
45	V	71	
46	W	72	
47	X	330	

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Mol	Chain	Length	Quality of chain
48	Y	106	
49	a	142	
50	U	828	
51	Z	625	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	FES	G	803	-	-	X	-
59	SF4	B	201	-	-	X	-
59	SF4	I	201	-	-	X	-
59	SF4	I	202	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 74493 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

- Molecule 3 is a protein called Cytochrome b.

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

There are 6 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 25 is a protein called complex I.

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

- Molecule 26 is a protein called complex I.

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

- Molecule 27 is a protein called complex I.

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

- Molecule 28 is a protein called complex I.

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

- Molecule 29 is a protein called complex I.

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

- Molecule 30 is a protein called complex I.

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

- Molecule 31 is a protein called complex I.

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

- Molecule 32 is a protein called complex I.

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

- Molecule 33 is a protein called complex I.

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

- Molecule 34 is a protein called complex I.

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

- Molecule 35 is a protein called complex I.

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

- Molecule 36 is a protein called complex I.

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

- Molecule 37 is a protein called complex I.

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

- Molecule 38 is a protein called complex I.

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

- Molecule 39 is a protein called complex I.

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

- Molecule 40 is a protein called complex I.

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

- Molecule 41 is a protein called complex I.

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

- Molecule 42 is a protein called complex I.

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

- Molecule 43 is a protein called complex I.

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

- Molecule 44 is a protein called complex I.

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

- Molecule 45 is a protein called complex I.

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

- Molecule 46 is a protein called complex I.

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

- Molecule 47 is a protein called complex I.

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

- Molecule 48 is a protein called complex I.

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

- Molecule 49 is a protein called complex I.

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

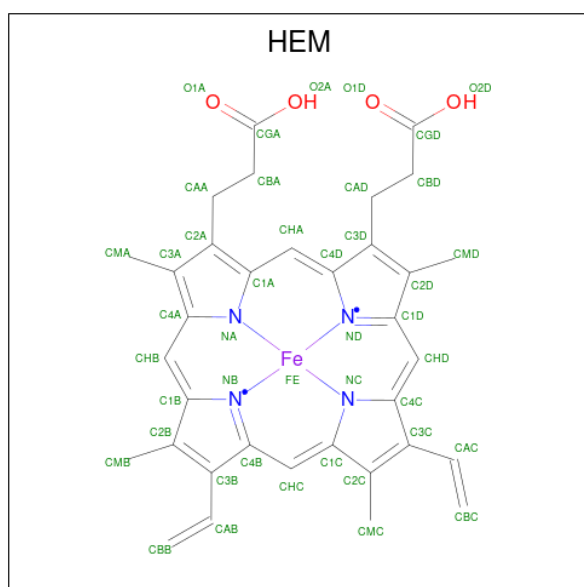
- Molecule 50 is a protein called complex I.

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

- Molecule 51 is a protein called complex I.

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

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



-
- HEC**
- ORTEP diagram of the HEC molecule. The structure shows a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The molecule is labeled with atom names (C1A, C2A, etc.) and bond lengths (e.g., C1A-C2A 1.38 Å). The title 'HEC' is centered above the structure.

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

-
- Diagram illustrating the structure of a ferredoxin (FES) molecule, showing a square planar arrangement of two iron (Fe) and two sulfur (S) atoms. The atoms are labeled S1, FE2, FE1, and S2 in green text. The bonds are colored yellow and purple.

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



WORLD WIDE
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PROTEIN DATA BANK

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

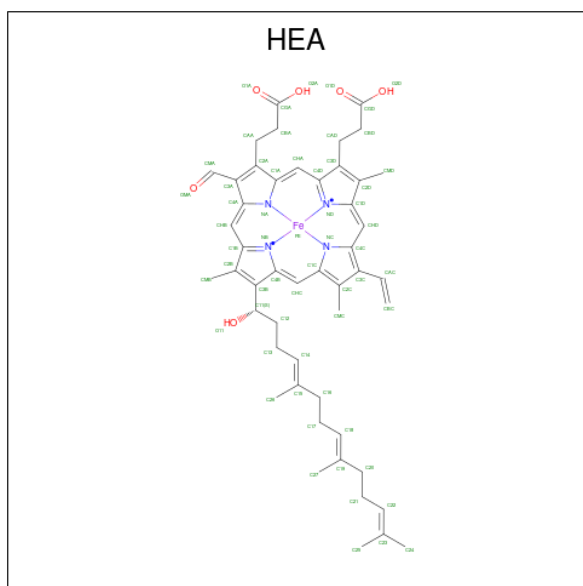
- Molecule 55 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

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

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

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

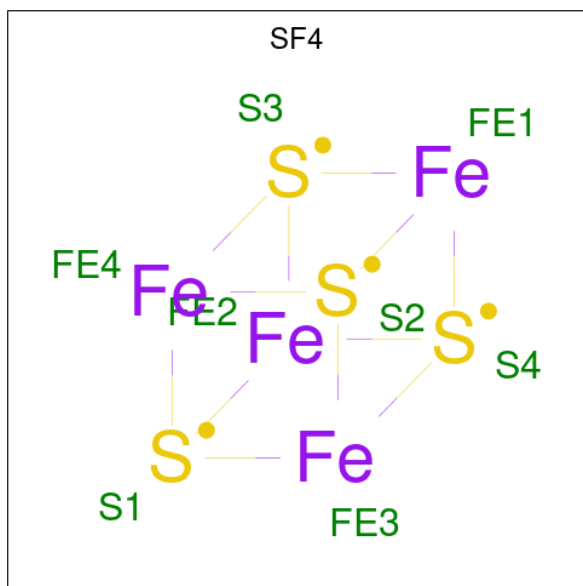


Mol	Chain	Residues	Atoms					AltConf
57	x	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
57	x	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

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

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

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

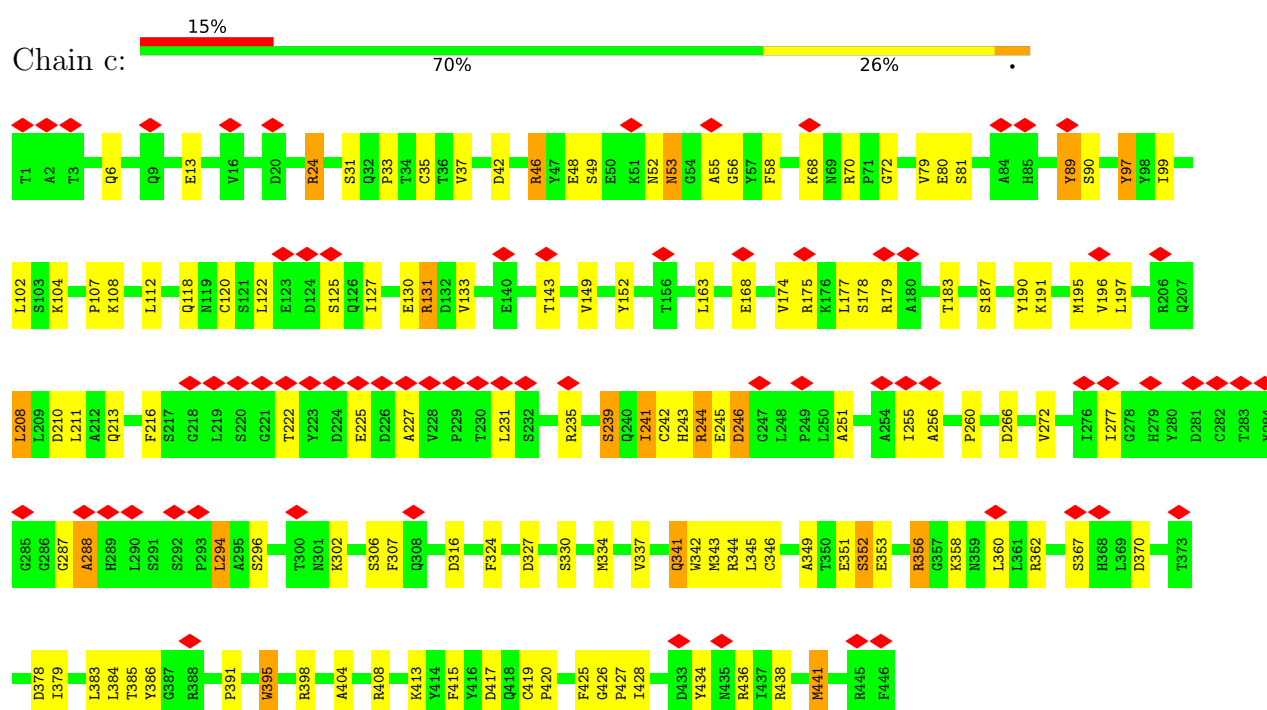


Mol	Chain	Residues	Atoms			AltConf
59	B	1	Total	Fe	S	0
			8	4	4	
59	F	1	Total	Fe	S	0
			8	4	4	
59	G	1	Total	Fe	S	0
			8	4	4	
59	G	1	Total	Fe	S	0
			8	4	4	
59	I	1	Total	Fe	S	0
			8	4	4	
59	I	1	Total	Fe	S	0
			8	4	4	

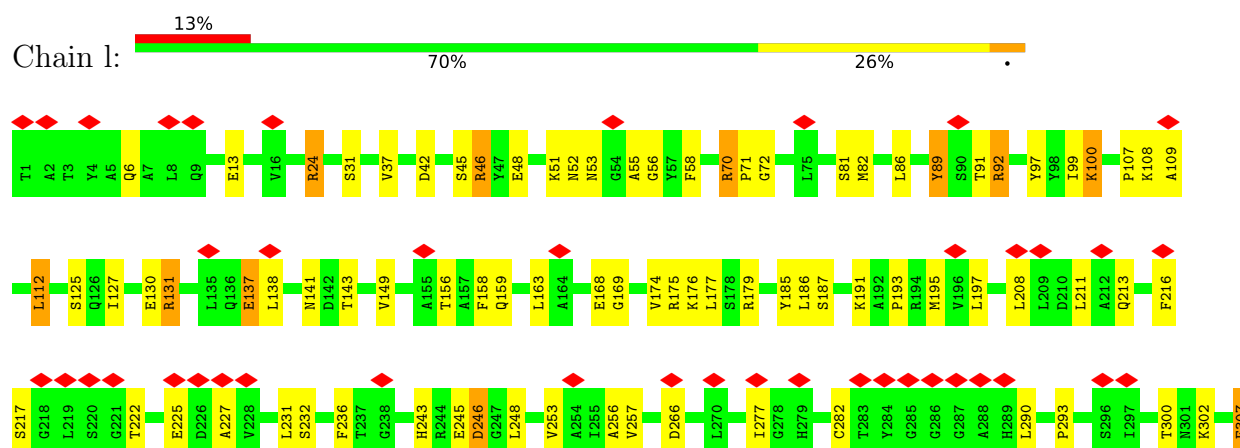
3 Residue-property plots

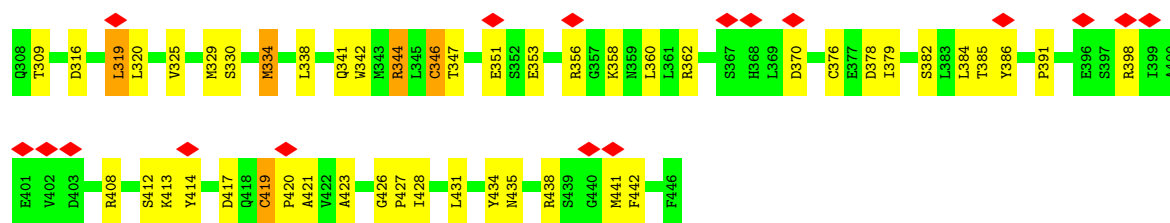
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Cytochrome b-c1 complex subunit 1, mitochondrial

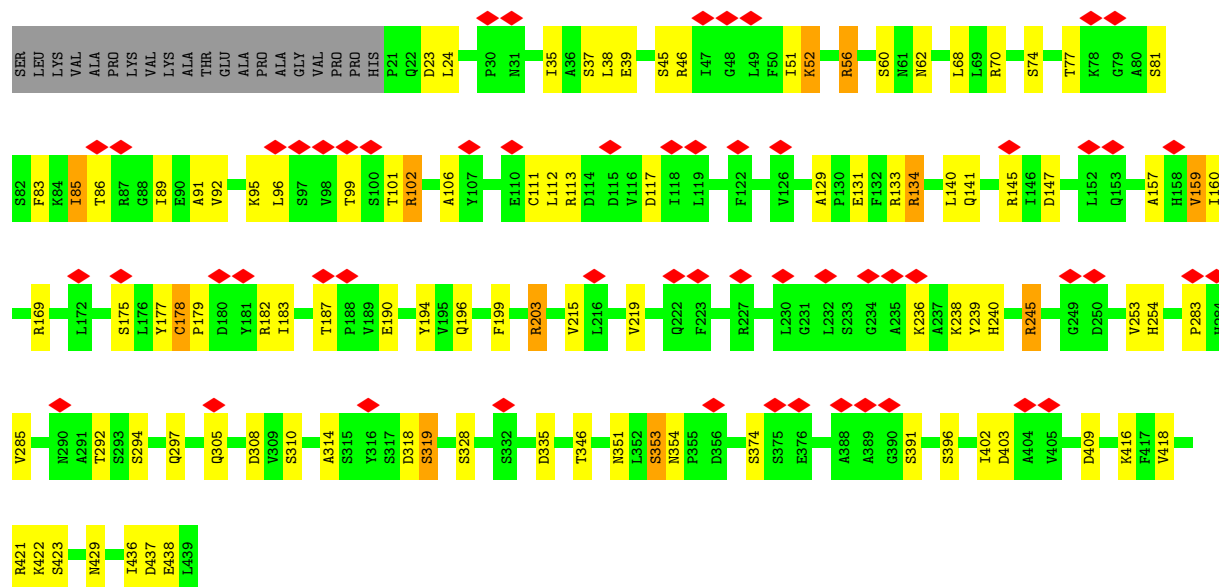
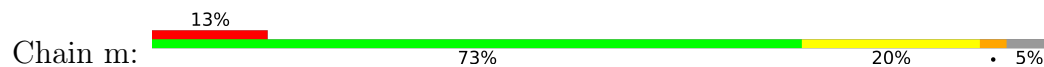


- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

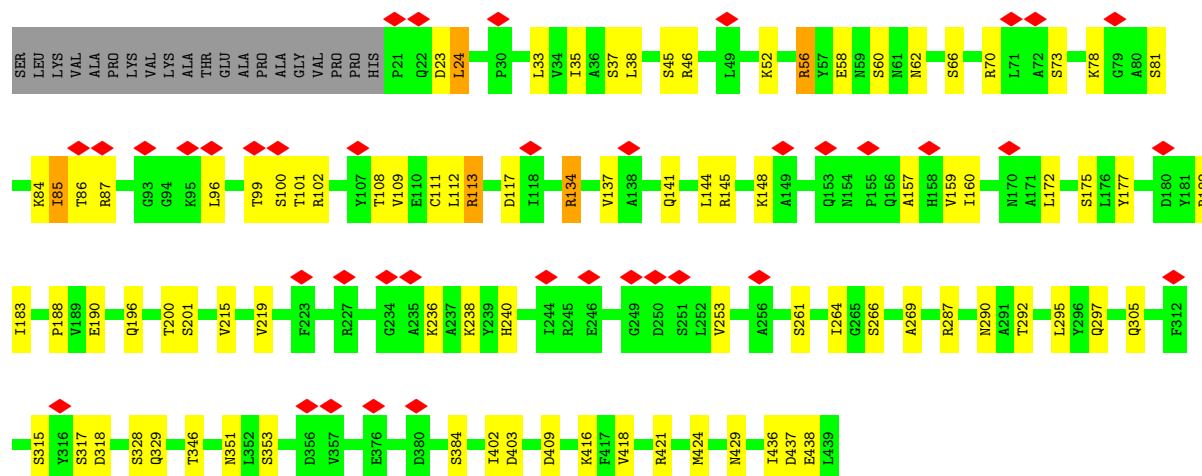
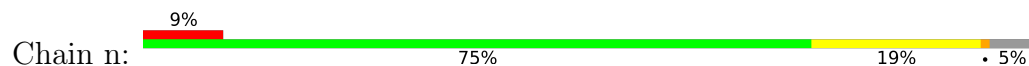




• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

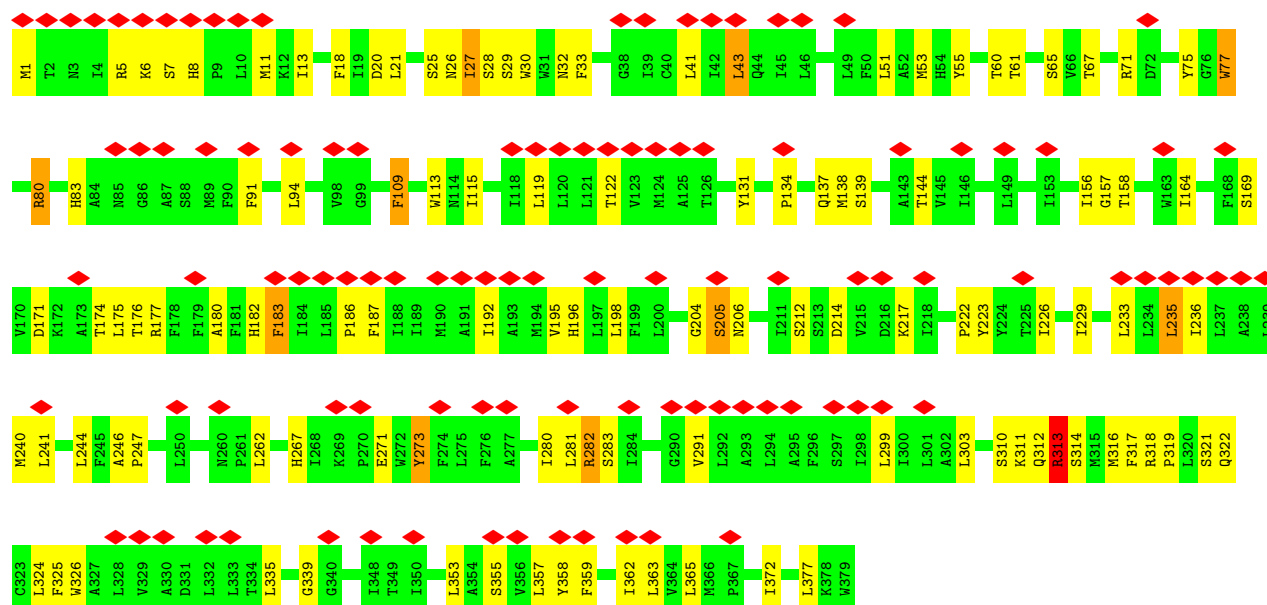


• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

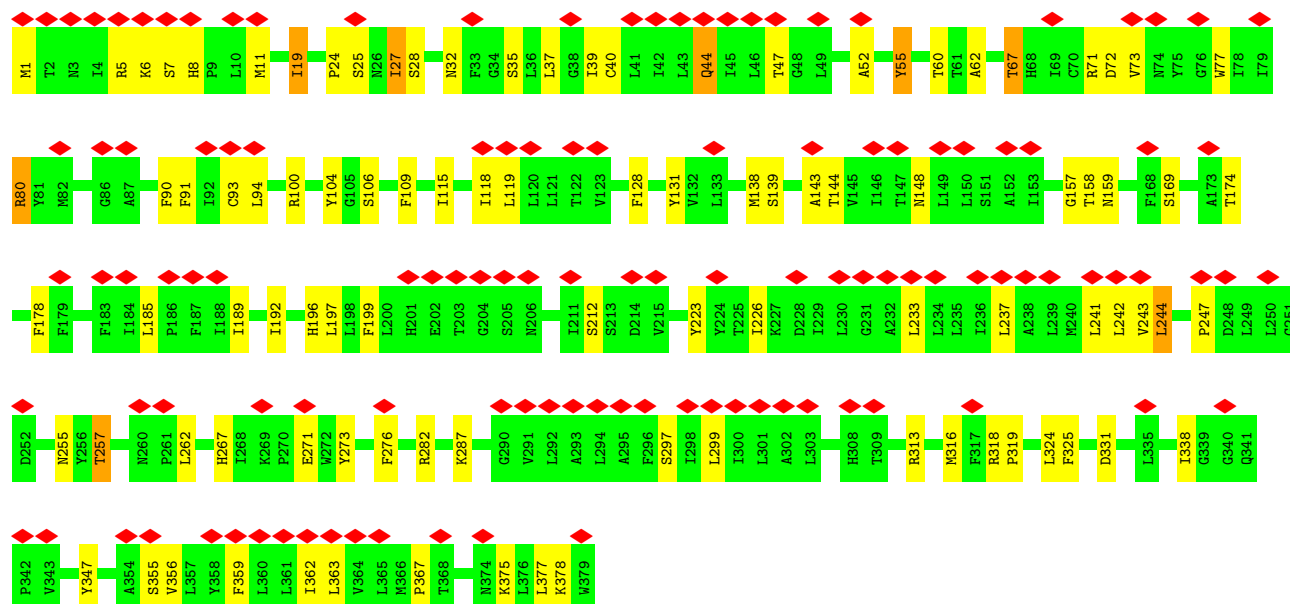
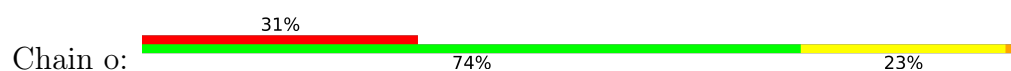


• Molecule 3: Cytochrome b

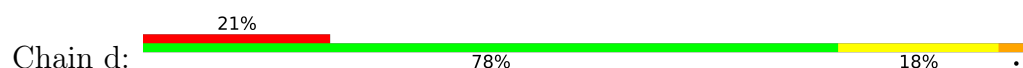




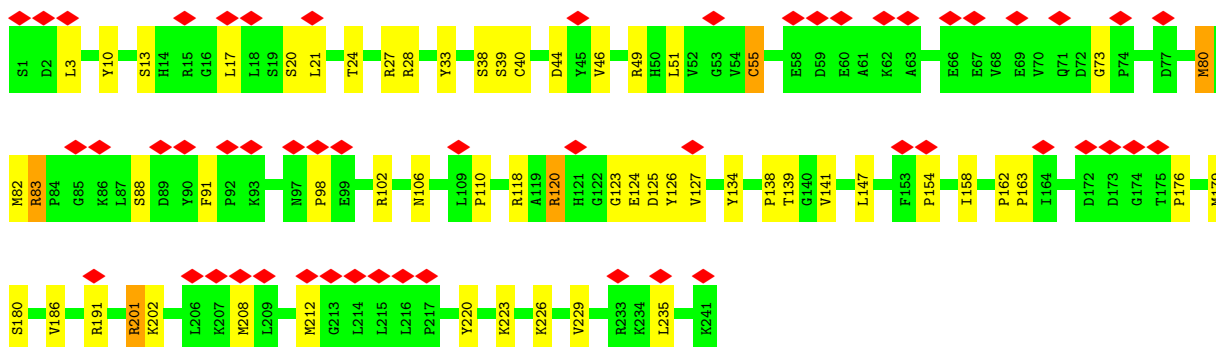
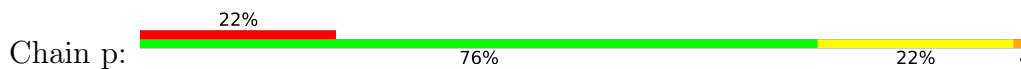
• Molecule 3: Cytochrome b



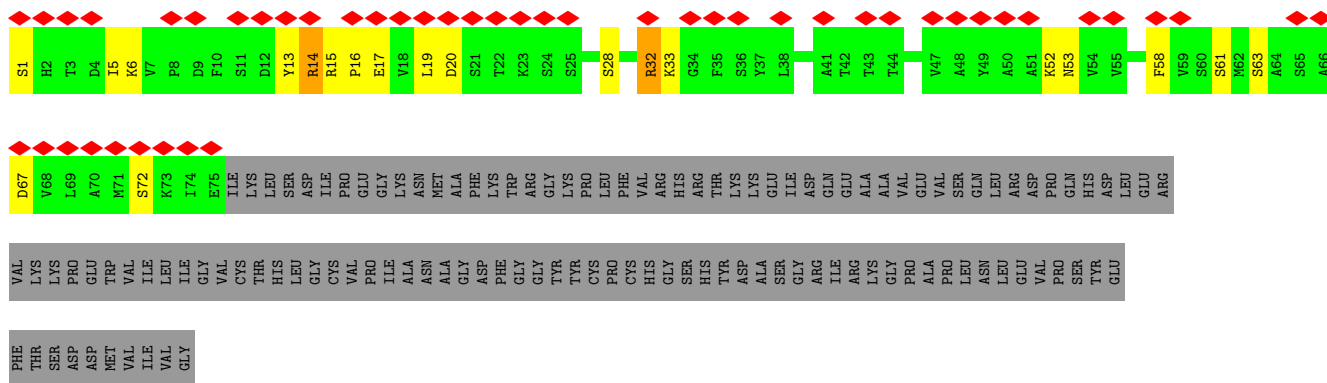
• Molecule 4: Cytochrome c1, heme protein, mitochondrial



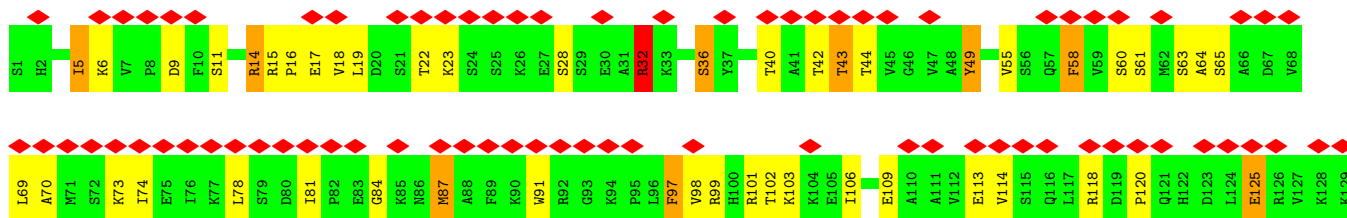
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

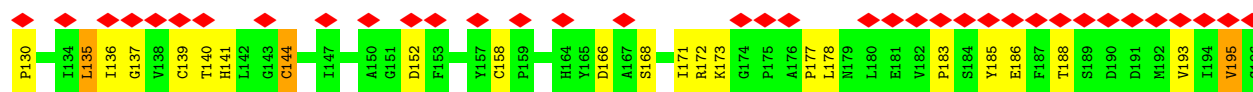


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

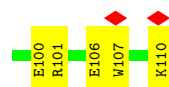
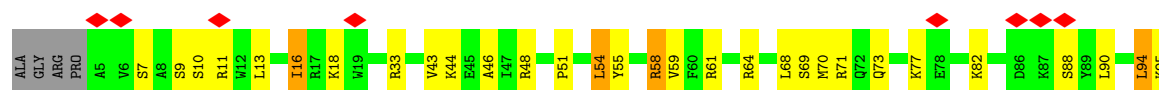


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

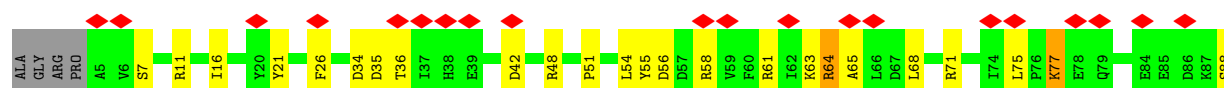




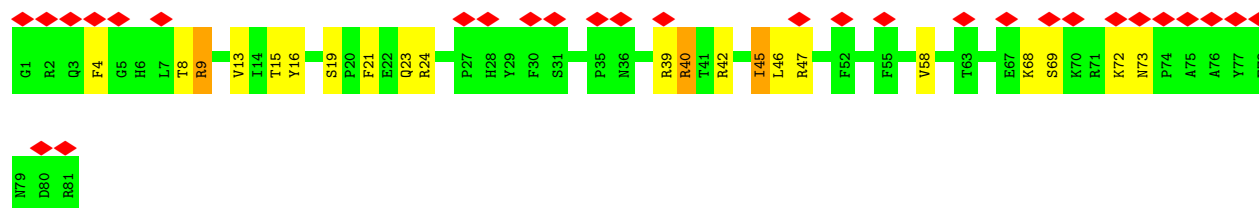
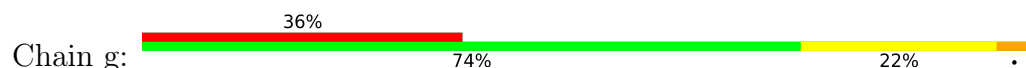
• Molecule 6: Cytochrome b-c1 complex subunit 7



• Molecule 6: Cytochrome b-c1 complex subunit 7



• Molecule 7: Cytochrome b-c1 complex subunit 8



• Molecule 7: Cytochrome b-c1 complex subunit 8



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

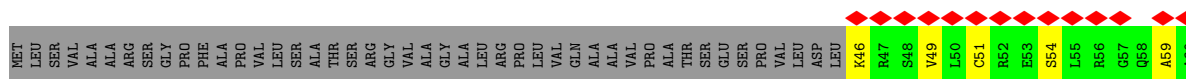




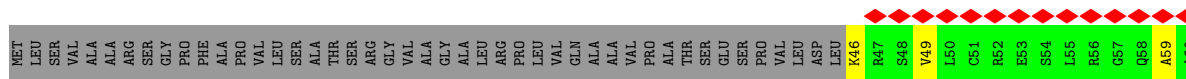
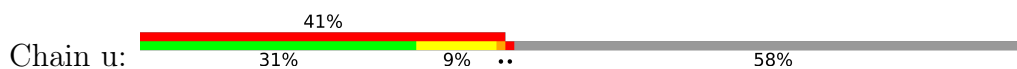
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



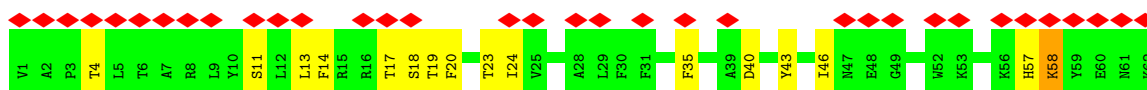
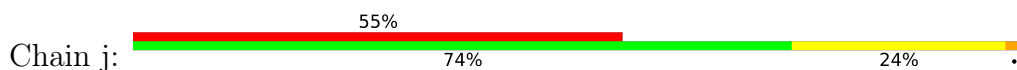
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



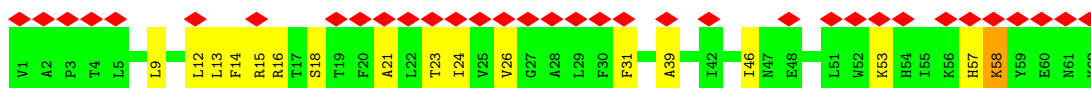
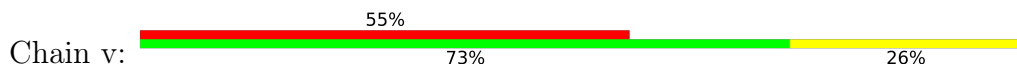
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



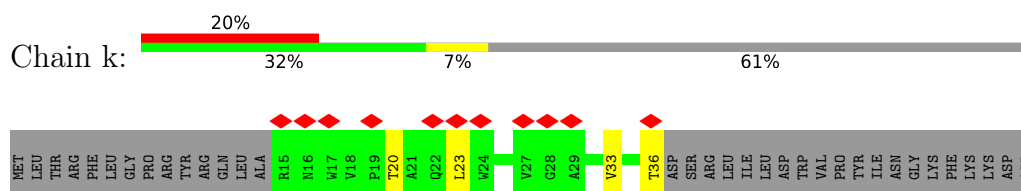
- Molecule 10: Cytochrome b-c1 complex subunit 9



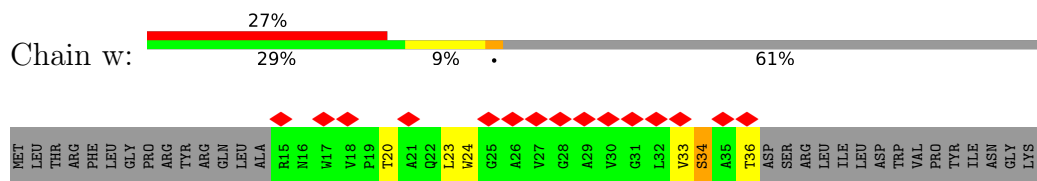
- Molecule 10: Cytochrome b-c1 complex subunit 9



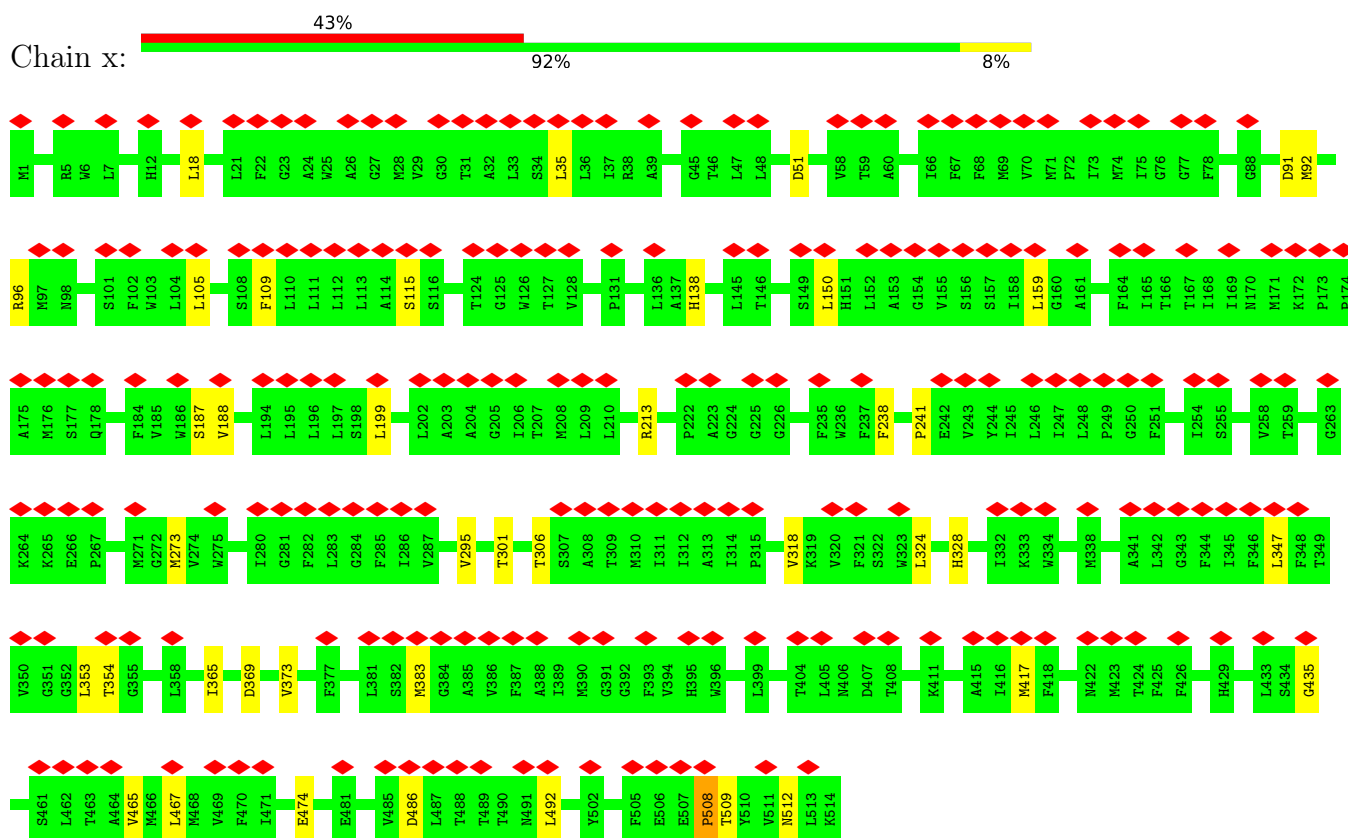
- Molecule 11: Cytochrome b-c1 complex subunit 10



