



wwPDB EM Validation Summary Report ⓘ

Oct 12, 2024 – 01:03 PM EDT

PDB ID : 5KZ5
EMDB ID : EMD-8301
Title : Architecture of the Human Mitochondrial Iron-Sulfur Cluster Assembly Machinery: the Complex Formed by the Iron Donor, the Sulfur Donor, and the Scaffold
Authors : Gakh, O.; Ranatunga, W.; Smith, D.Y.; Ahlgren, E.C.; Al-Karadaghi, S.; Thompson, J.R.; Isaya, G.
Deposited on : 2016-07-22
Resolution : 14.30 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
MolProbity : 4.02b-467
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

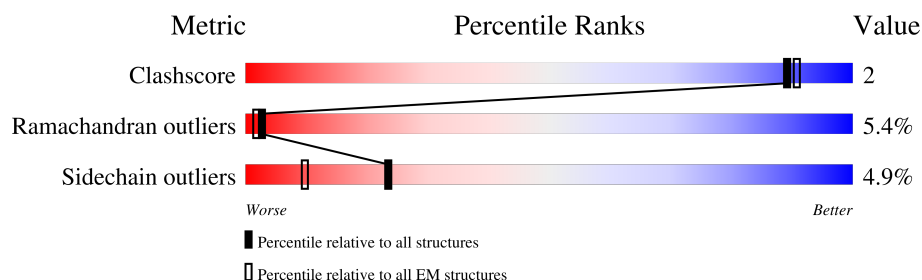
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 14.30 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	1	391	<div> <div>51%</div> <div>81%</div> <div>15%</div> <div>.</div> </div>
1	2	391	<div> <div>54%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
1	3	391	<div> <div>59%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>
1	4	391	<div> <div>50%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
1	M	391	<div> <div>56%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	N	391	<div> <div>60%</div> <div>91%</div> <div>9%</div> <div>.</div> </div>
1	O	391	<div> <div>63%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	P	391	<div> <div>59%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Q	391	61% 90% 9% .
1	R	391	62% 88% 11% .
1	S	391	59% 90% 10%
1	T	391	63% 89% 9% .
2	A	169	56% 79% 18% .
2	B	169	50% 88% 9% .
2	C	169	58% 82% 15% .
2	D	169	56% 85% 12% .
2	E	169	56% 79% 16% . .
2	F	169	58% 87% 10% . .
2	G	169	56% 86% 11% . .
2	H	169	54% 86% 11% . .
2	I	169	55% 80% 16% . .
2	J	169	49% 83% 16% .
2	K	169	57% 80% 16% .
2	L	169	60% 80% 17% . .
3	a	118	52% 89% 10% .
3	b	118	63% 93% 7%
3	c	118	38% 95% . .
3	d	118	49% 92% 8% .
3	e	118	65% 92% 8% .
3	f	118	41% 90% 10%
3	g	118	49% 88% 12%
3	h	118	59% 94% 5% .
3	i	118	47% 91% 6% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	j	118	<div><div>58%</div><div>83%</div><div>16%</div><div></div></div>
3	k	118	<div><div>53%</div><div>92%</div><div>7%</div><div></div></div>
3	l	118	<div><div>53%</div><div>90%</div><div>9%</div><div></div></div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 62880 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 Cysteine desulfurase, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	391	Total 3040	C 1905	N 540	O 576	S 19	0	0
1	2	391	Total 3040	C 1905	N 540	O 576	S 19	0	0
1	3	391	Total 3040	C 1905	N 540	O 576	S 19	0	0
1	4	391	Total 3040	C 1905	N 540	O 576	S 19	0	0
1	M	391	Total 3040	C 1905	N 540	O 576	S 19	0	0
1	N	391	Total 3040	C 1905	N 540	O 576	S 19	0	0
1	O	391	Total 3040	C 1905	N 540	O 576	S 19	0	0
1	P	391	Total 3040	C 1905	N 540	O 576	S 19	0	0
1	Q	391	Total 3040	C 1905	N 540	O 576	S 19	0	0
1	R	391	Total 3040	C 1905	N 540	O 576	S 19	0	0
1	S	391	Total 3040	C 1905	N 540	O 576	S 19	0	0
1	T	391	Total 3040	C 1905	N 540	O 576	S 19	0	0

- Molecule 2 is a protein called Frataxin, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	169	Total 1328	C 837	N 225	O 264	S 2	0	0
2	B	169	Total 1328	C 837	N 225	O 264	S 2	0	0
2	C	169	Total 1328	C 837	N 225	O 264	S 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	169	Total	C	N	O	S	0	0
			1328	837	225	264	2		
2	E	169	Total	C	N	O	S	0	0
			1328	837	225	264	2		
2	F	169	Total	C	N	O	S	0	0
			1328	837	225	264	2		
2	G	169	Total	C	N	O	S	0	0
			1328	837	225	264	2		
2	H	169	Total	C	N	O	S	0	0
			1328	837	225	264	2		
2	I	169	Total	C	N	O	S	0	0
			1328	837	225	264	2		
2	J	169	Total	C	N	O	S	0	0
			1328	837	225	264	2		
2	K	169	Total	C	N	O	S	0	0
			1328	837	225	264	2		
2	L	169	Total	C	N	O	S	0	0
			1328	837	225	264	2		

- Molecule 3 is a protein called Iron-sulfur cluster assembly enzyme ISCU, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	118	Total	C	N	O	S	0	0
			872	549	147	170	6		
3	b	118	Total	C	N	O	S	0	0
			872	549	147	170	6		
3	c	118	Total	C	N	O	S	0	0
			872	549	147	170	6		
3	d	118	Total	C	N	O	S	0	0
			872	549	147	170	6		
3	e	118	Total	C	N	O	S	0	0
			872	549	147	170	6		
3	f	118	Total	C	N	O	S	0	0
			872	549	147	170	6		
3	g	118	Total	C	N	O	S	0	0
			872	549	147	170	6		
3	h	118	Total	C	N	O	S	0	0
			872	549	147	170	6		
3	i	118	Total	C	N	O	S	0	0
			872	549	147	170	6		
3	j	118	Total	C	N	O	S	0	0
			872	549	147	170	6		

Continued on next page...

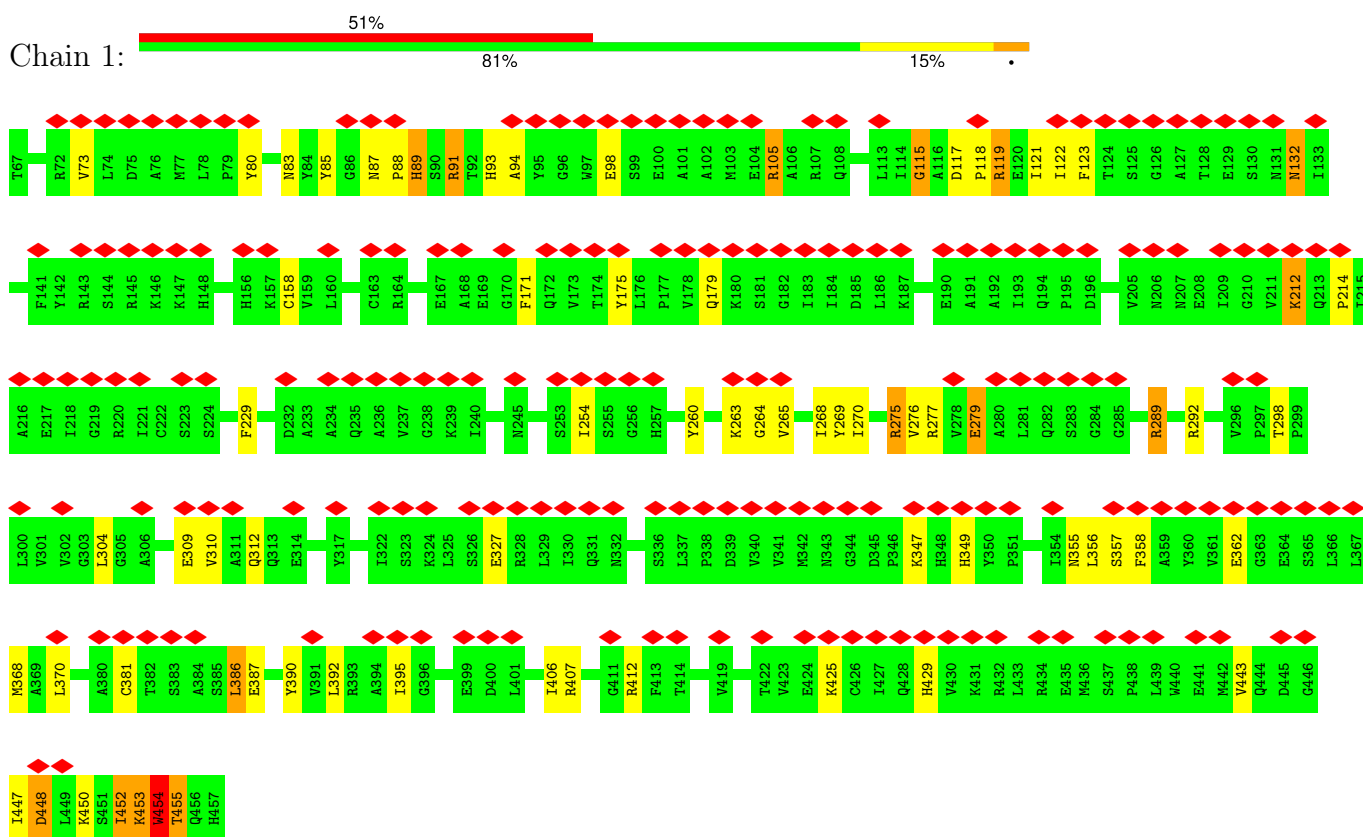
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	k	118	Total	C	N	O	S	0	0
			872	549	147	170	6		
3	l	118	Total	C	N	O	S	0	0
			872	549	147	170	6		

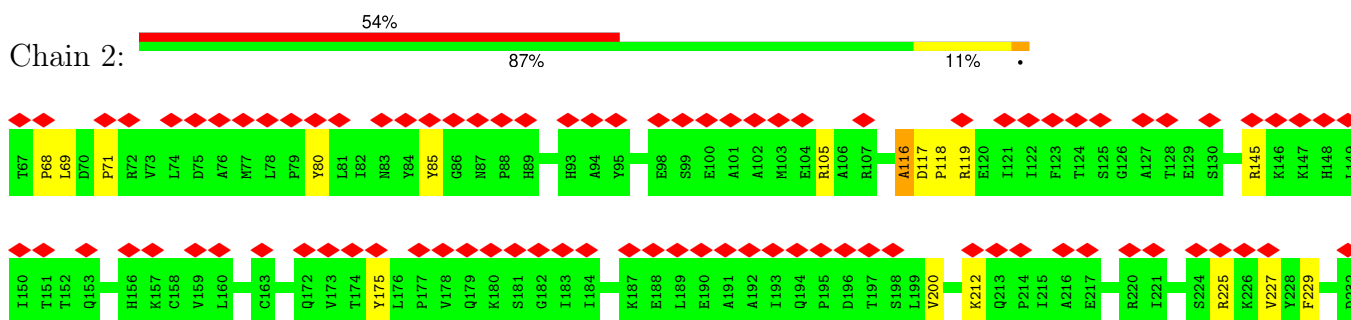
3 Residue-property plots

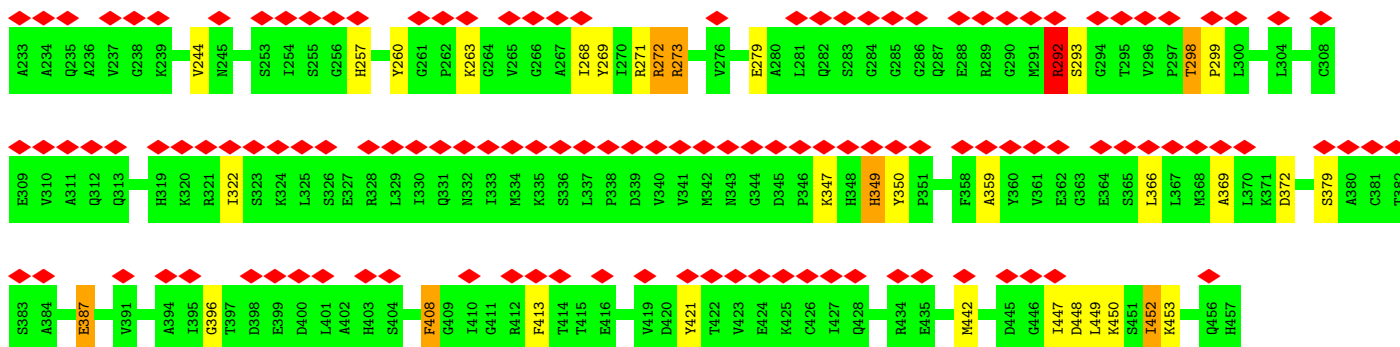
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