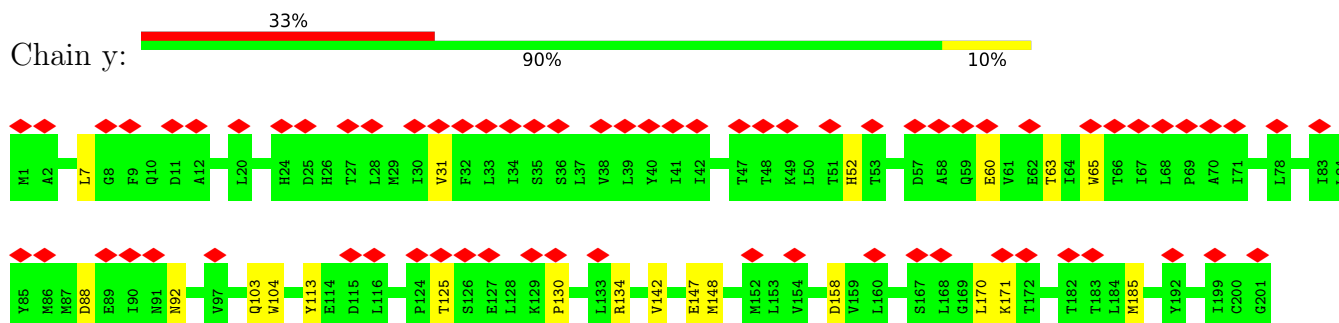
• Molecule 11: Cytochrome b-c1 complex subunit 10



• Molecule 12: Cytochrome c oxidase subunit 1

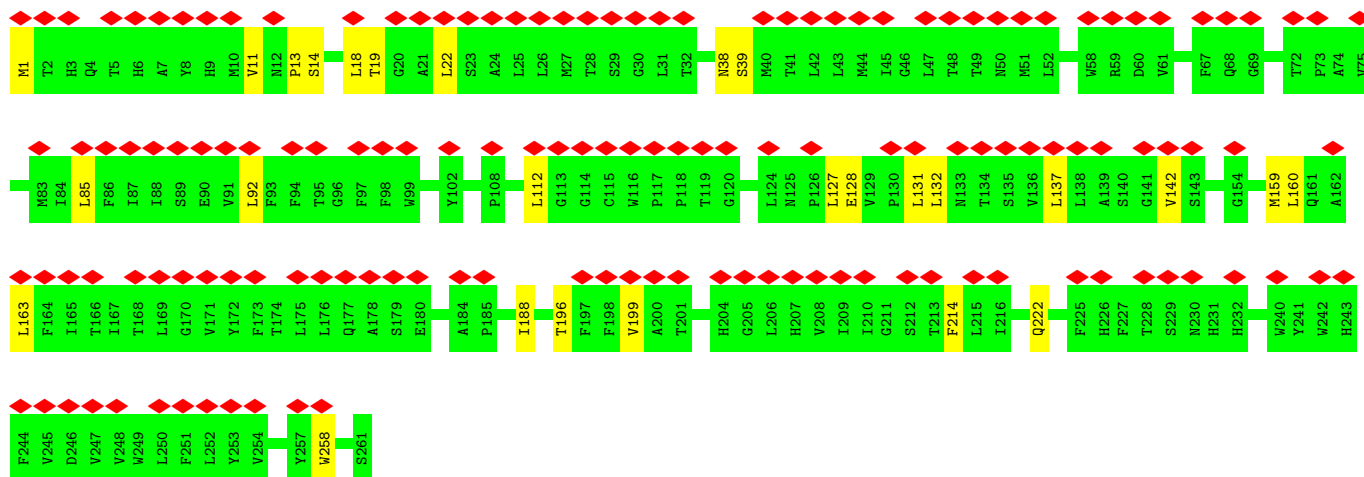
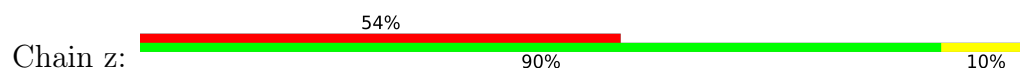


• Molecule 13: Cytochrome c oxidase subunit 2

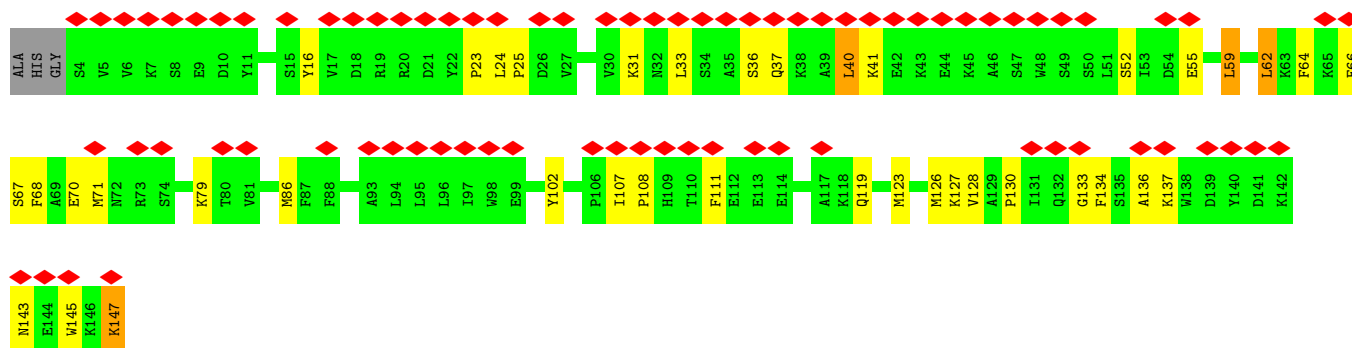
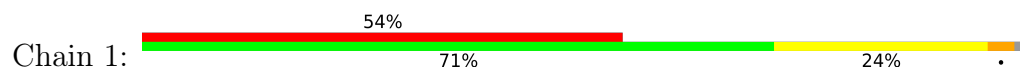




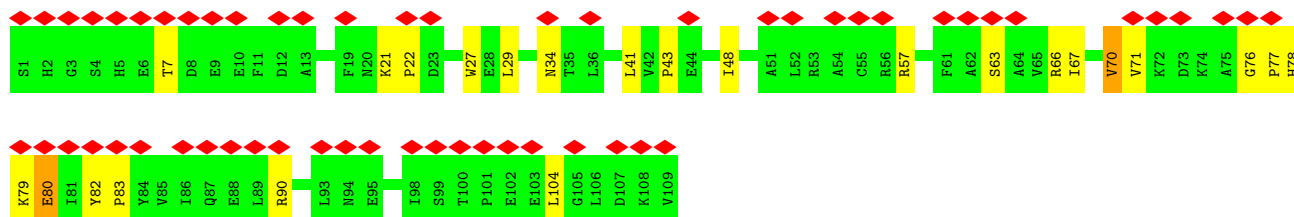
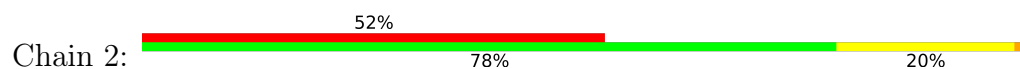
• Molecule 14: Cytochrome c oxidase subunit 3



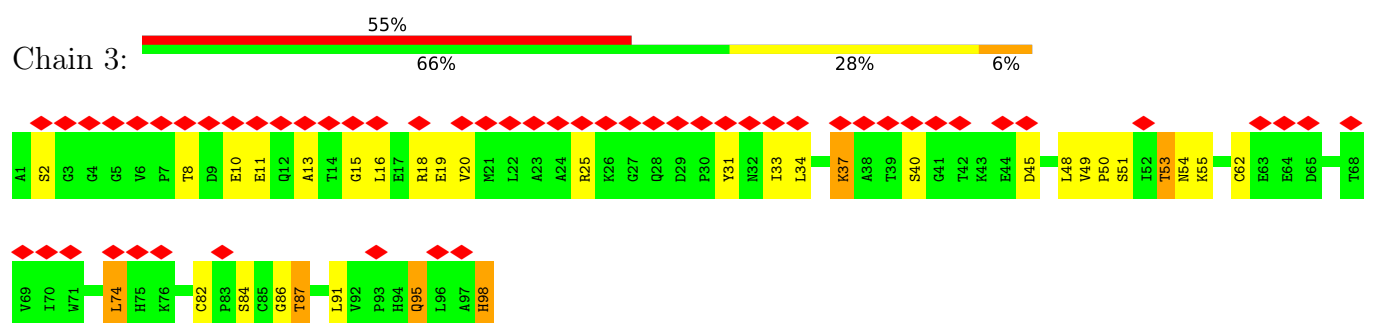
• Molecule 15: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



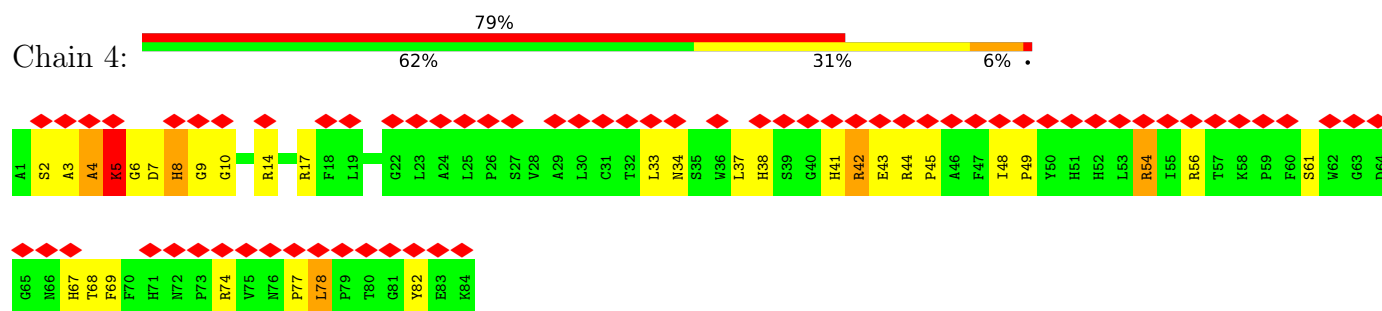
• Molecule 16: Cytochrome c oxidase subunit 5A, mitochondrial



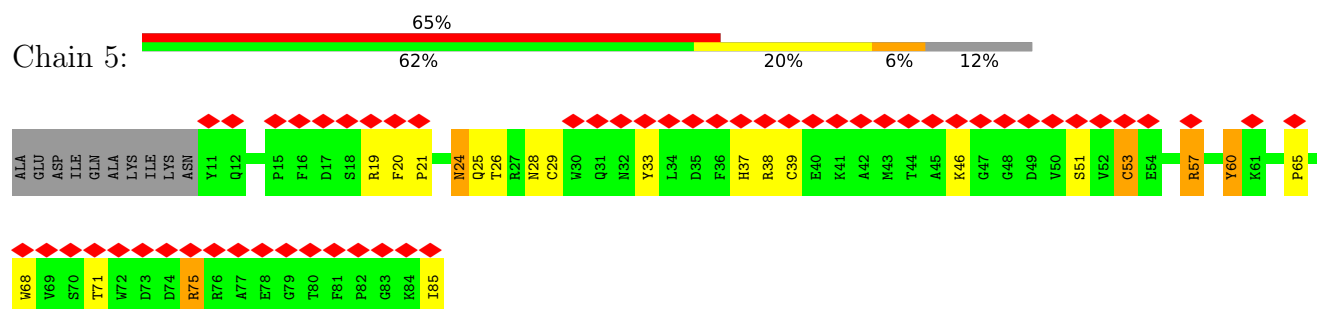
• Molecule 17: Cytochrome c oxidase subunit 5B, mitochondrial



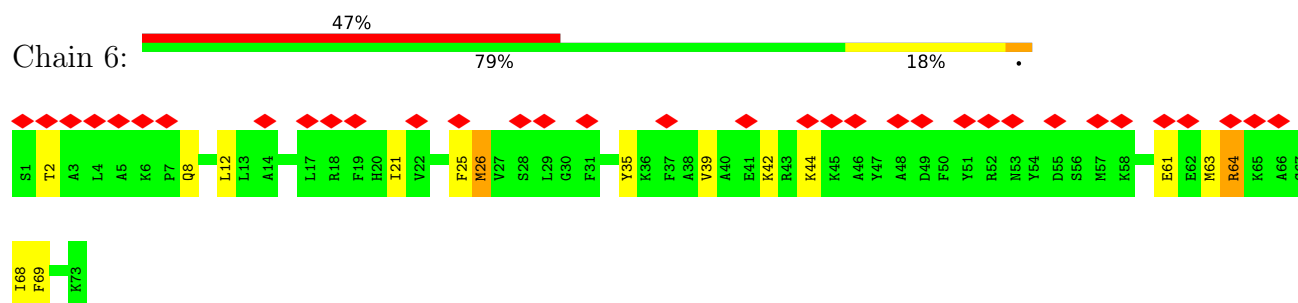
- Molecule 18: Cytochrome c oxidase subunit 6A2, mitochondrial



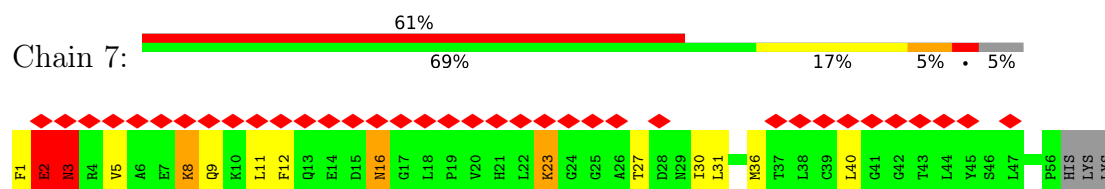
- Molecule 19: Cytochrome c oxidase subunit 6B1



- Molecule 20: Cytochrome c oxidase subunit 6C



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



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

Chain 8:

Chain 9:

Chain 0:

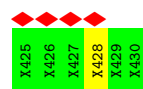
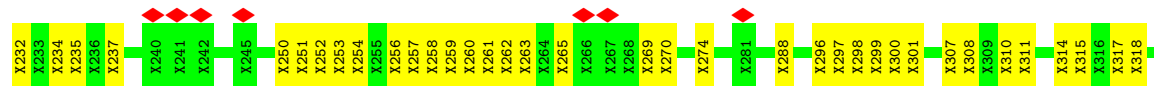
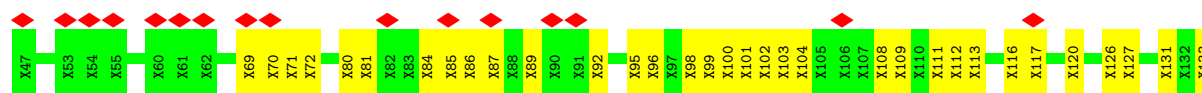
Chain A:

Chain B:

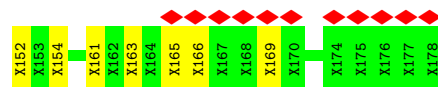
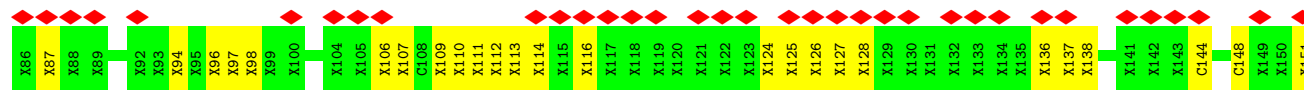
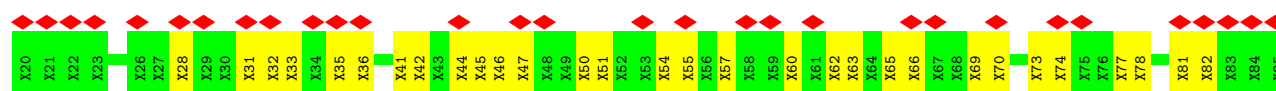
Chain C:



• Molecule 28: complex I

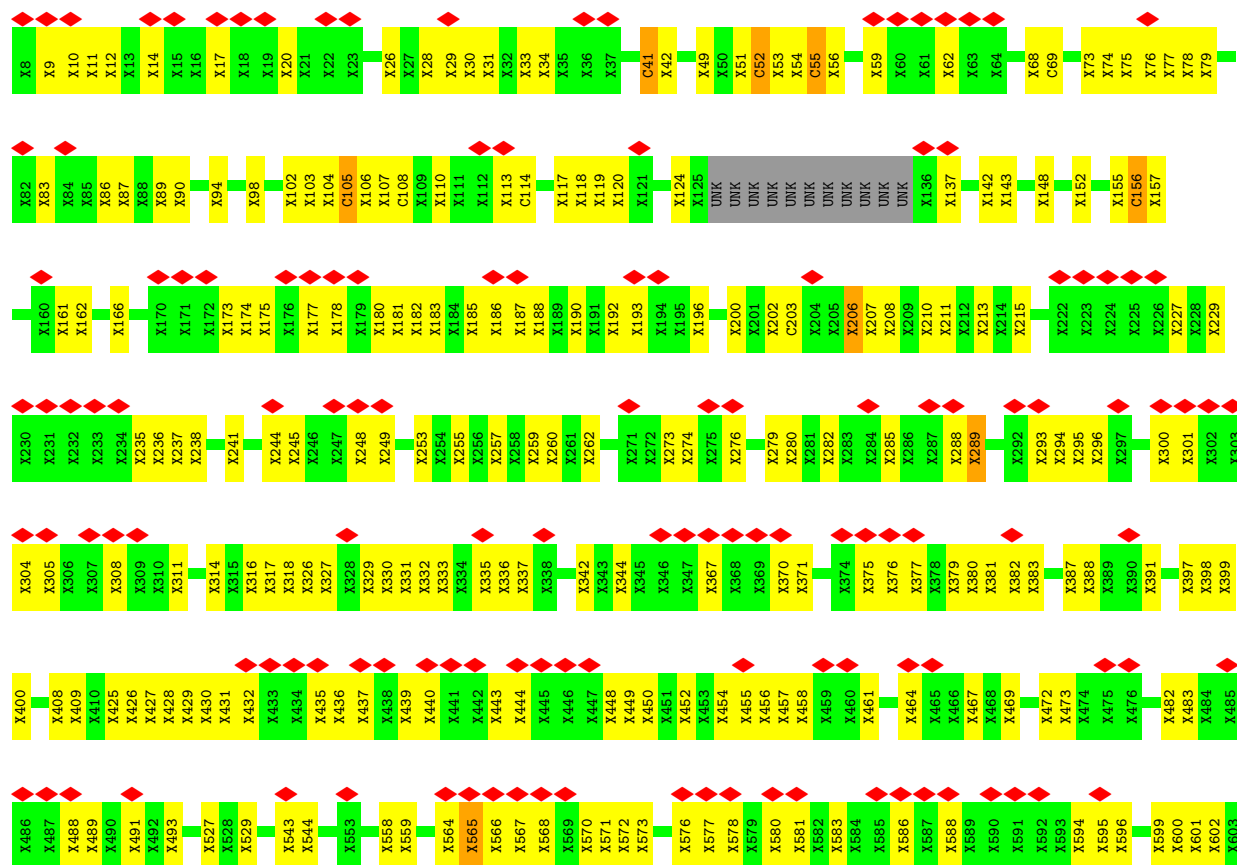


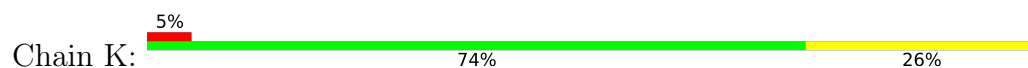
• Molecule 29: complex I

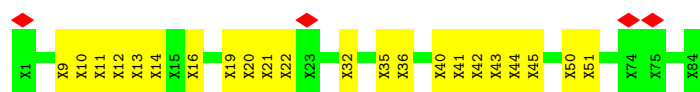


• Molecule 30: complex I



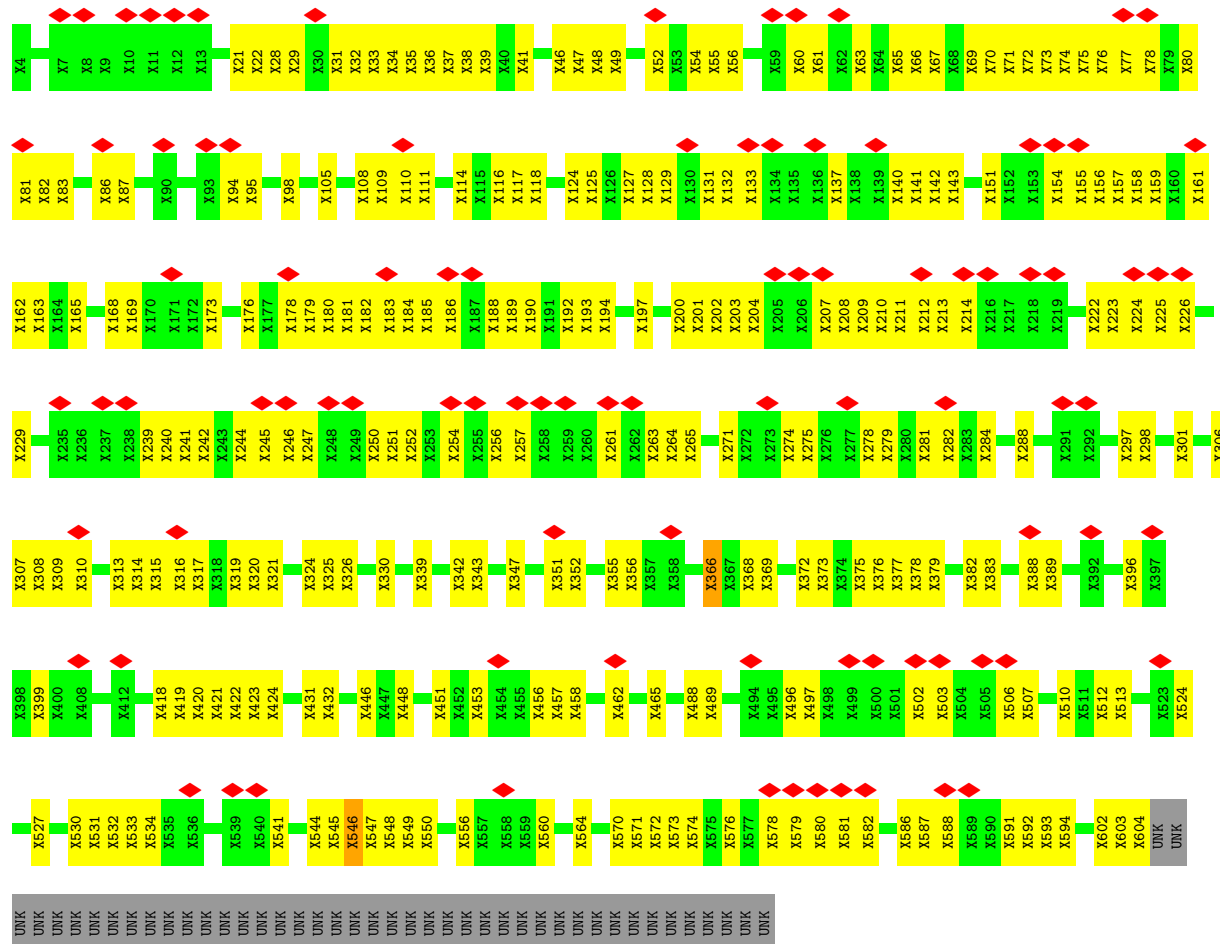






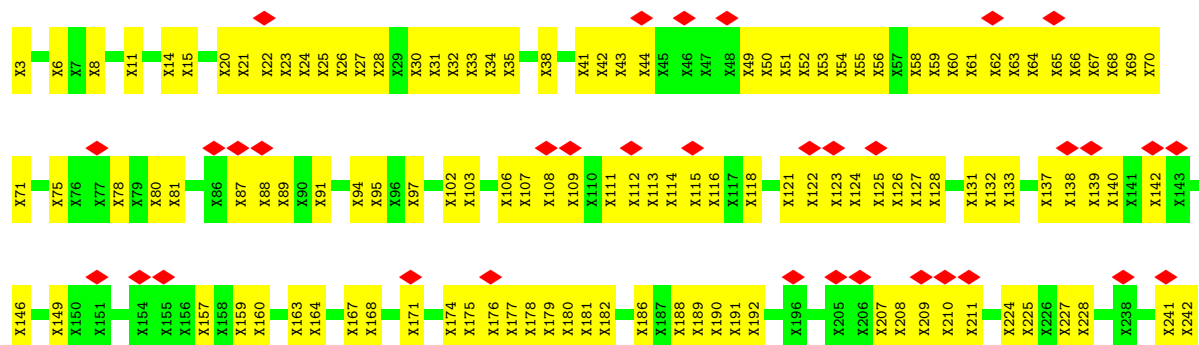
• Molecule 36: complex I

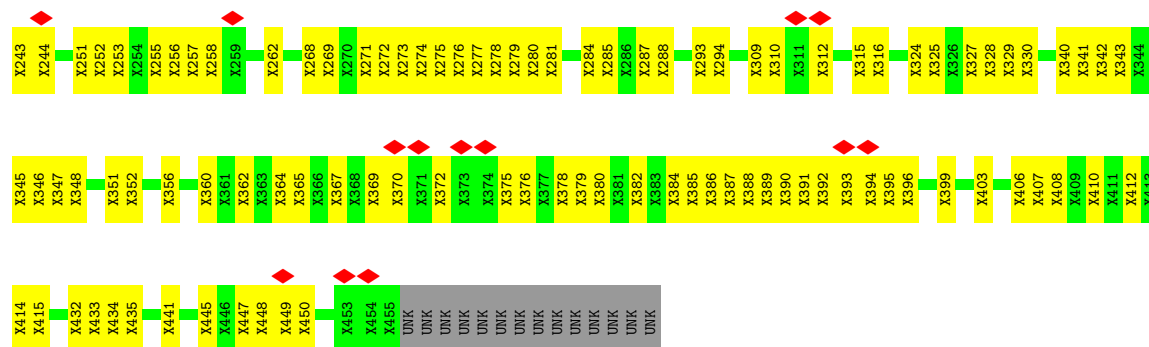
Chain L: 15% 50% 43% 7%



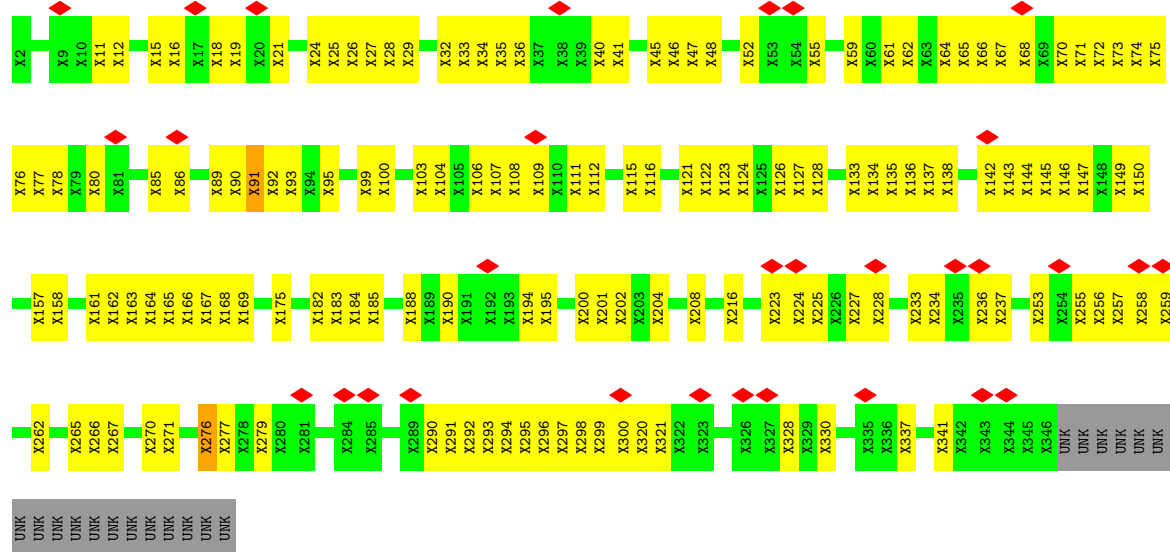
• Molecule 37: complex I

Chain M: 10% 48% 49%

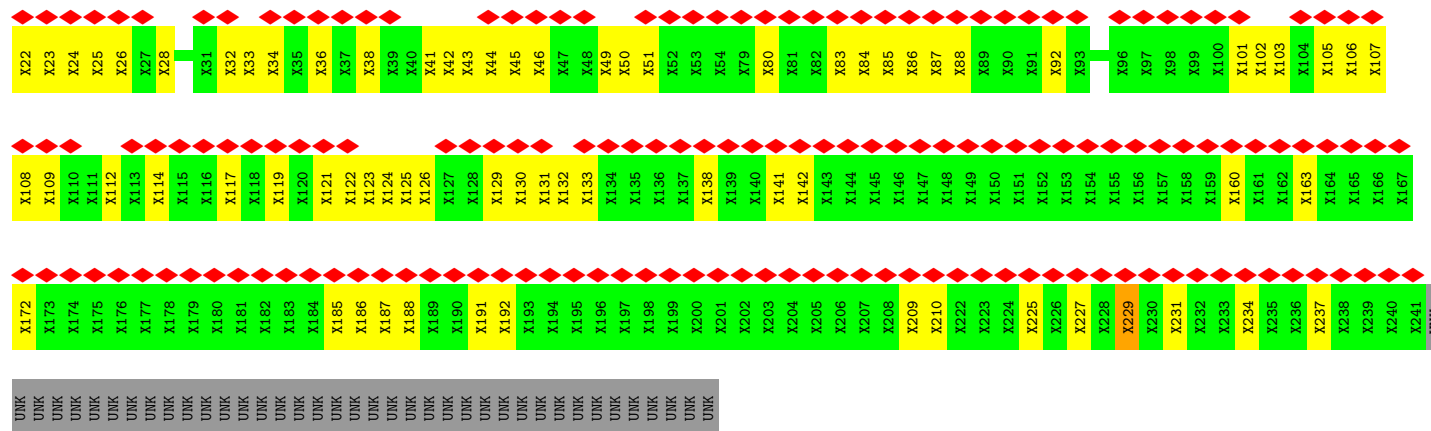
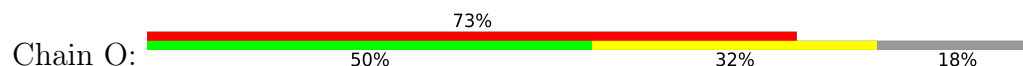




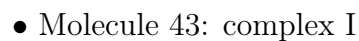
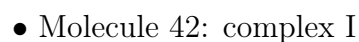
• Molecule 38: complex I