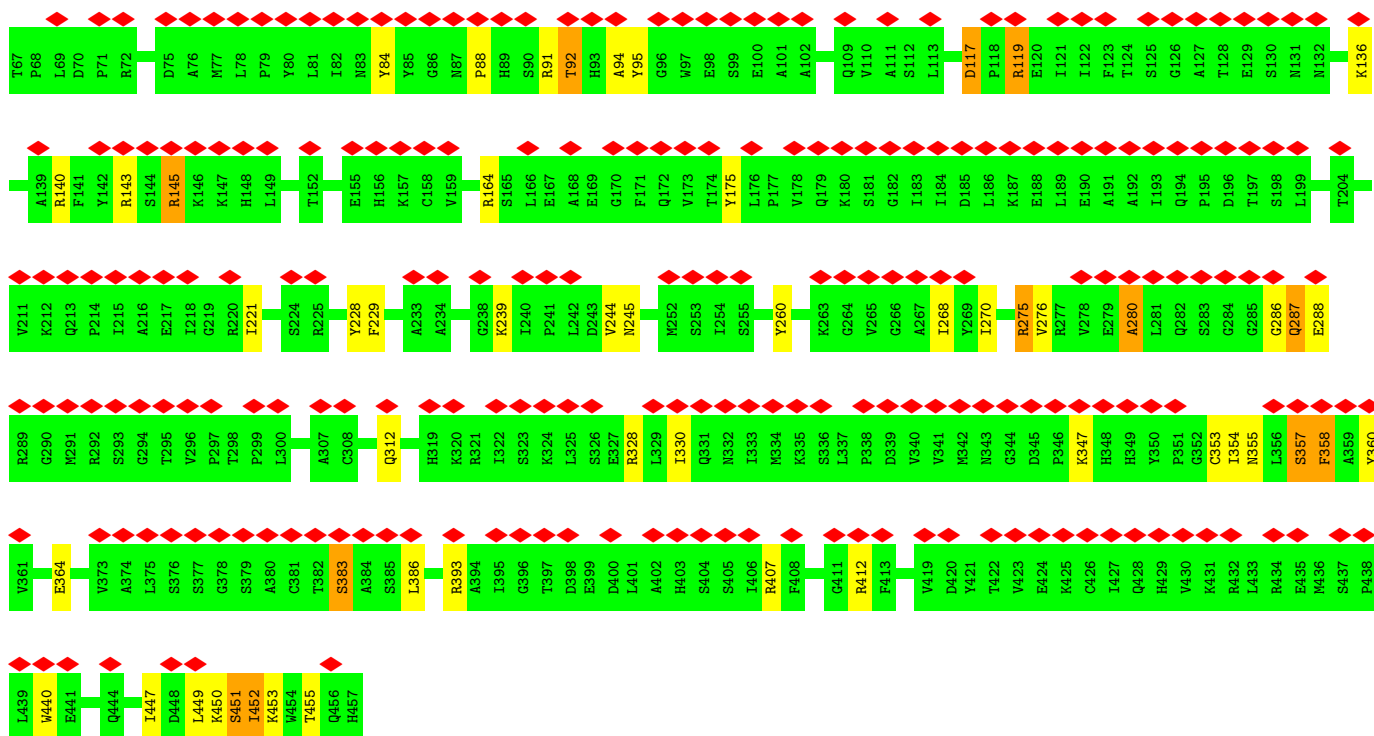
- Molecule 1: Cysteine desulfurase, mitochondrial





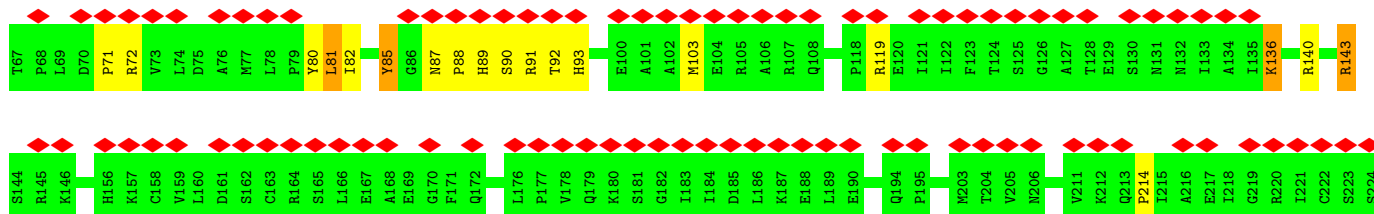
• Molecule 1: Cysteine desulfurase, mitochondrial

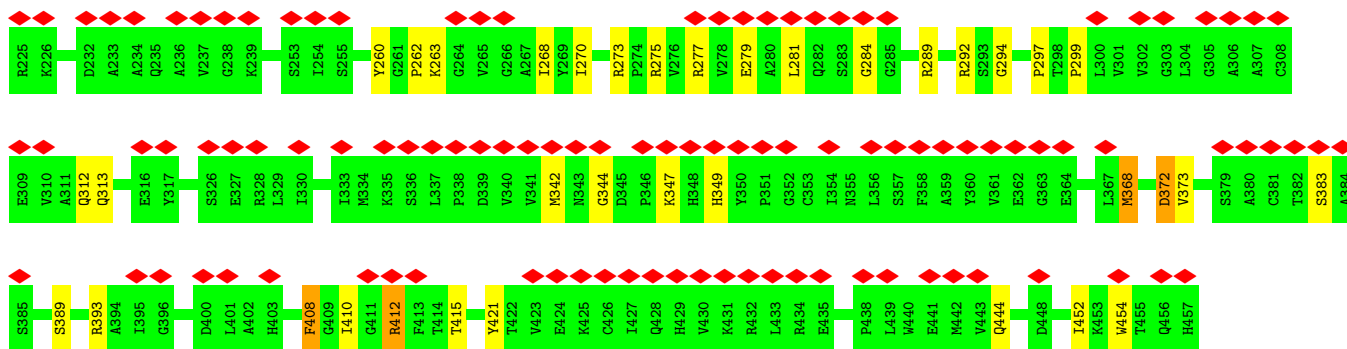
Chain 3: 59% 86% 10% •



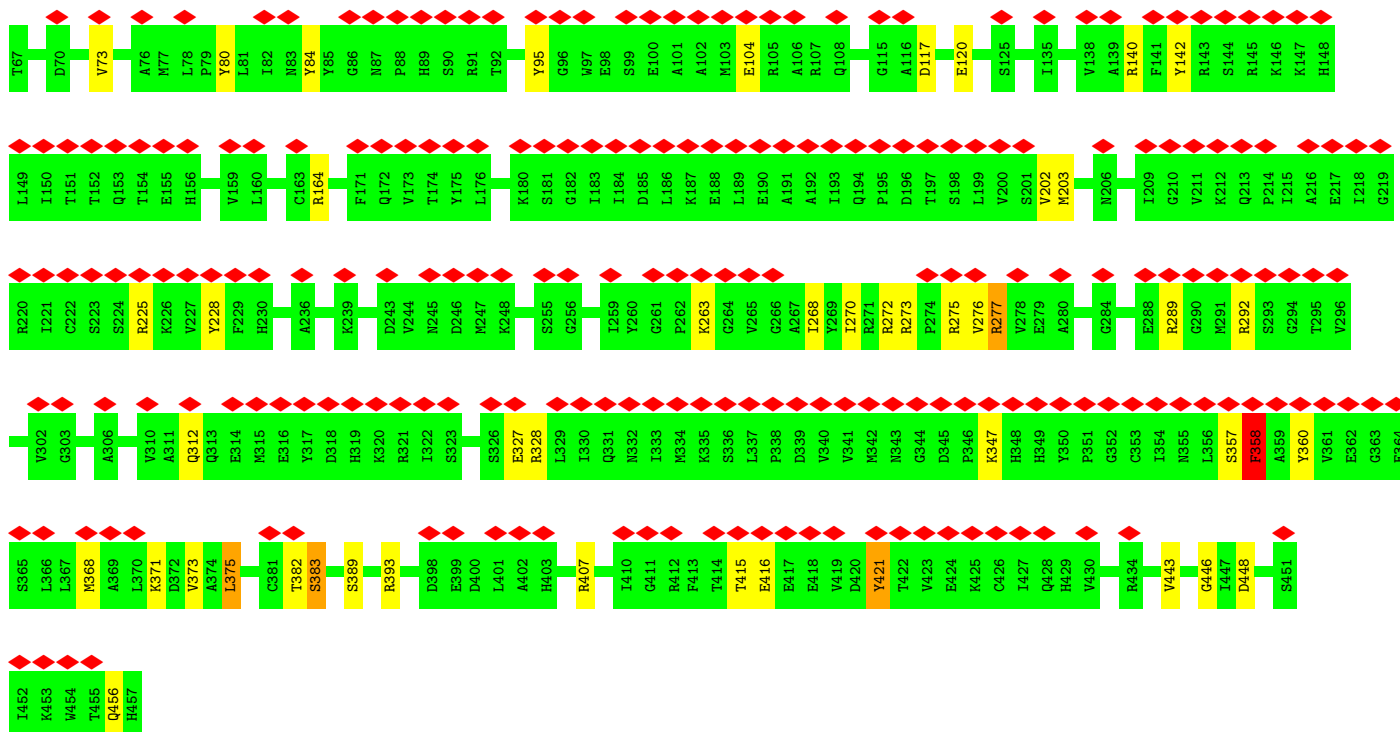
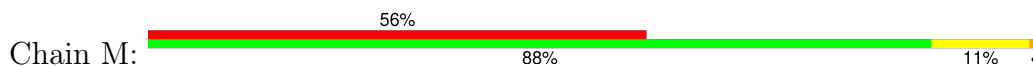
• Molecule 1: Cysteine desulfurase, mitochondrial

Chain 4: 50% 86% 12% •

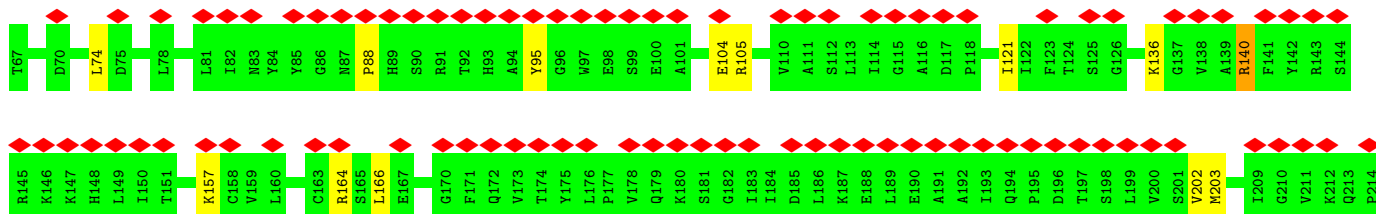
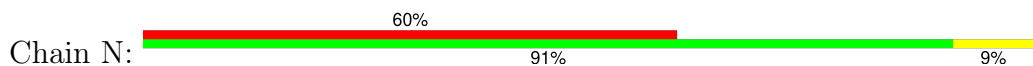