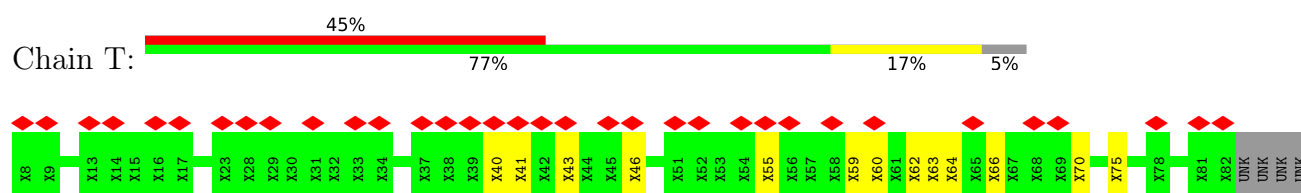


• Molecule 39: complex I

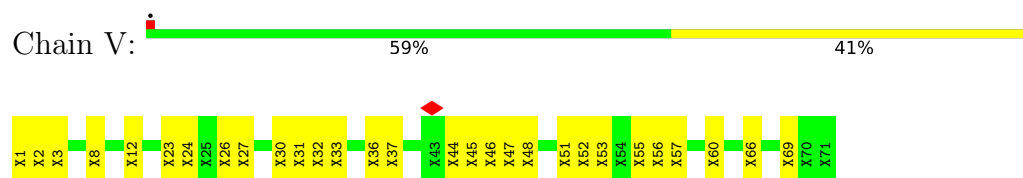


• Molecule 40: complex I

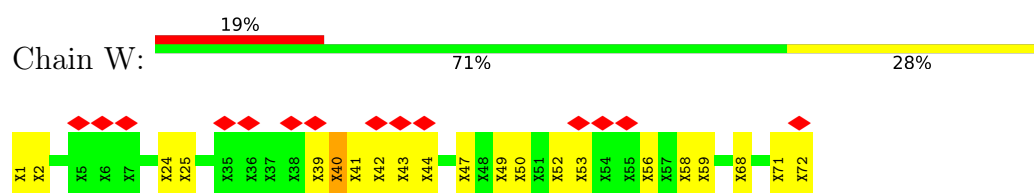




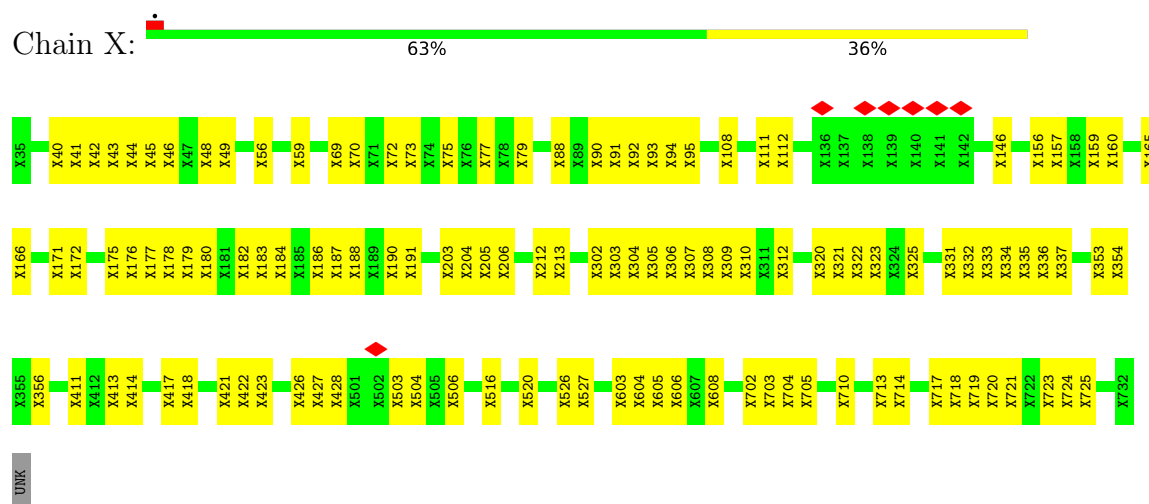
- Molecule 45: complex I



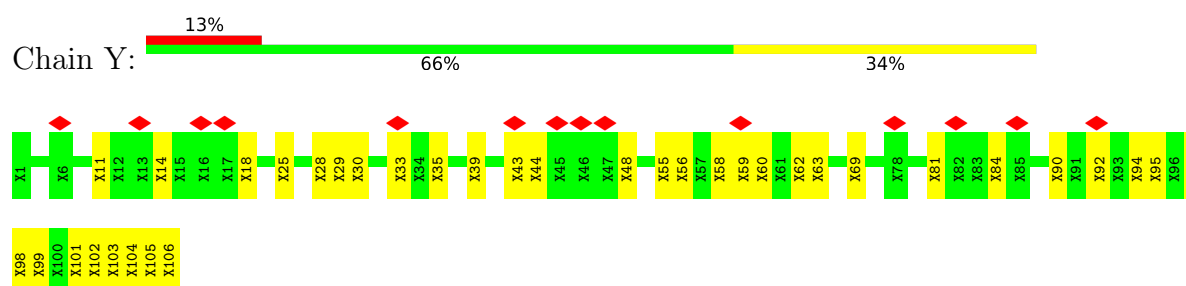
- Molecule 46: complex I



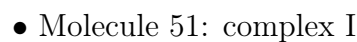
- Molecule 47: complex I

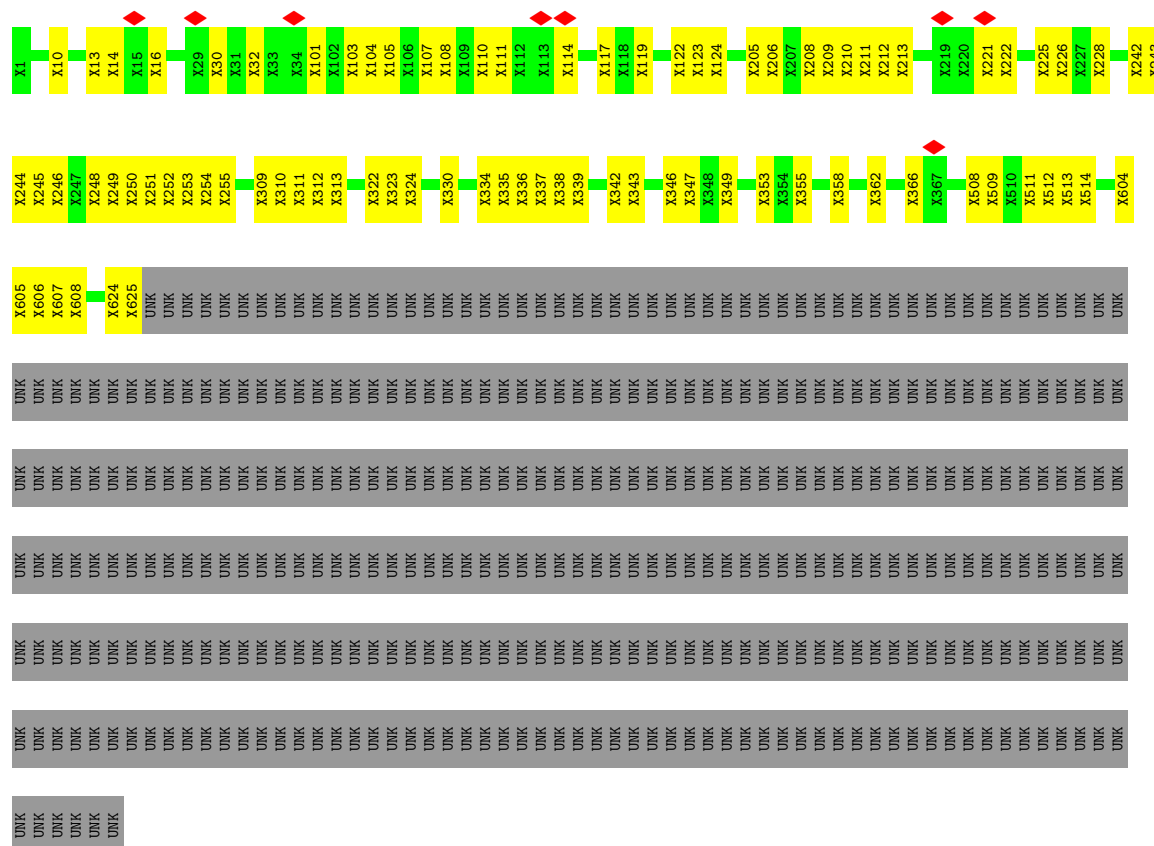


- Molecule 48: complex I



- Molecule 49: complex I





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17093	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	4300	Depositor
Magnification	57797	Depositor
Image detector	OTHER	Depositor
Maximum map value	0.368	Depositor
Minimum map value	-0.164	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.081	Depositor
Map size (\AA)	509.76, 509.76, 509.76	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.77, 1.77, 1.77	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, ZN, MG, HEM, SF4, CU, HEA, 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	$\# Z > 5$
1	c	0.60	2/3531 (0.1%)	1.58	43/4792 (0.9%)
1	l	0.63	3/3531 (0.1%)	1.61	58/4792 (1.2%)
2	m	0.51	0/3198	1.46	31/4336 (0.7%)
2	n	0.51	0/3198	1.33	11/4336 (0.3%)
3	b	0.71	2/3108 (0.1%)	1.73	62/4252 (1.5%)
3	o	0.69	3/3108 (0.1%)	1.62	50/4252 (1.2%)
4	d	0.55	0/1978	1.50	23/2684 (0.9%)
4	p	0.55	0/1978	1.40	24/2684 (0.9%)
5	e	0.60	0/574	1.62	7/775 (0.9%)
5	q	0.61	0/1551	1.68	28/2097 (1.3%)
6	f	0.57	0/935	1.56	18/1253 (1.4%)
6	r	0.57	0/935	1.66	24/1253 (1.9%)
7	g	0.61	1/704 (0.1%)	1.41	9/951 (0.9%)
7	s	0.59	0/704	1.30	5/951 (0.5%)
8	h	0.41	0/529	1.12	0/708
8	t	0.39	0/529	1.06	0/708
9	i	0.48	0/250	1.31	2/335 (0.6%)
9	u	0.48	0/250	1.32	1/335 (0.3%)
10	j	0.51	0/525	1.31	5/707 (0.7%)
10	v	0.51	0/525	1.42	6/707 (0.8%)
11	k	0.42	0/163	1.01	0/225
11	w	0.46	0/163	1.17	0/225
12	x	0.60	0/4164	0.76	1/5688 (0.0%)
13	y	0.57	0/1868	0.79	0/2544
14	z	0.56	0/2211	0.68	0/3023
15	1	0.57	0/1229	0.64	1/1658 (0.1%)
16	2	0.50	0/898	0.66	0/1218
17	3	0.56	0/765	0.81	0/1038
18	4	0.54	0/699	0.73	1/950 (0.1%)
19	5	0.55	0/648	0.73	0/877
20	6	0.60	0/611	0.65	0/810
21	7	0.61	0/451	0.72	0/610

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
22	8	0.57	0/398	0.66	0/546
23	9	0.63	0/399	0.62	0/534
24	0	0.51	0/345	0.65	0/470
26	B	1.57	1/21 (4.8%)	2.68	2/23 (8.7%)
29	E	0.77	0/20	1.58	0/20
30	F	2.57	1/20 (5.0%)	2.24	0/20
31	G	1.04	0/65	1.60	0/67
33	I	2.33	2/40 (5.0%)	1.47	0/40
All	All	0.59	15/46819 (0.0%)	1.33	412/63494 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	c	0	13
1	l	0	3
2	m	0	9
2	n	0	5
3	b	0	14
3	o	0	6
4	d	0	5
4	p	0	4
5	e	0	1
5	q	0	9
6	f	0	2
7	g	0	2
7	s	0	3
8	t	0	1
9	i	0	1
9	u	0	1
10	j	0	1
11	w	0	1
26	B	0	2
27	C	0	1
28	D	0	1
30	F	0	2
31	G	0	6
33	I	0	1
36	L	0	4
38	N	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
39	O	0	2
40	P	0	3
41	Q	0	1
43	S	0	1
46	W	0	1
47	X	0	1
All	All	0	109

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

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

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

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

There are no chirality outliers.

5 of 109 planarity outliers are listed below:

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 51.

The worst 5 of 2394 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:148:UNK:CB	26:B:151:UNK:CA	1.77	1.59
30:F:405:CYS:CB	30:F:406:UNK:CB	1.78	1.56
30:F:405:CYS:HB2	30:F:406:UNK:CB	1.04	1.48
36:L:321:UNK:CB	36:L:324:UNK:CB	1.92	1.45
29:E:148:CYS:SG	30:F:103:UNK:CB	2.04	1.44

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	c	444/446 (100%)	355 (80%)	66 (15%)	23 (5%)	1	15
1	l	444/446 (100%)	370 (83%)	54 (12%)	20 (4%)	2	17
2	m	417/439 (95%)	341 (82%)	67 (16%)	9 (2%)	5	29
2	n	417/439 (95%)	344 (82%)	62 (15%)	11 (3%)	4	26
3	b	377/379 (100%)	303 (80%)	60 (16%)	14 (4%)	2	20
3	o	377/379 (100%)	316 (84%)	50 (13%)	11 (3%)	3	23
4	d	239/241 (99%)	188 (79%)	36 (15%)	15 (6%)	1	13
4	p	239/241 (99%)	195 (82%)	32 (13%)	12 (5%)	1	16
5	e	73/196 (37%)	57 (78%)	14 (19%)	2 (3%)	4	25
5	q	194/196 (99%)	148 (76%)	35 (18%)	11 (6%)	1	14
6	f	104/110 (94%)	89 (86%)	13 (12%)	2 (2%)	6	32
6	r	104/110 (94%)	87 (84%)	15 (14%)	2 (2%)	6	32
7	g	79/81 (98%)	63 (80%)	13 (16%)	3 (4%)	2	19
7	s	79/81 (98%)	60 (76%)	16 (20%)	3 (4%)	2	19
8	h	62/78 (80%)	52 (84%)	10 (16%)	0	100	100
8	t	62/78 (80%)	51 (82%)	10 (16%)	1 (2%)	8	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	i	31/78 (40%)	19 (61%)	10 (32%)	2 (6%)	1	12
9	u	31/78 (40%)	17 (55%)	11 (36%)	3 (10%)	0	7
10	j	60/62 (97%)	41 (68%)	13 (22%)	6 (10%)	0	7
10	v	60/62 (97%)	44 (73%)	12 (20%)	4 (7%)	1	12
11	k	20/56 (36%)	17 (85%)	2 (10%)	1 (5%)	1	16
11	w	20/56 (36%)	15 (75%)	3 (15%)	2 (10%)	0	7
12	x	512/514 (100%)	480 (94%)	28 (6%)	4 (1%)	16	55
13	y	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	10	43
14	z	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
15	1	142/147 (97%)	135 (95%)	7 (5%)	0	100	100
16	2	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
17	3	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	2	17
18	4	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	1	13
19	5	73/85 (86%)	64 (88%)	8 (11%)	1 (1%)	9	41
20	6	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
21	7	54/59 (92%)	48 (89%)	4 (7%)	2 (4%)	2	20
22	8	47/56 (84%)	41 (87%)	6 (13%)	0	100	100
23	9	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
24	0	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
26	B	4/143 (3%)	3 (75%)	0	1 (25%)	0	1
29	E	4/159 (2%)	3 (75%)	1 (25%)	0	100	100
30	F	4/411 (1%)	4 (100%)	0	0	100	100
31	G	12/538 (2%)	9 (75%)	1 (8%)	2 (17%)	0	2
33	I	8/162 (5%)	7 (88%)	0	1 (12%)	0	4
All	All	5719/7551 (76%)	4821 (84%)	718 (13%)	180 (3%)	5	22

5 of 180 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	c	370/370 (100%)	289 (78%)	81 (22%)	1	5
1	l	370/370 (100%)	286 (77%)	84 (23%)	0	4
2	m	328/343 (96%)	260 (79%)	68 (21%)	1	6
2	n	328/343 (96%)	262 (80%)	66 (20%)	1	6
3	b	327/327 (100%)	269 (82%)	58 (18%)	1	8
3	o	327/327 (100%)	276 (84%)	51 (16%)	2	11
4	d	206/206 (100%)	179 (87%)	27 (13%)	3	14
4	p	206/206 (100%)	179 (87%)	27 (13%)	3	14
5	e	65/168 (39%)	51 (78%)	14 (22%)	1	5
5	q	167/168 (99%)	123 (74%)	44 (26%)	0	3
6	f	96/98 (98%)	74 (77%)	22 (23%)	0	4
6	r	96/98 (98%)	78 (81%)	18 (19%)	1	7
7	g	71/71 (100%)	58 (82%)	13 (18%)	1	8
7	s	71/71 (100%)	57 (80%)	14 (20%)	1	7
8	h	61/74 (82%)	51 (84%)	10 (16%)	2	10
8	t	61/74 (82%)	51 (84%)	10 (16%)	2	10
9	i	27/60 (45%)	19 (70%)	8 (30%)	0	2
9	u	27/60 (45%)	20 (74%)	7 (26%)	0	3
10	j	52/52 (100%)	46 (88%)	6 (12%)	4	16
10	v	52/52 (100%)	43 (83%)	9 (17%)	1	9
11	k	15/46 (33%)	12 (80%)	3 (20%)	1	6
11	w	15/46 (33%)	11 (73%)	4 (27%)	0	3
12	x	427/427 (100%)	389 (91%)	38 (9%)	8	25
13	y	211/211 (100%)	191 (90%)	20 (10%)	7	22
14	z	226/226 (100%)	199 (88%)	27 (12%)	4	16
15	l	128/129 (99%)	120 (94%)	8 (6%)	15	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	2	95/95 (100%)	89 (94%)	6 (6%)	15	36
17	3	81/81 (100%)	76 (94%)	5 (6%)	15	36
18	4	68/68 (100%)	50 (74%)	18 (26%)	0	3
19	5	67/75 (89%)	58 (87%)	9 (13%)	3	13
20	6	58/58 (100%)	53 (91%)	5 (9%)	8	26
21	7	47/50 (94%)	40 (85%)	7 (15%)	2	11
22	8	39/46 (85%)	37 (95%)	2 (5%)	20	41
23	9	40/40 (100%)	38 (95%)	2 (5%)	20	41
24	0	37/38 (97%)	34 (92%)	3 (8%)	9	28
26	B	4/4 (100%)	2 (50%)	2 (50%)	0	0
29	E	4/4 (100%)	4 (100%)	0	100	100
30	F	4/4 (100%)	3 (75%)	1 (25%)	0	3
31	G	12/12 (100%)	8 (67%)	4 (33%)	0	1
33	I	8/8 (100%)	7 (88%)	1 (12%)	3	15
All	All	4894/5206 (94%)	4092 (84%)	802 (16%)	4	10

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

Mol	Chain	Res	Type
3	o	7	SER
5	q	144	CYS
31	G	55	CYS
3	o	118	ILE
3	o	6	LYS

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

Mol	Chain	Res	Type
1	l	243	HIS
19	5	23	GLN
3	o	26	ASN
18	4	52	HIS
22	8	15	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 5 are monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	SF4	F	501	30	0,12,12	-	-	-		
52	HEM	b	401	3	41,50,50	1.48	4 (9%)	45,82,82	1.87	10 (22%)
52	HEM	o	402	3	41,50,50	1.57	4 (9%)	45,82,82	1.96	14 (31%)
59	SF4	I	202	33	0,12,12	-	-	-		
52	HEM	o	401	3	41,50,50	1.59	5 (12%)	45,82,82	2.55	19 (42%)
52	HEM	b	402	3	41,50,50	1.39	4 (9%)	45,82,82	2.16	13 (28%)
54	FES	q	201	5	0,4,4	-	-	-		
59	SF4	B	201	26	0,12,12	-	-	-		
57	HEA	x	604	12	57,67,67	1.47	6 (10%)	61,103,103	1.45	11 (18%)
54	FES	E	201	29	0,4,4	-	-	-		
59	SF4	G	801	31	0,12,12	-	-	-		
53	HEC	d	301	4	32,50,50	2.20	4 (12%)	24,82,82	2.10	12 (50%)
59	SF4	G	802	31	0,12,12	-	-	-		
53	HEC	p	301	4	32,50,50	2.24	5 (15%)	24,82,82	1.92	9 (37%)
59	SF4	I	201	33	0,12,12	-	-	-		
54	FES	G	803	31	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	HEA	x	603	12	57,67,67	1.25	6 (10%)	61,103,103	1.47	12 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	F	501	30	-	-	0/6/5/5
52	HEM	b	401	3	-	4/12/54/54	-
52	HEM	o	402	3	-	4/12/54/54	-
59	SF4	I	202	33	-	-	0/6/5/5
52	HEM	o	401	3	-	6/12/54/54	-
52	HEM	b	402	3	-	6/12/54/54	-
54	FES	q	201	5	-	-	0/1/1/1
59	SF4	B	201	26	-	-	0/6/5/5
57	HEA	x	604	12	-	5/32/76/76	-
54	FES	E	201	29	-	-	0/1/1/1
59	SF4	G	801	31	-	-	0/6/5/5
53	HEC	d	301	4	-	3/10/54/54	-
59	SF4	G	802	31	-	-	0/6/5/5
53	HEC	p	301	4	-	6/10/54/54	-
59	SF4	I	201	33	-	-	0/6/5/5
54	FES	G	803	31	-	-	0/1/1/1
57	HEA	x	603	12	-	7/32/76/76	-

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	p	301	HEC	C3C-C2C	-7.19	1.33	1.40
53	d	301	HEC	C2B-C3B	-7.02	1.33	1.40
53	p	301	HEC	C2B-C3B	-6.85	1.33	1.40
53	d	301	HEC	C3C-C2C	-6.55	1.33	1.40
57	x	604	HEA	C3A-C2A	-6.39	1.31	1.40

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	o	401	HEM	CMA-C3A-C4A	-6.84	117.95	128.46
52	o	401	HEM	C3B-C2B-C1B	-5.58	102.35	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	b	402	HEM	CMA-C3A-C4A	-5.42	120.13	128.46
52	b	402	HEM	C4B-CHC-C1C	4.99	129.15	122.56
52	o	402	HEM	C3B-C2B-C1B	4.93	110.15	106.49

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

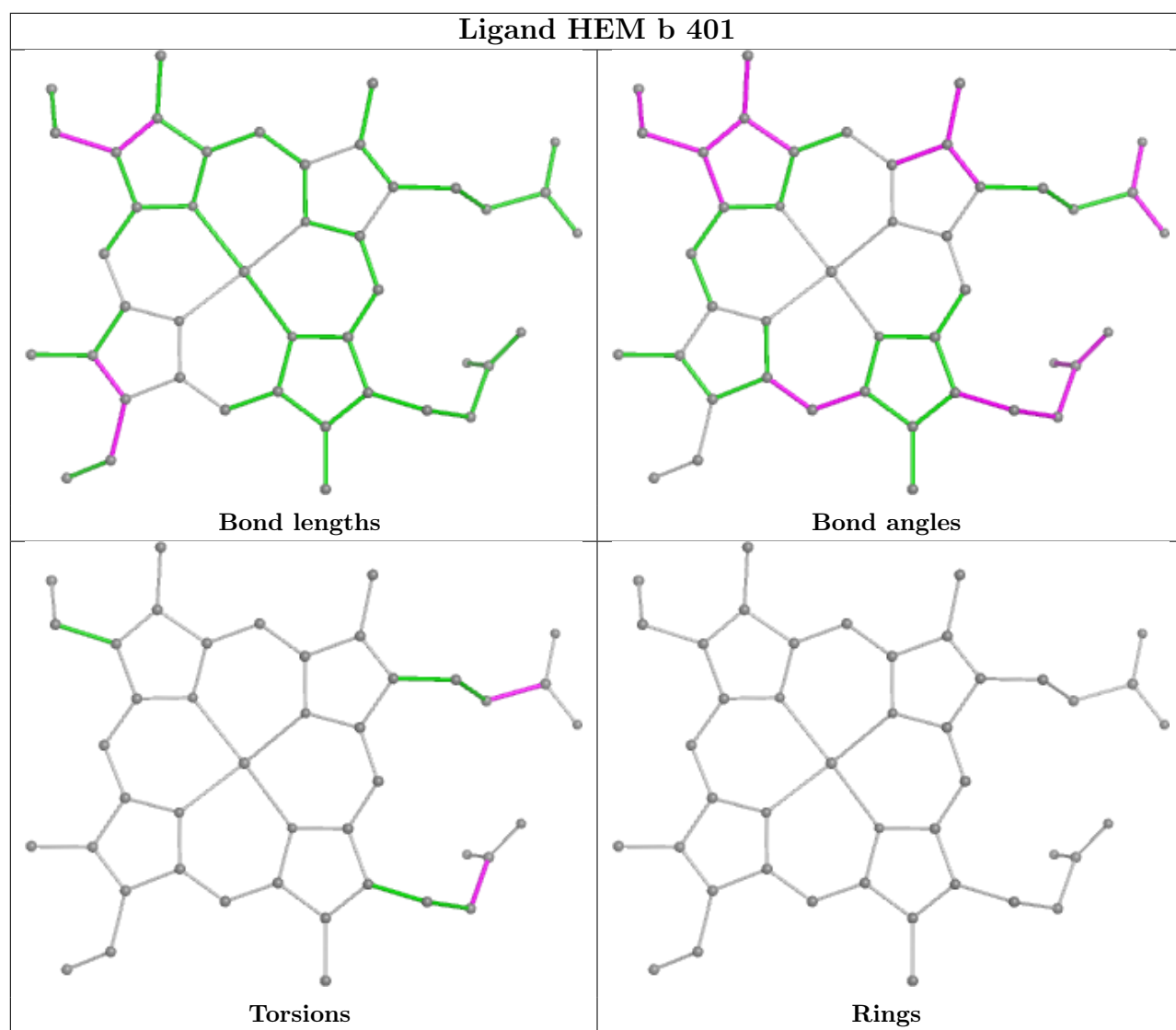
Mol	Chain	Res	Type	Atoms
52	o	401	HEM	C2B-C3B-CAB-CBB
57	x	603	HEA	C12-C11-C3B-C2B
57	x	603	HEA	C15-C16-C17-C18
52	o	401	HEM	C4B-C3B-CAB-CBB
52	b	402	HEM	C2B-C3B-CAB-CBB