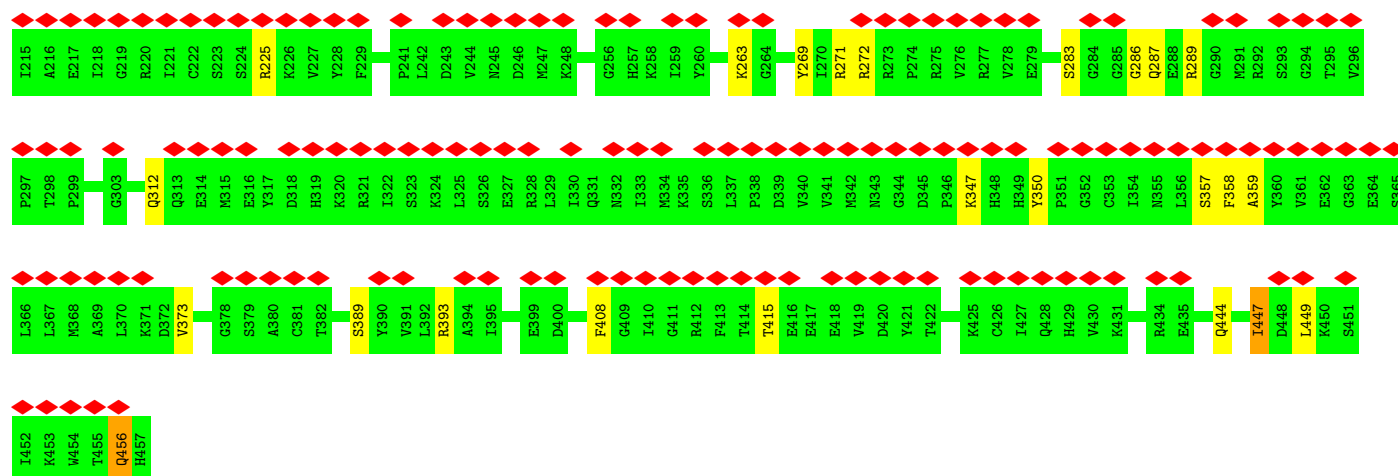


• Molecule 1: Cysteine desulfurase, mitochondrial

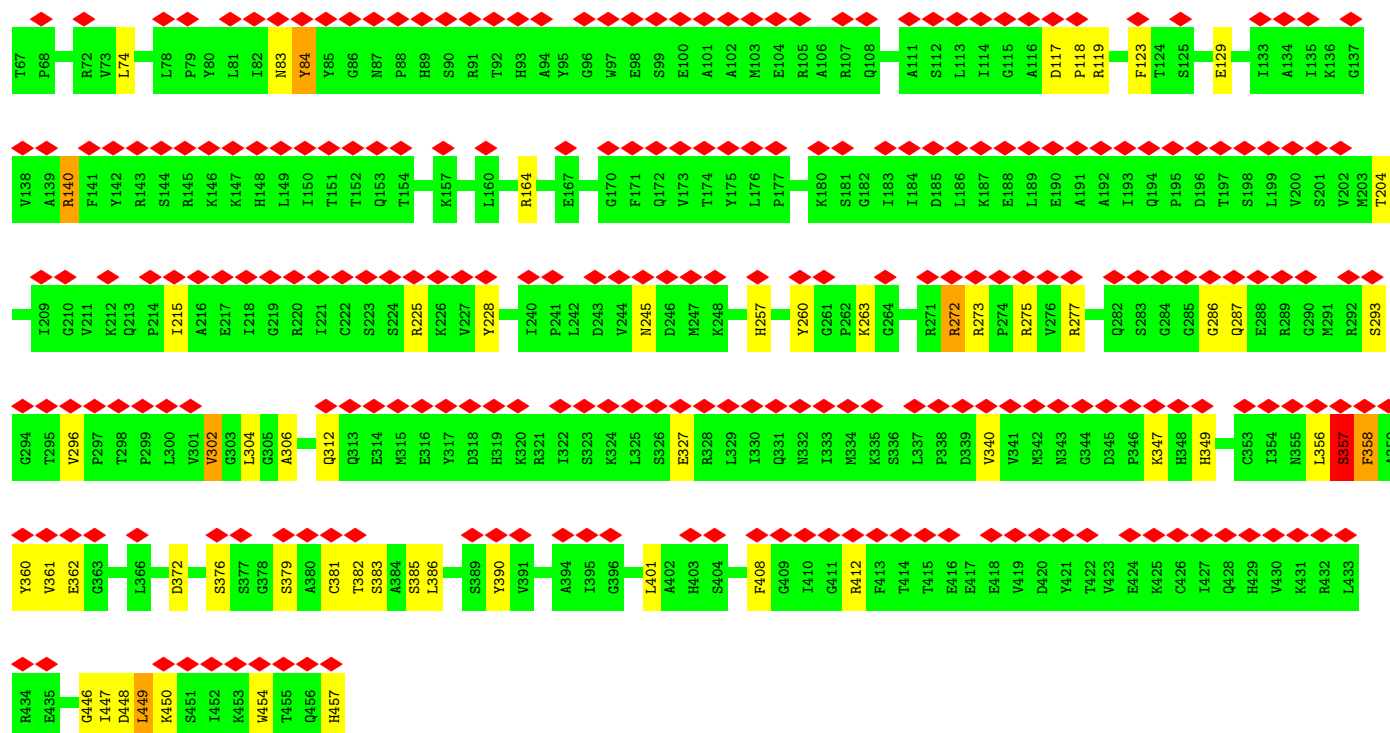
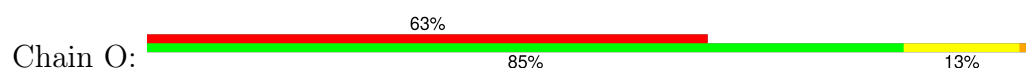


• Molecule 1: Cysteine desulfurase, mitochondrial

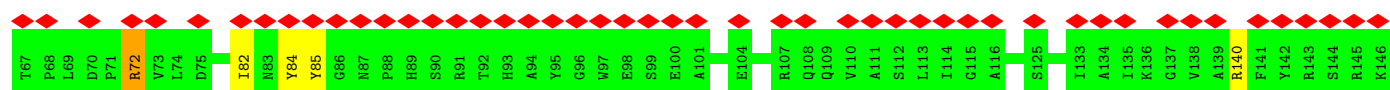
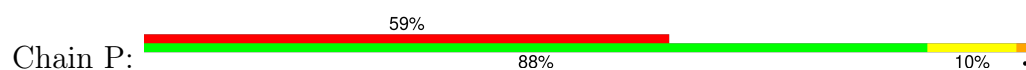