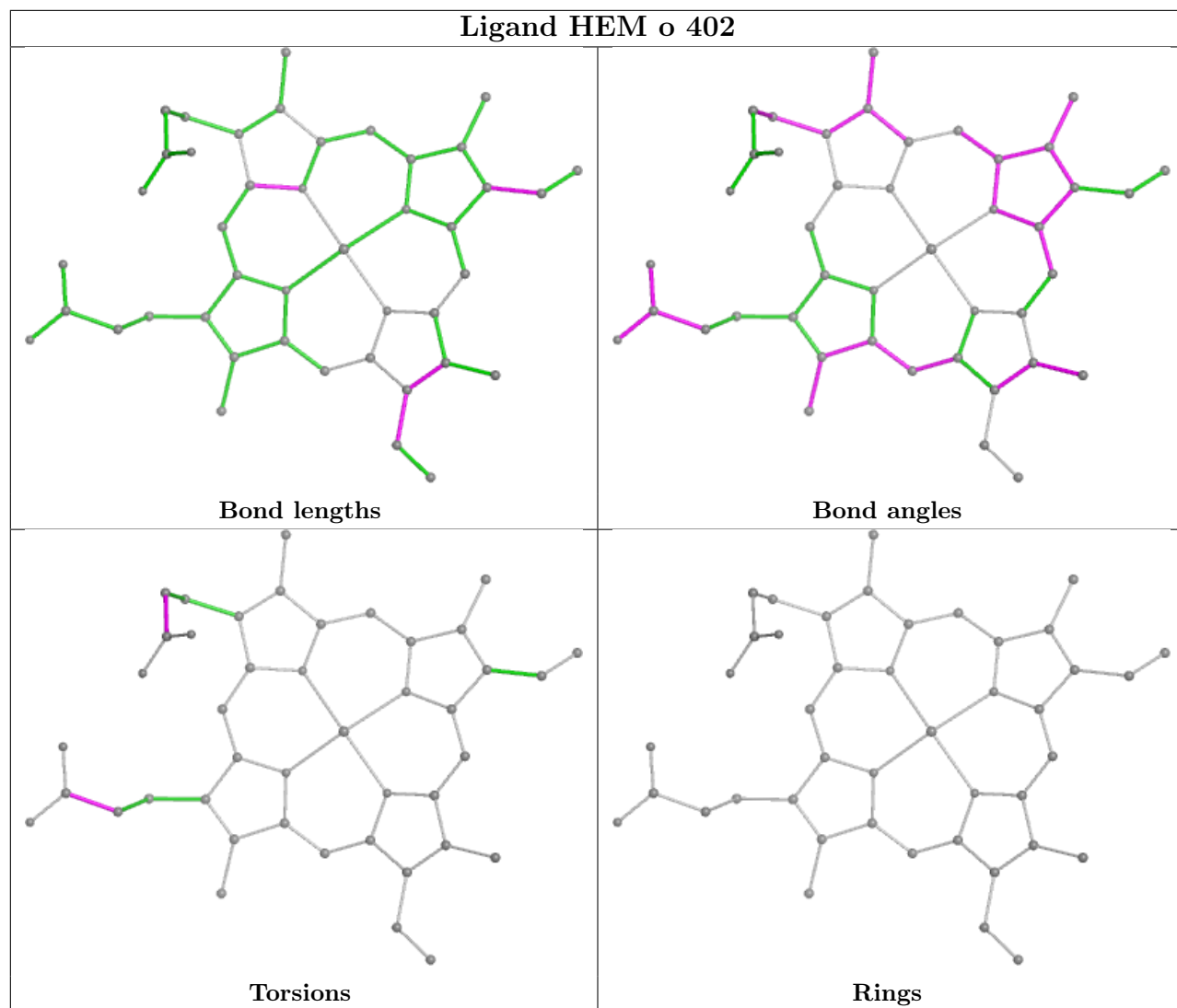
There are no ring outliers.

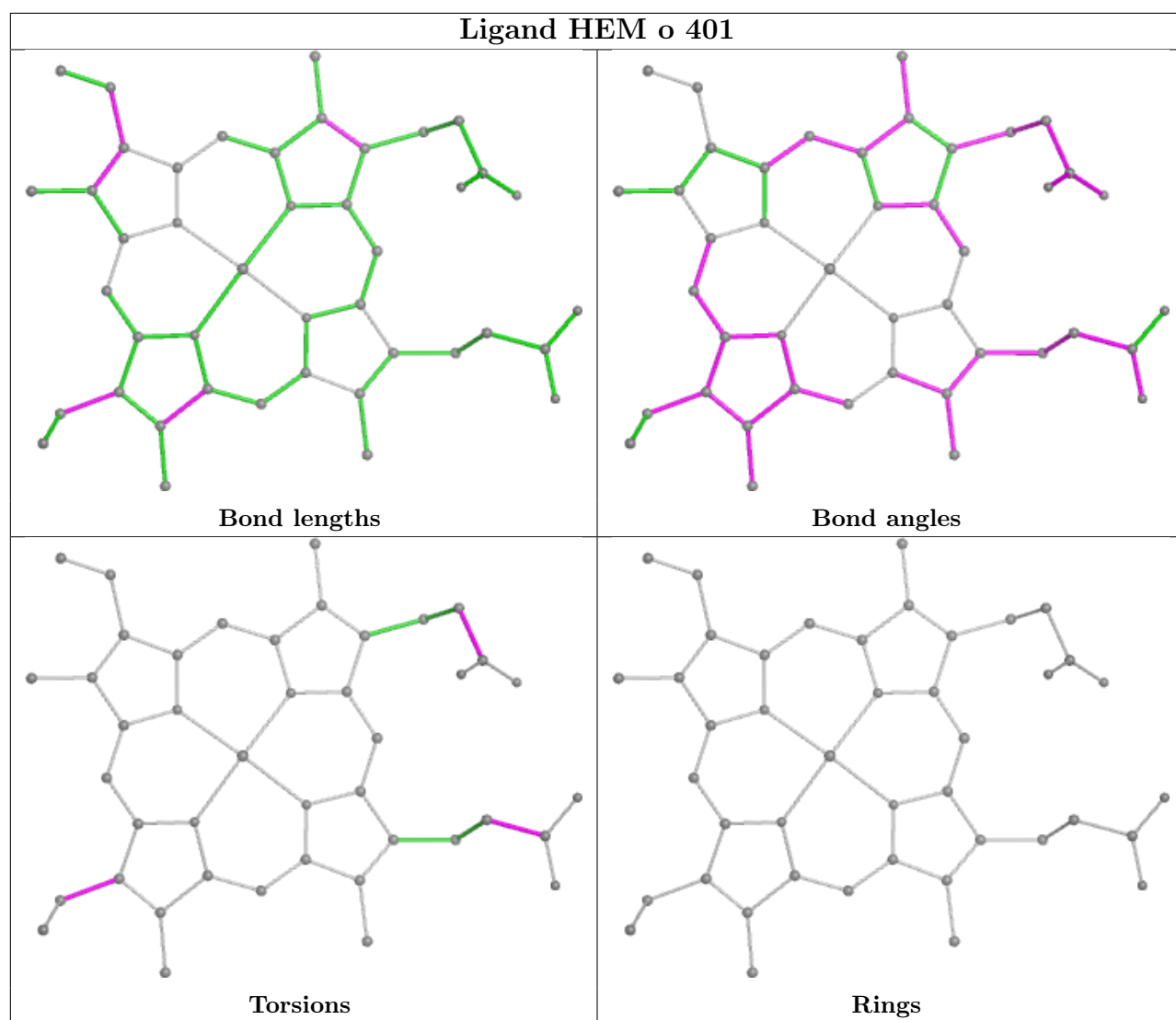
5 monomers are involved in 15 short contacts:

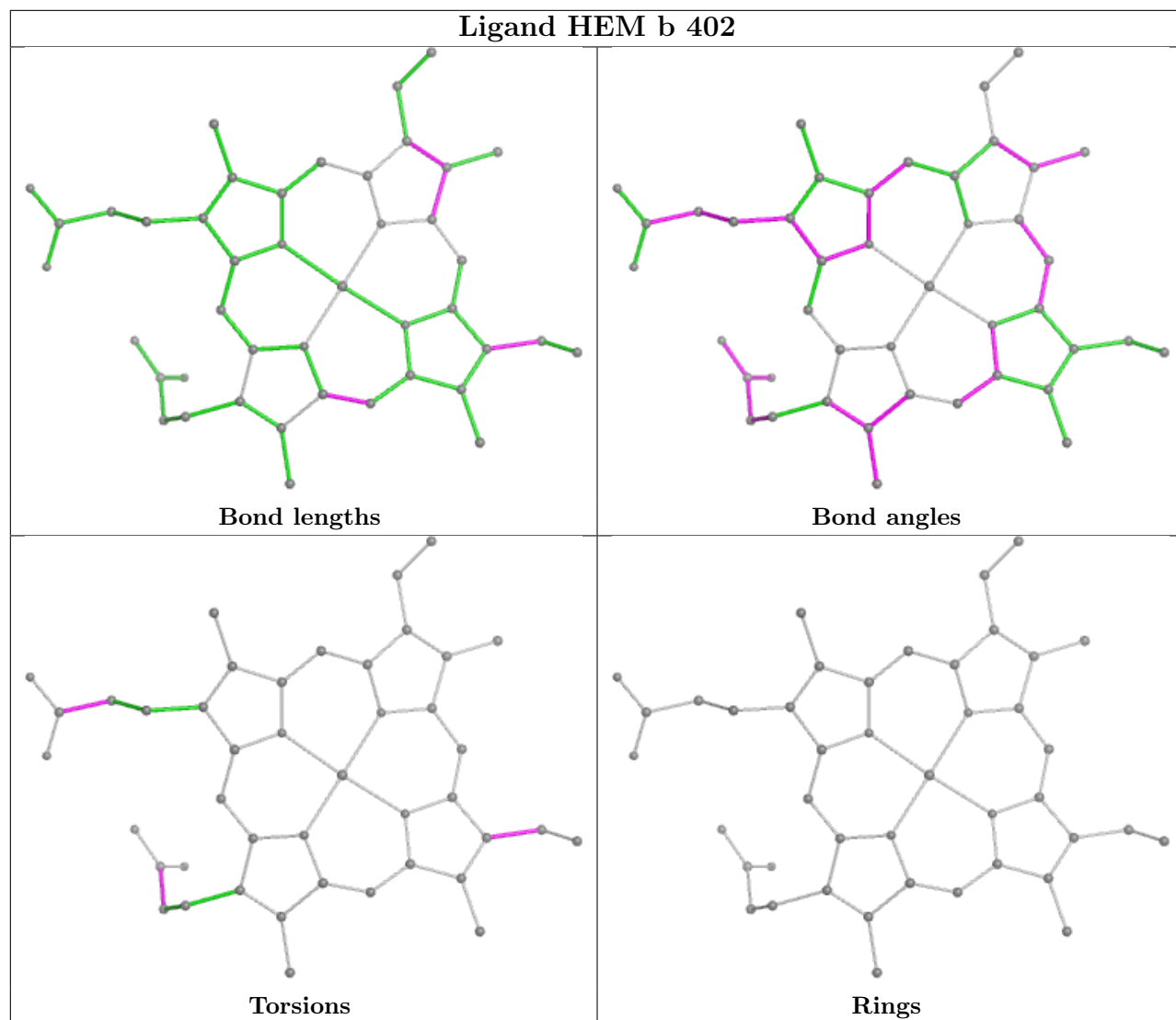
Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	F	501	SF4	1	0
59	I	202	SF4	3	0
59	B	201	SF4	6	0
59	I	201	SF4	2	0
54	G	803	FES	3	0

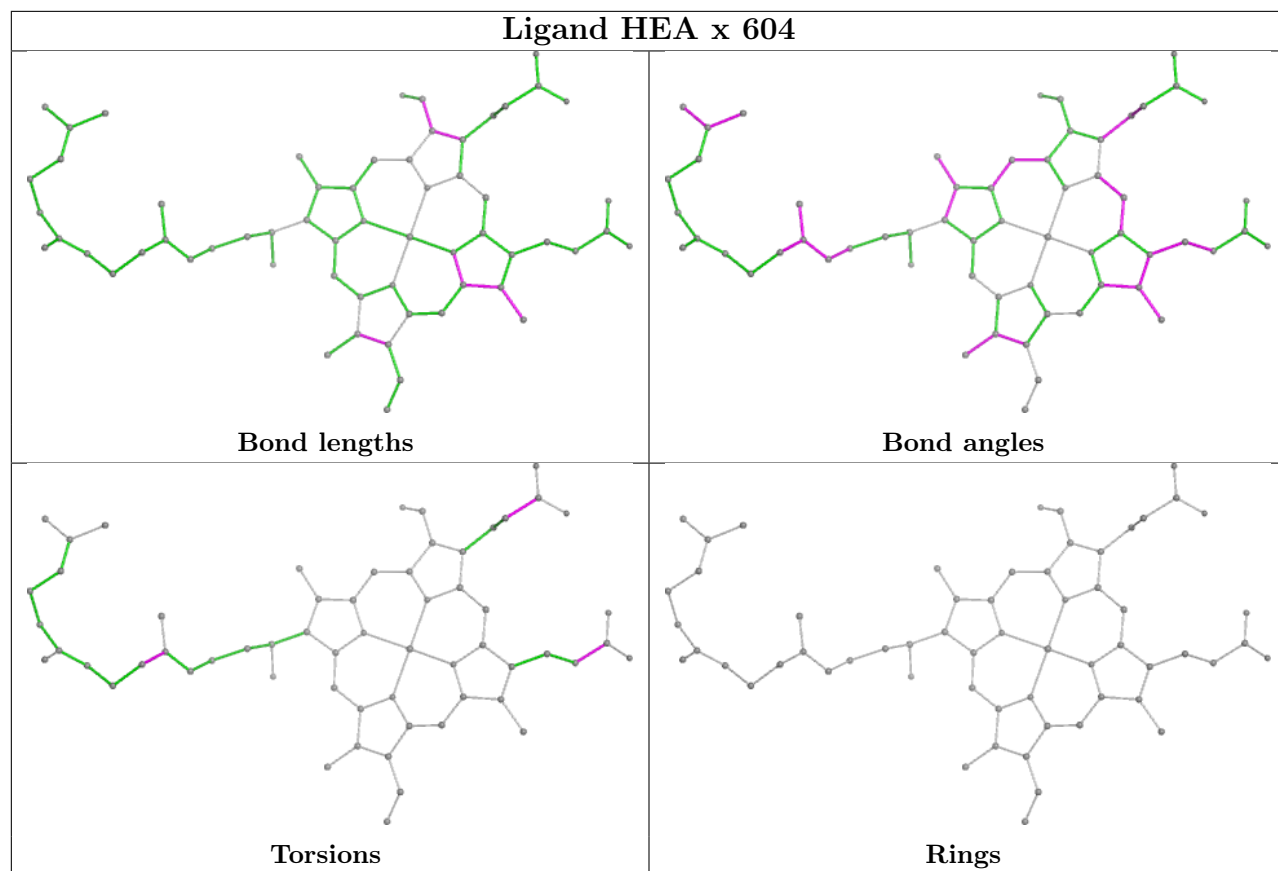
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