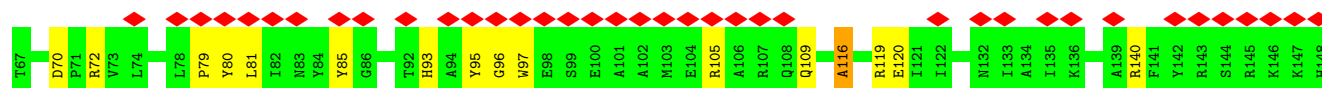


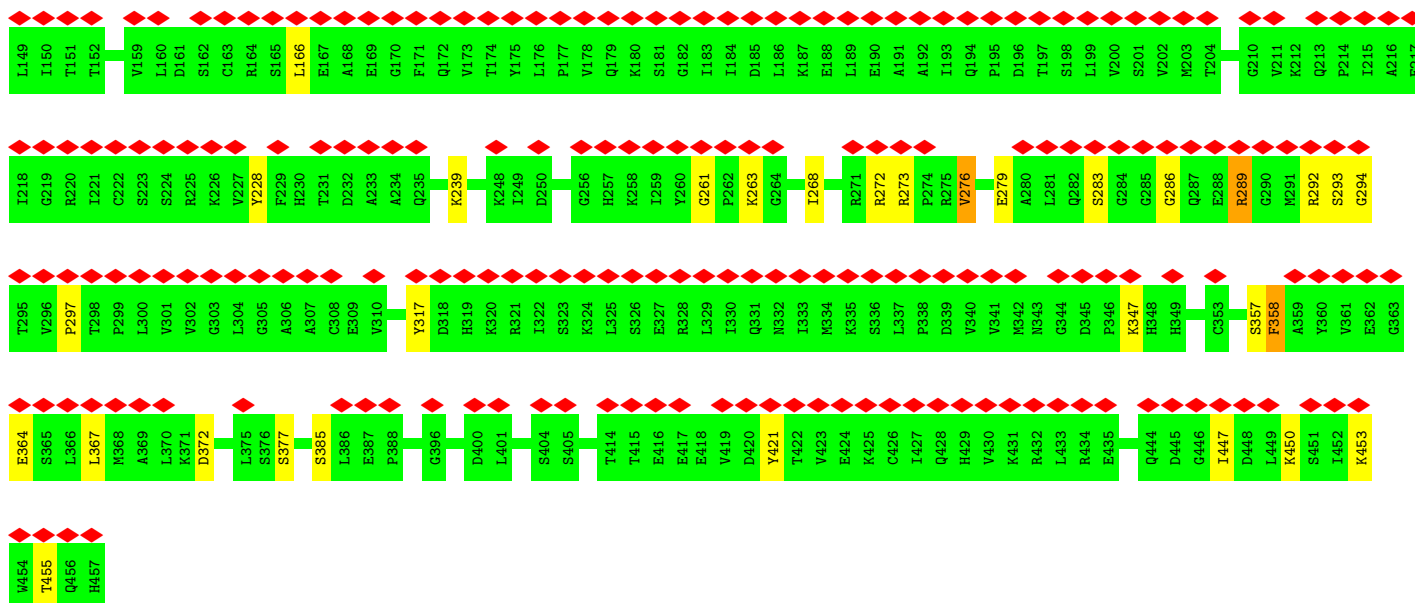
• Molecule 1: Cysteine desulfurase, mitochondrial



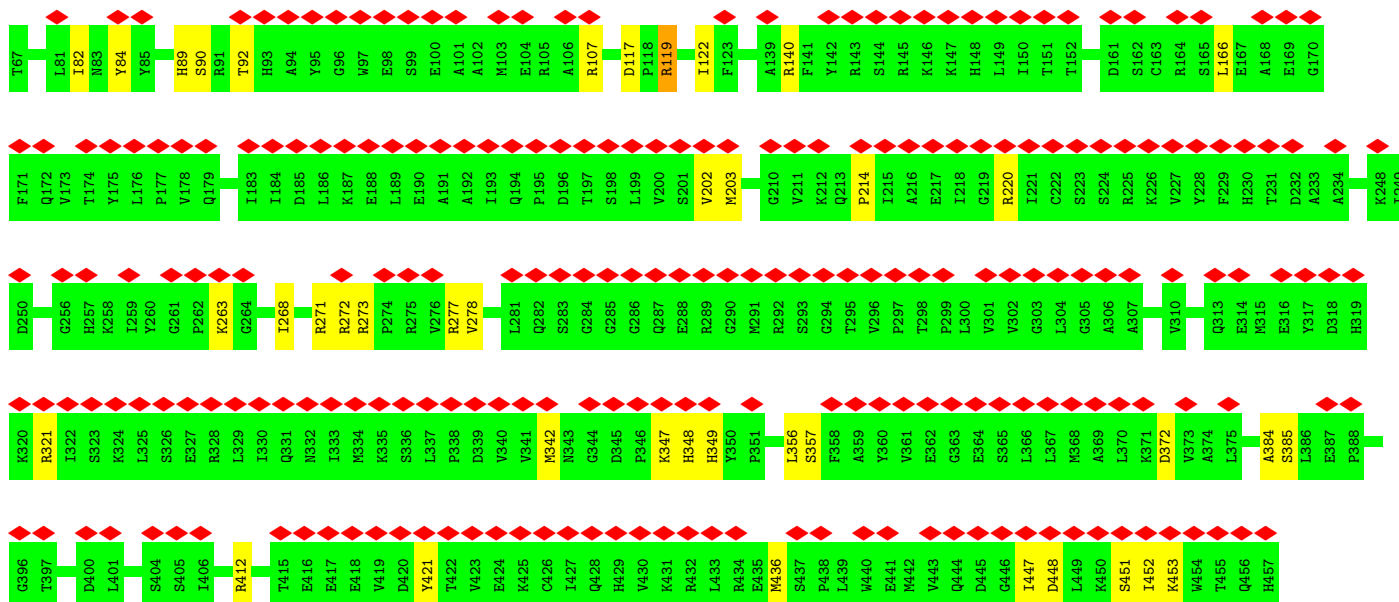
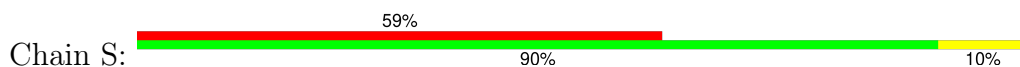
• Molecule 1: Cysteine desulfurase, mitochondrial



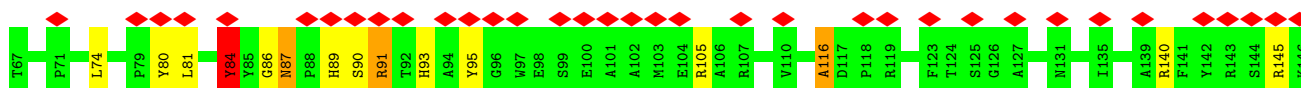
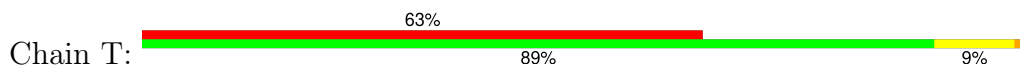


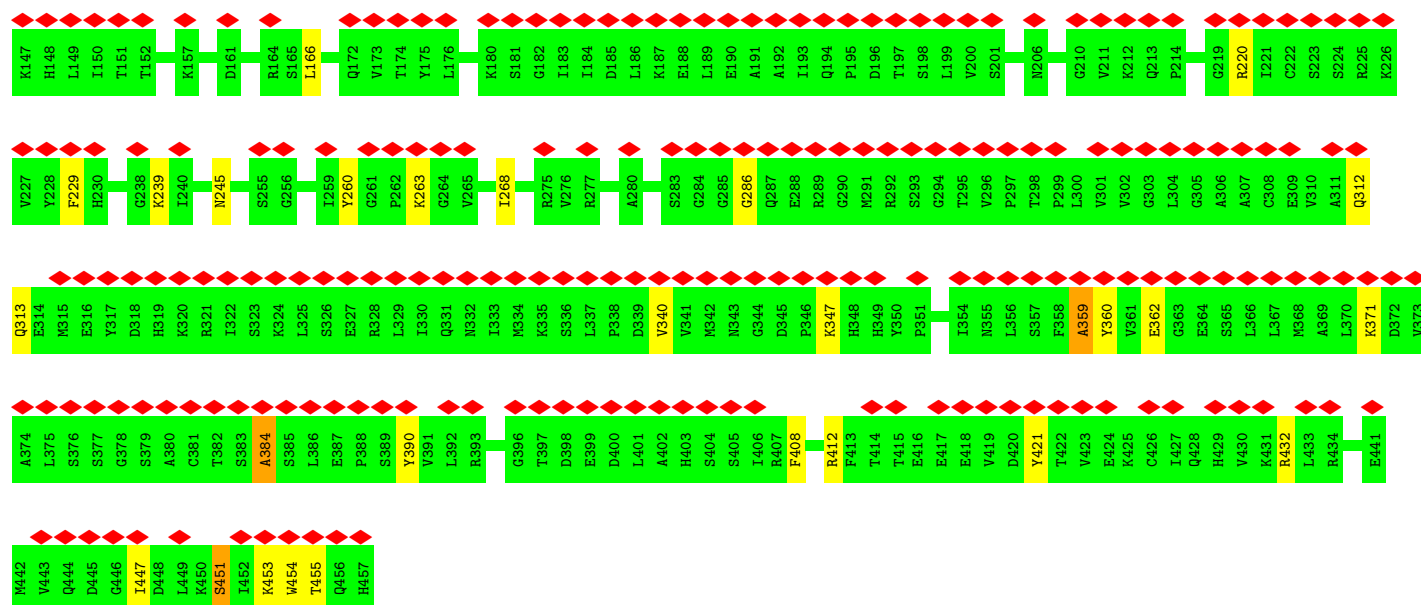


• Molecule 1: Cysteine desulfurase, mitochondrial

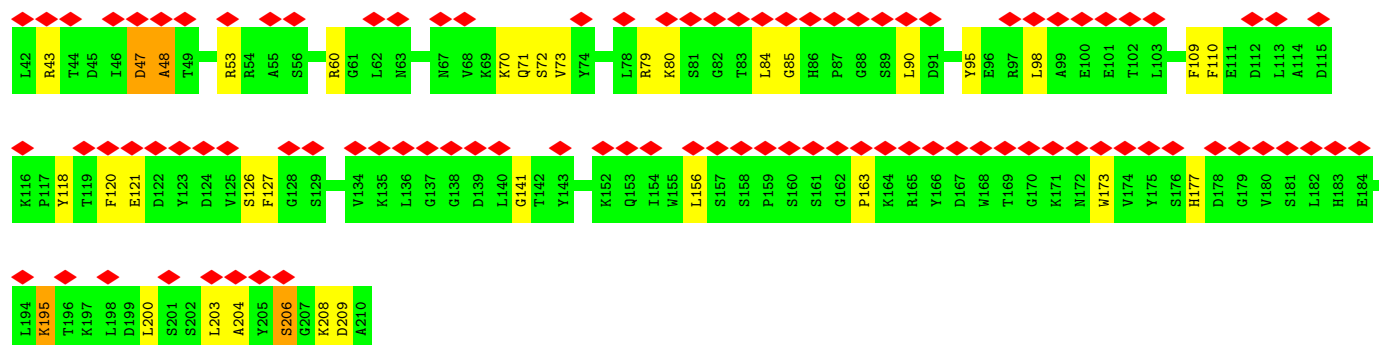
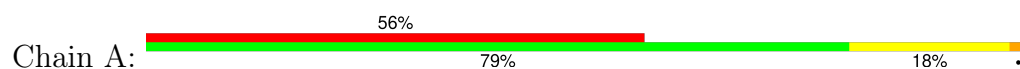