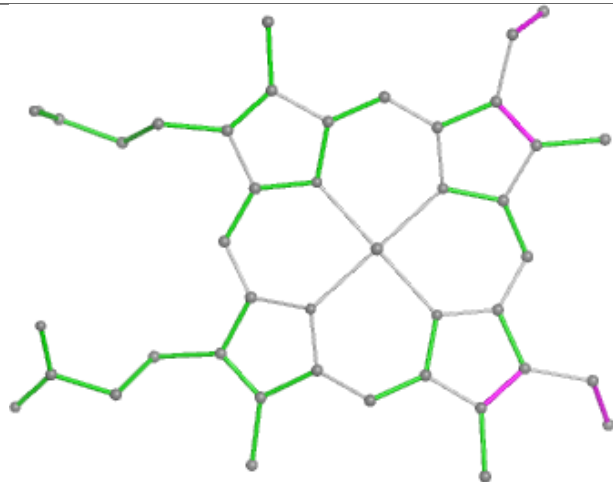




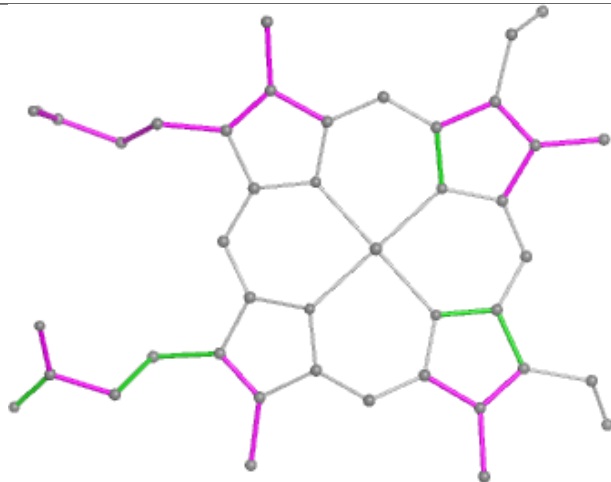




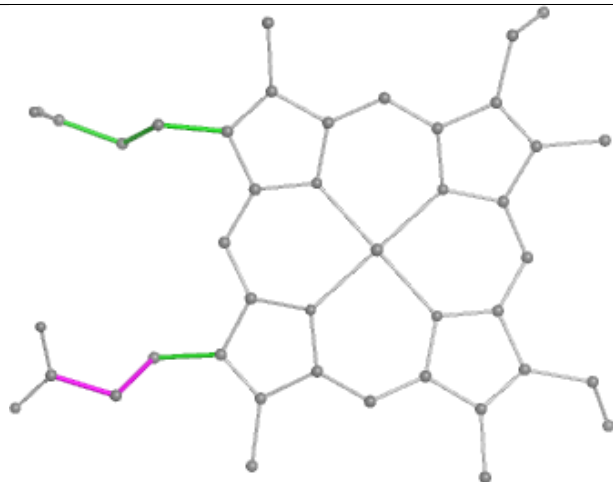
Ligand HEC d 301



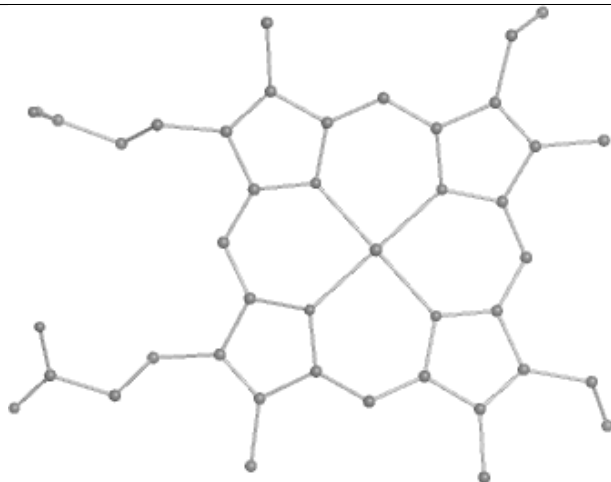
Bond lengths



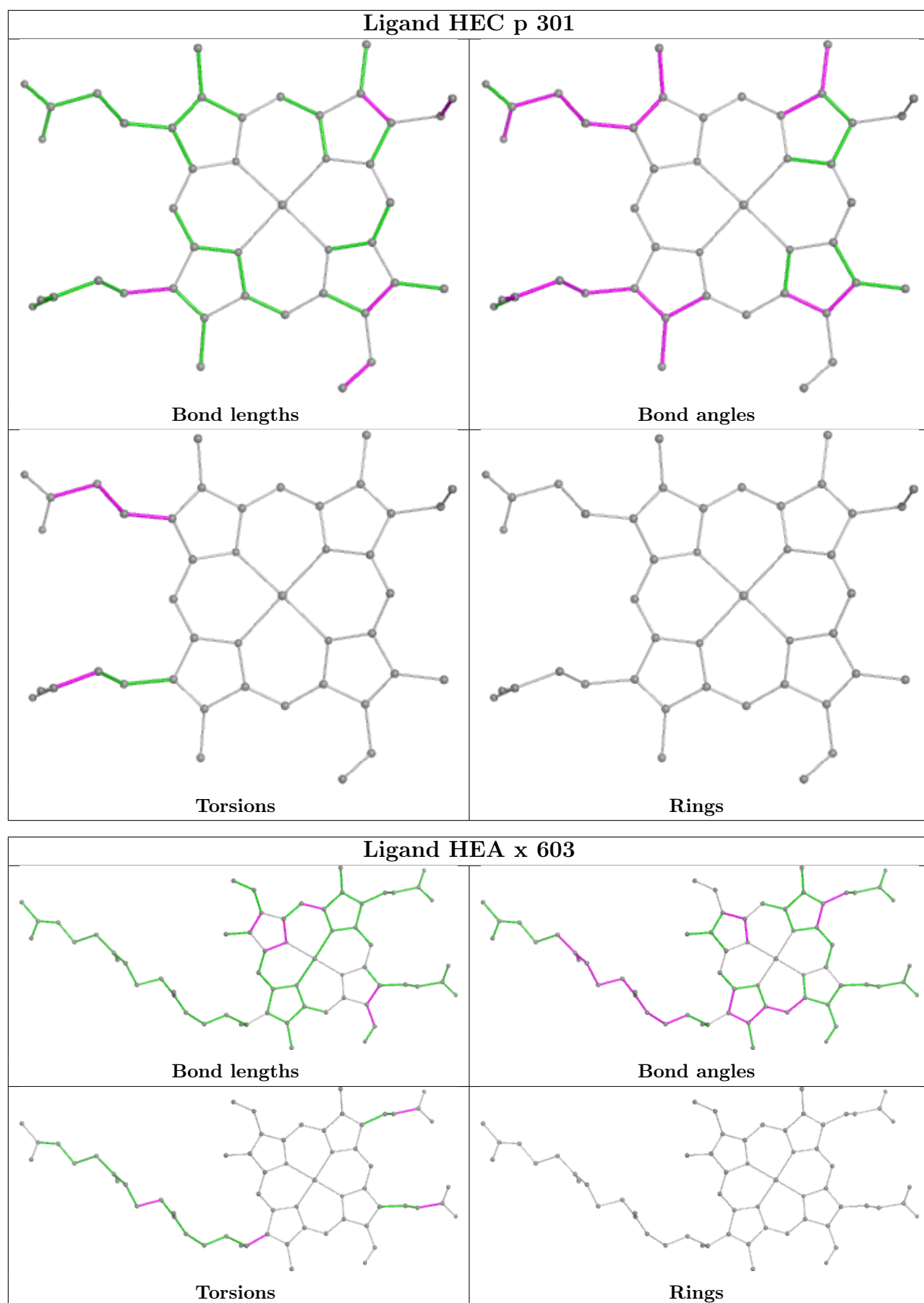
Bond angles



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
50	U	8
47	X	7
51	Z	6
31	G	6
36	L	5
39	O	3
34	J	2
40	P	2
32	H	2
44	T	2
49	a	1
25	A	1
38	N	1
37	M	1
41	Q	1

The worst 5 of 48 chain breaks are listed below:

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

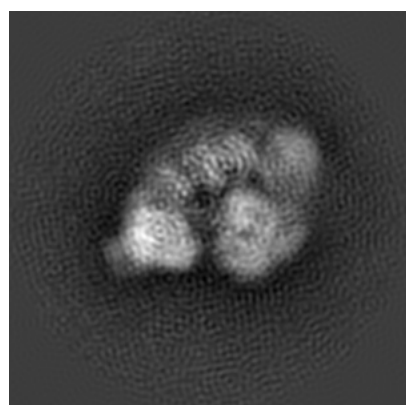
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4107. These allow visual inspection of the internal detail of the map and identification of artifacts.

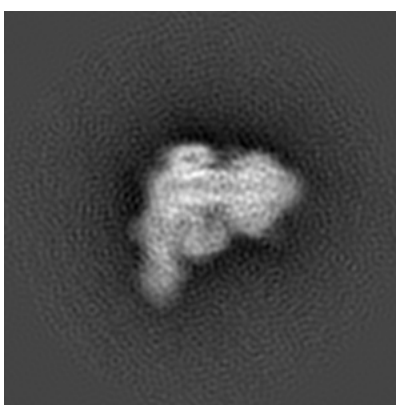
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

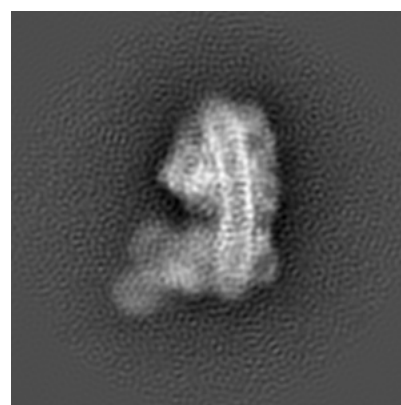
6.1.1 Primary map



X



Y

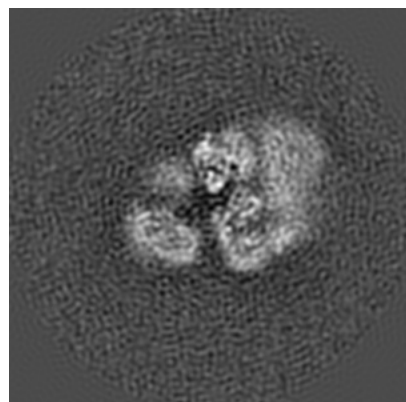


Z

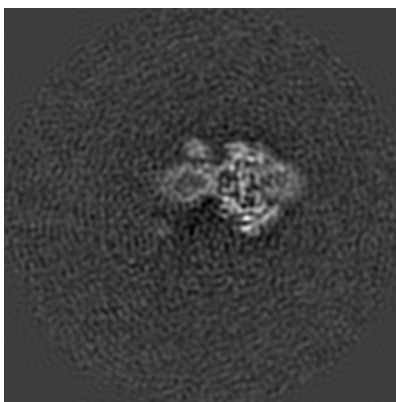
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

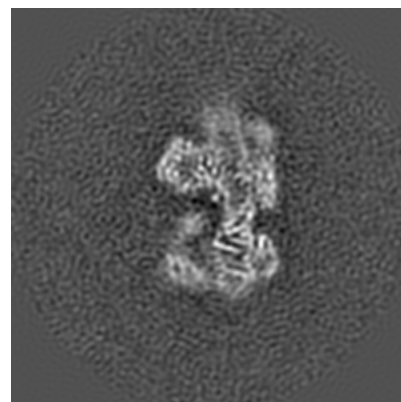
6.2.1 Primary map



X Index: 144



Y Index: 144

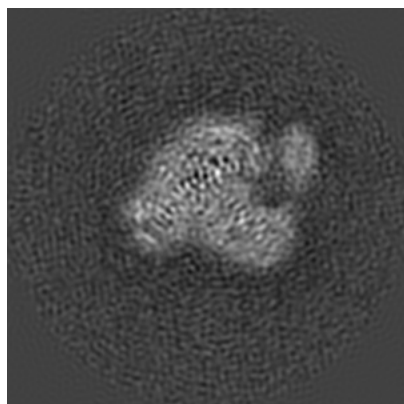


Z Index: 144

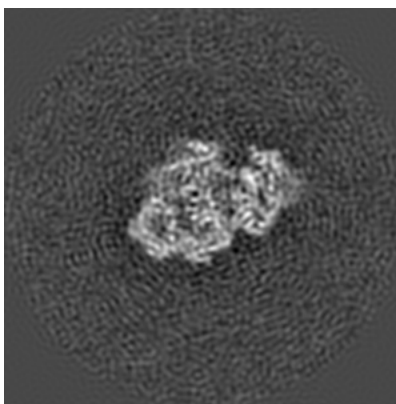
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

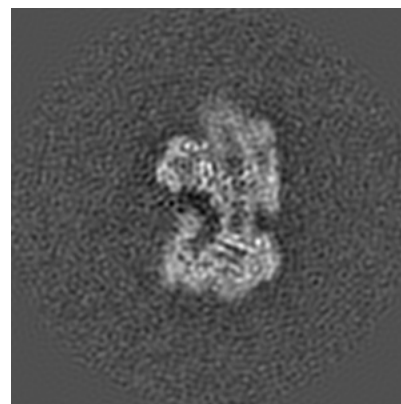
6.3.1 Primary map



X Index: 170



Y Index: 166

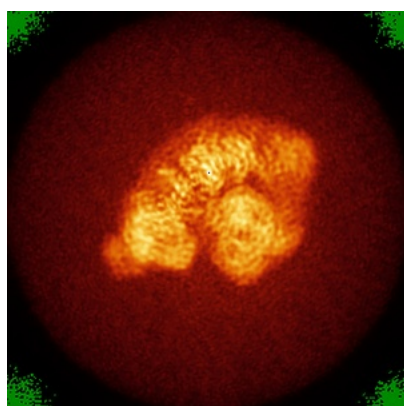


Z Index: 139

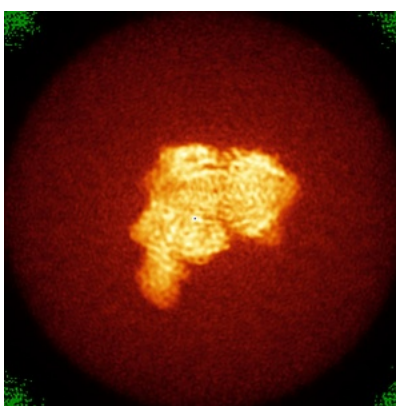
The images above show the largest variance slices of the map in three orthogonal directions.

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

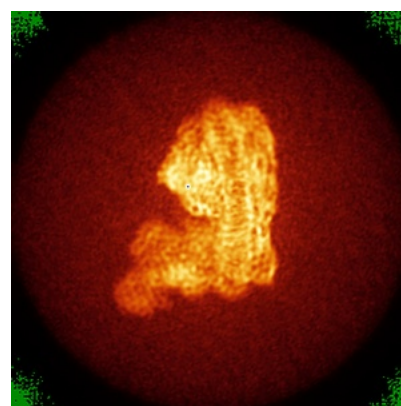
6.4.1 Primary map



X



Y

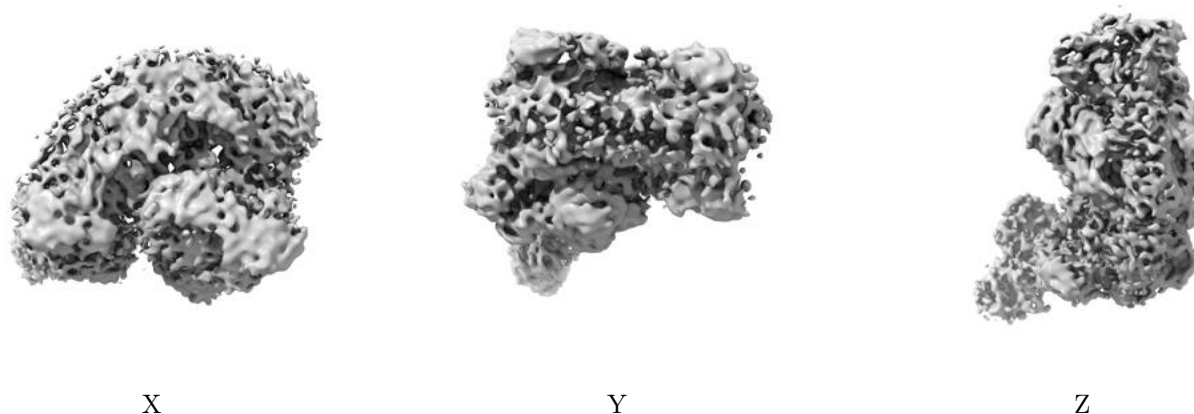


Z

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 0.081. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

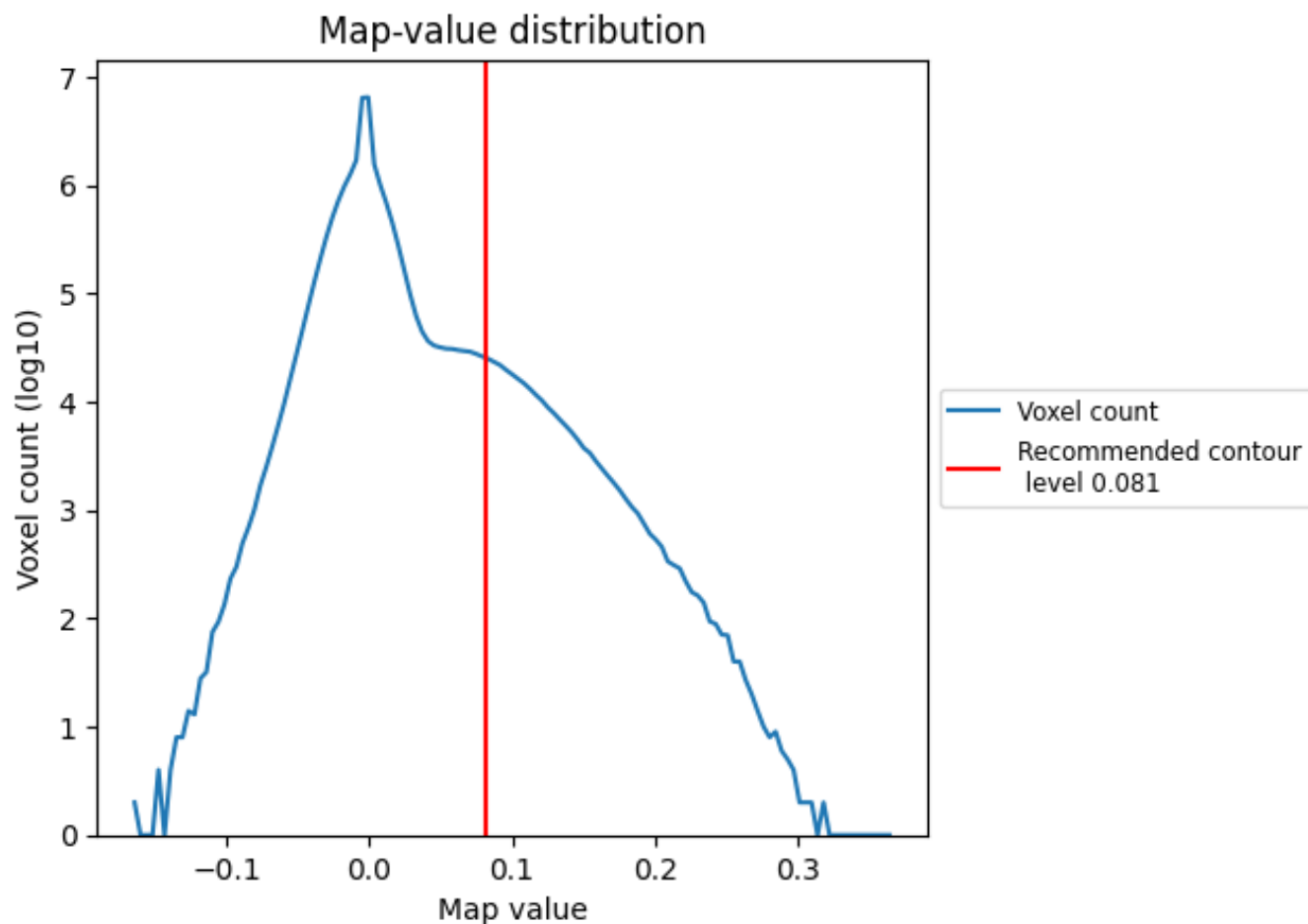
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

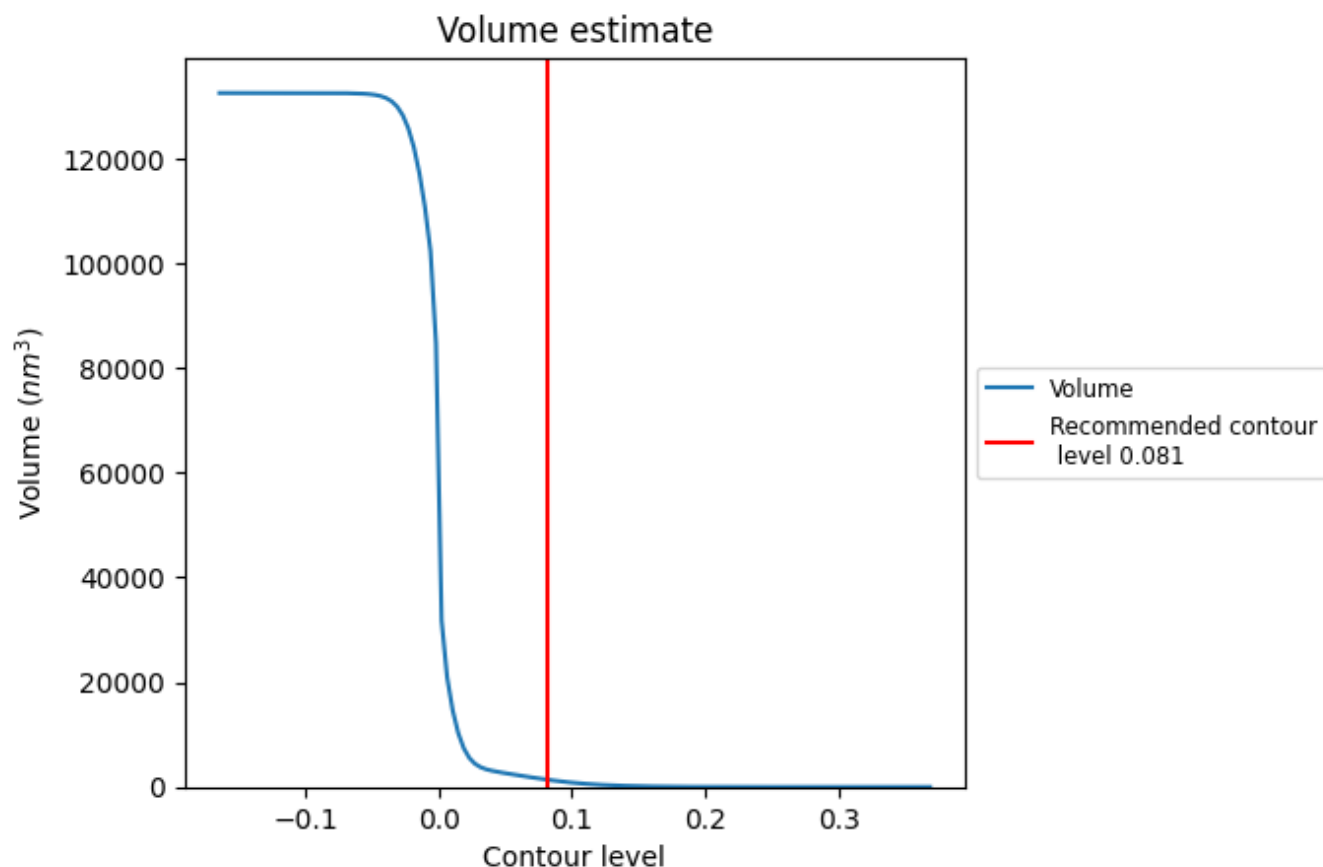
This section contains the results of statistical analysis of the map.

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.

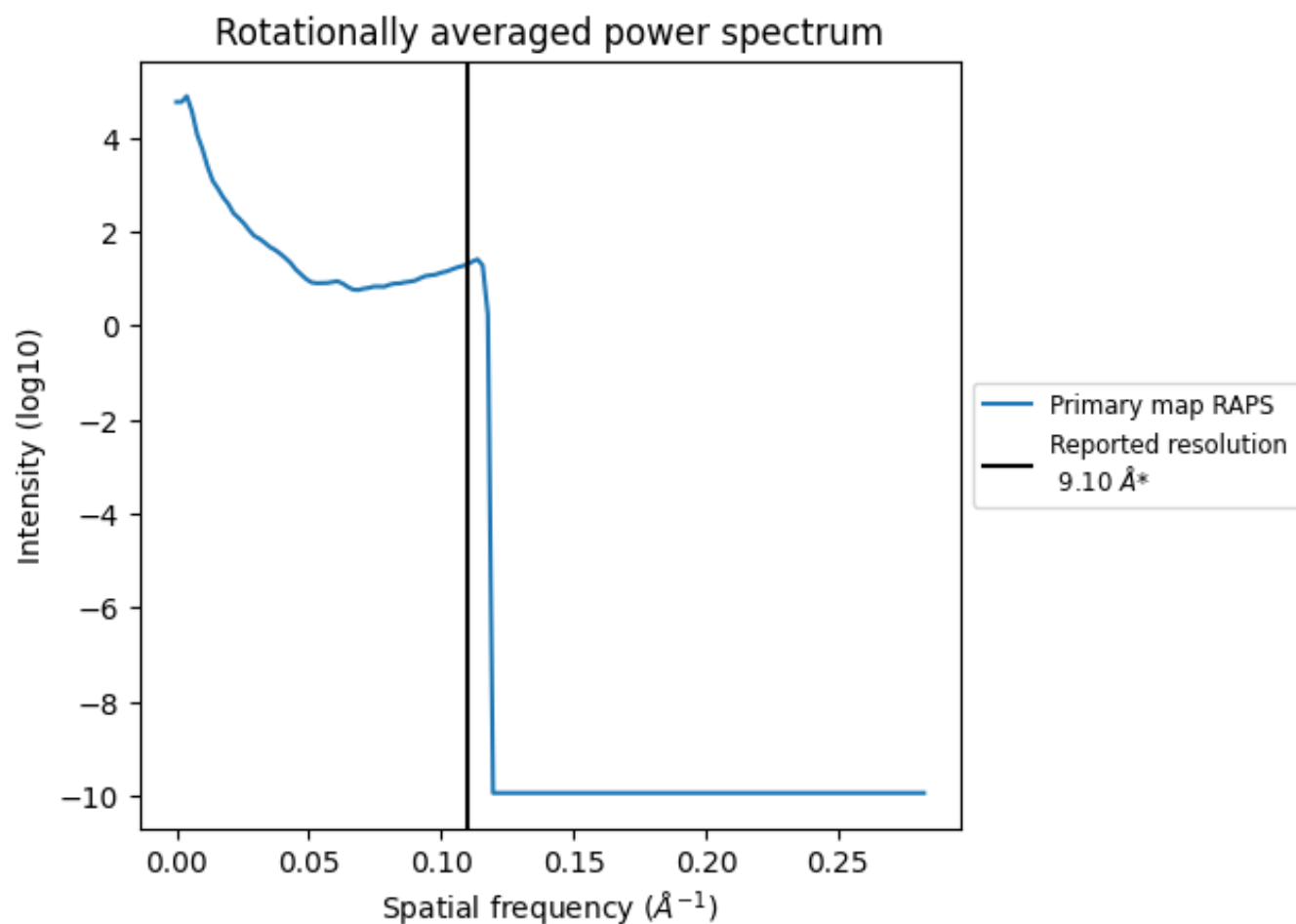
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1405 nm^3 ; this corresponds to an approximate mass of 1269 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 0.110 \AA^{-1}

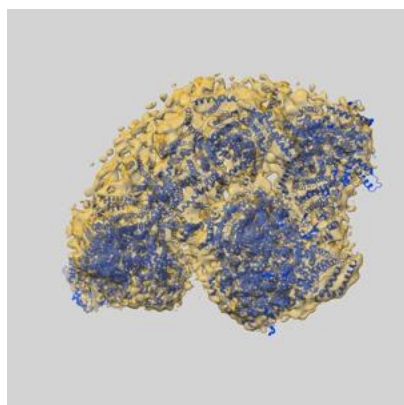
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

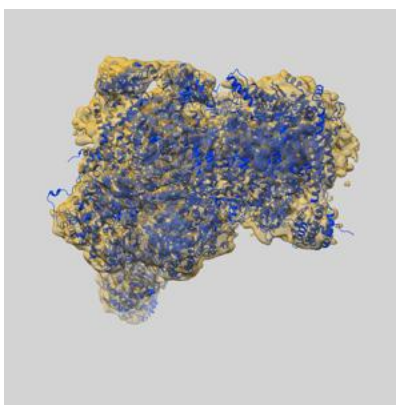
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4107 and PDB model 5LUF. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

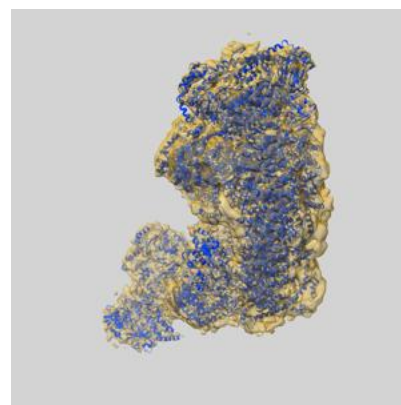
9.1 Map-model overlay [i](#)



X



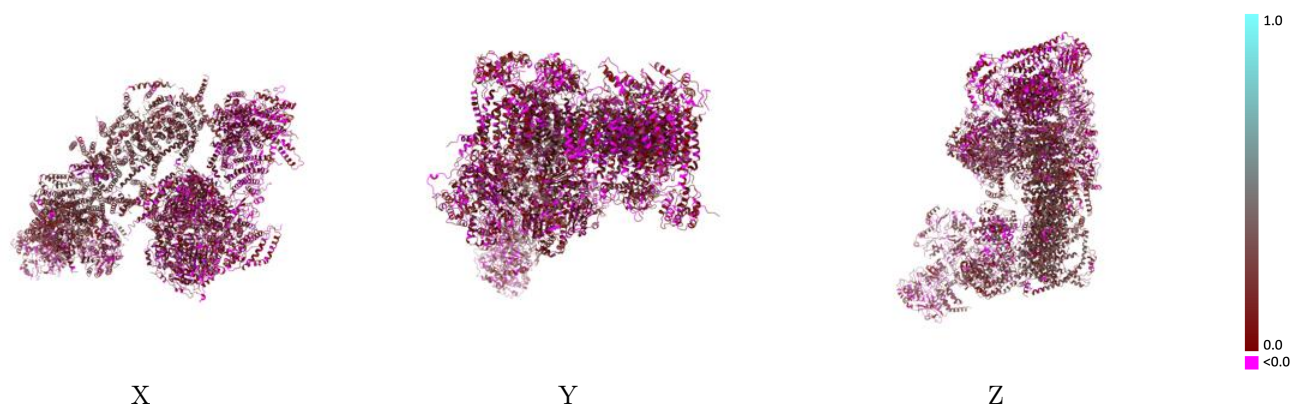
Y



Z

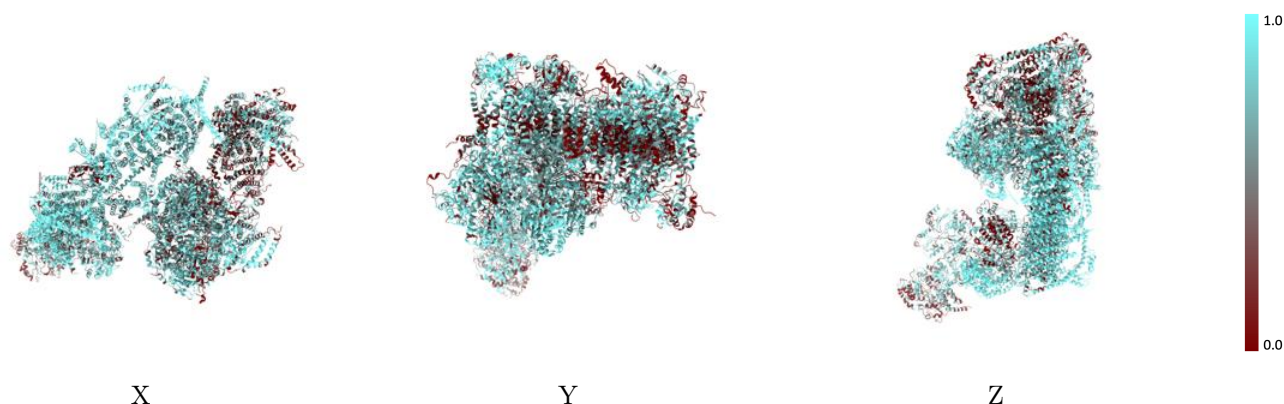
The images above show the 3D surface view of the map at the recommended contour level 0.081 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



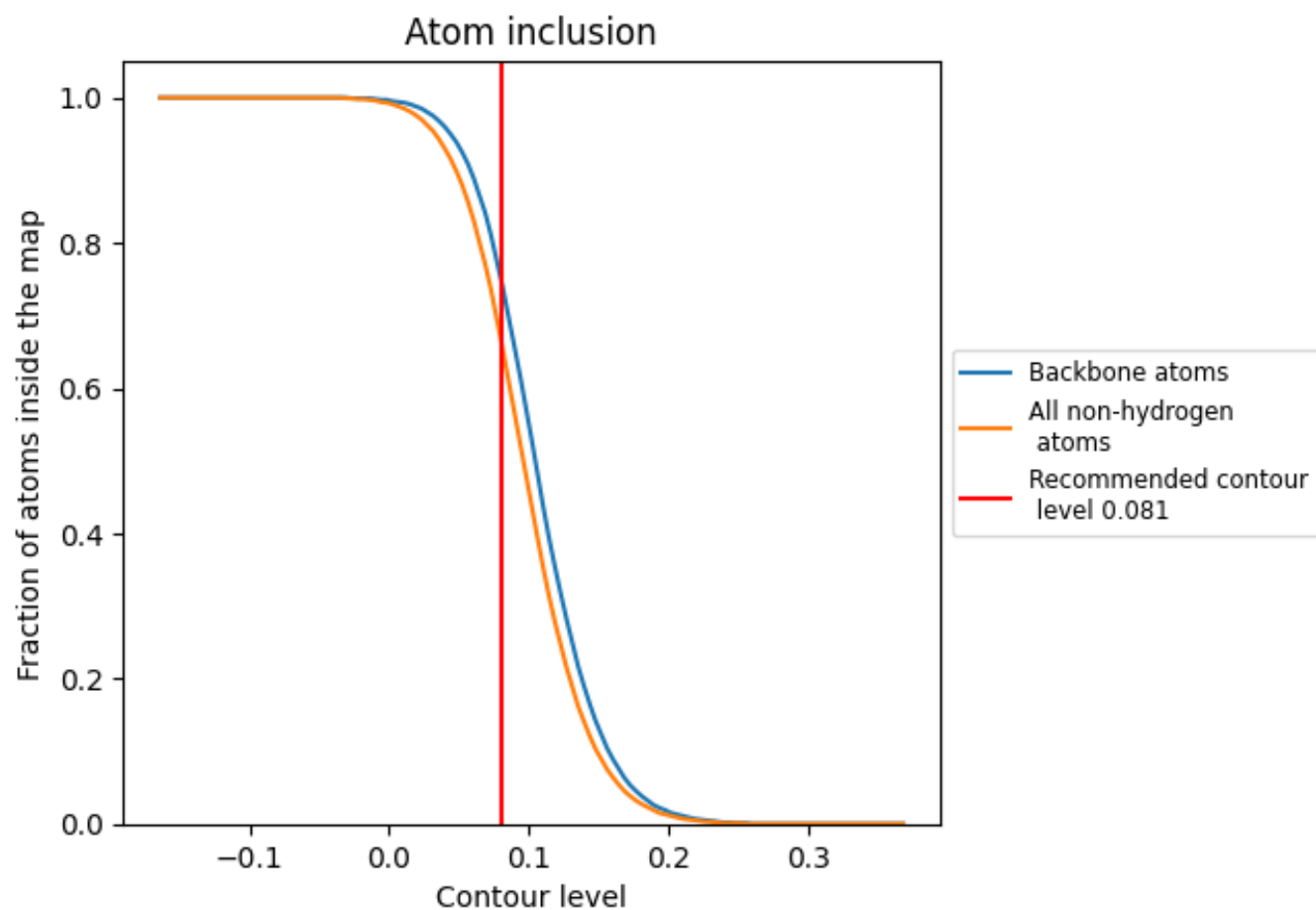
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.081).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 66% 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 (0.081) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6580	 0.1160
0	 0.5210	 0.1040
1	 0.4150	 0.0580
2	 0.4350	 0.0580
3	 0.4020	 0.0310
4	 0.2190	 -0.0020
5	 0.2610	 0.0540
6	 0.4550	 0.0650
7	 0.2790	 0.0510
8	 0.5330	 0.0780
9	 0.5000	 0.0550
A	 0.8100	 0.2640
B	 0.8170	 0.1760
C	 0.8440	 0.1700
D	 0.8540	 0.1700
E	 0.5040	 0.0580
F	 0.4690	 0.0870
G	 0.7290	 0.1010
H	 0.7990	 0.2150
I	 0.8670	 0.1290
J	 0.7830	 0.2180
K	 0.8570	 0.2430
L	 0.7950	 0.2180
M	 0.8390	 0.2470
N	 0.8620	 0.2510
O	 0.1380	 0.0250
P	 0.7630	 0.1270
Q	 0.5390	 0.1060
R	 0.3150	 0.0480
S	 0.6200	 0.1160
T	 0.5580	 0.1320
U	 0.8300	 0.2110
V	 0.9630	 0.2470
W	 0.7810	 0.1910
X	 0.9630	 0.2400



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Chain	Atom inclusion	Q-score
Y	 0.8400	 0.2070
Z	 0.9310	 0.2490
a	 0.8060	 0.2040
b	 0.6240	 0.1050
c	 0.7550	 0.0740
d	 0.7180	 0.0810
e	 0.3200	 0.0120
f	 0.7370	 0.1280
g	 0.5550	 0.0720
h	 0.7500	 0.0750
i	 0.0290	 -0.0600
j	 0.3780	 0.0430
k	 0.4450	 0.1510
l	 0.7210	 0.1030
m	 0.7670	 0.1000
n	 0.8220	 0.1160
o	 0.5950	 0.1030
p	 0.6710	 0.0830
q	 0.3810	 0.0600
r	 0.6440	 0.1280
s	 0.5880	 0.0990
t	 0.6740	 0.0770
u	 0.0550	 -0.0640
v	 0.4060	 0.0980
w	 0.3030	 0.0900
x	 0.5070	 0.0580
y	 0.6130	 0.0520
z	 0.4050	 0.0220