• Molecule 1: Cysteine desulfurase, mitochondrial

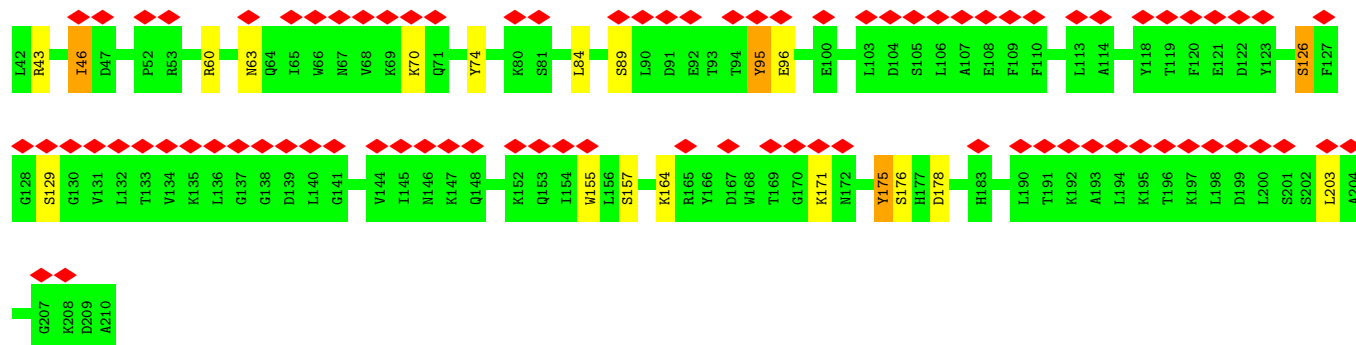
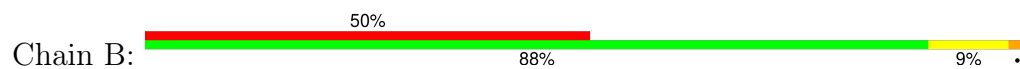




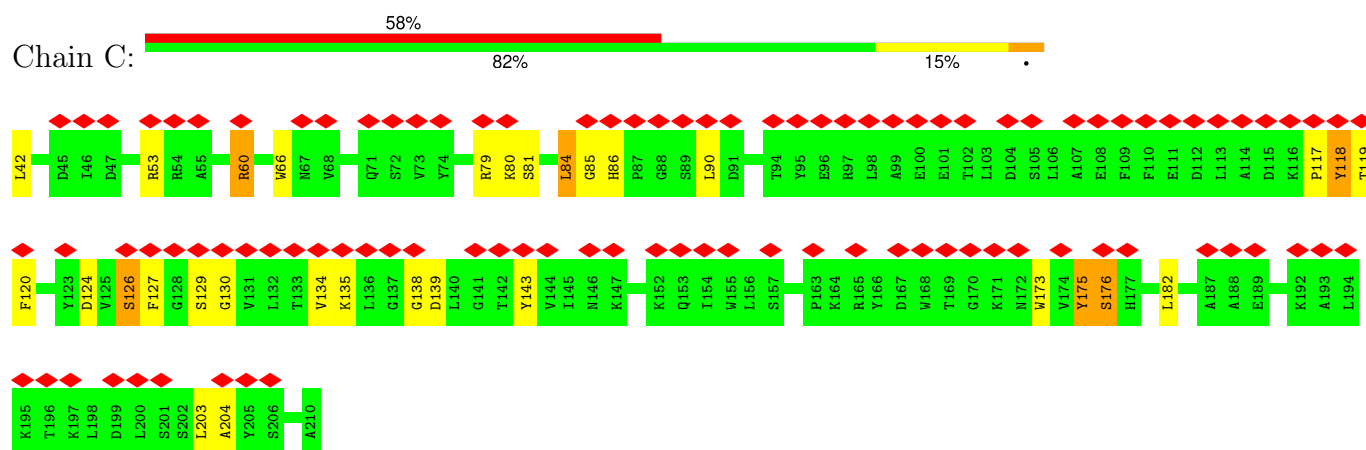
• Molecule 2: Frataxin, mitochondrial



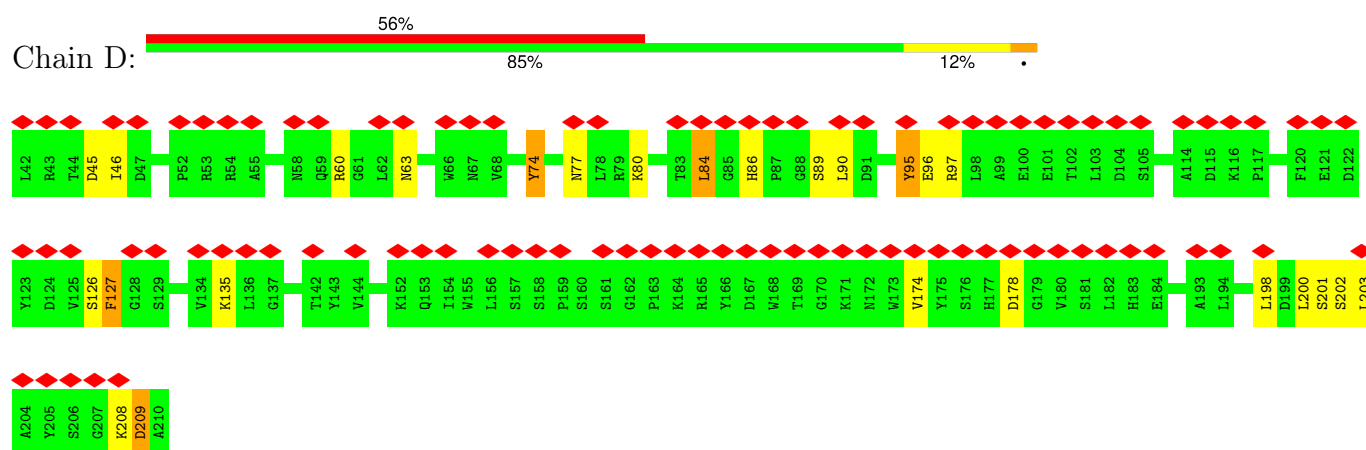
• Molecule 2: Frataxin, mitochondrial



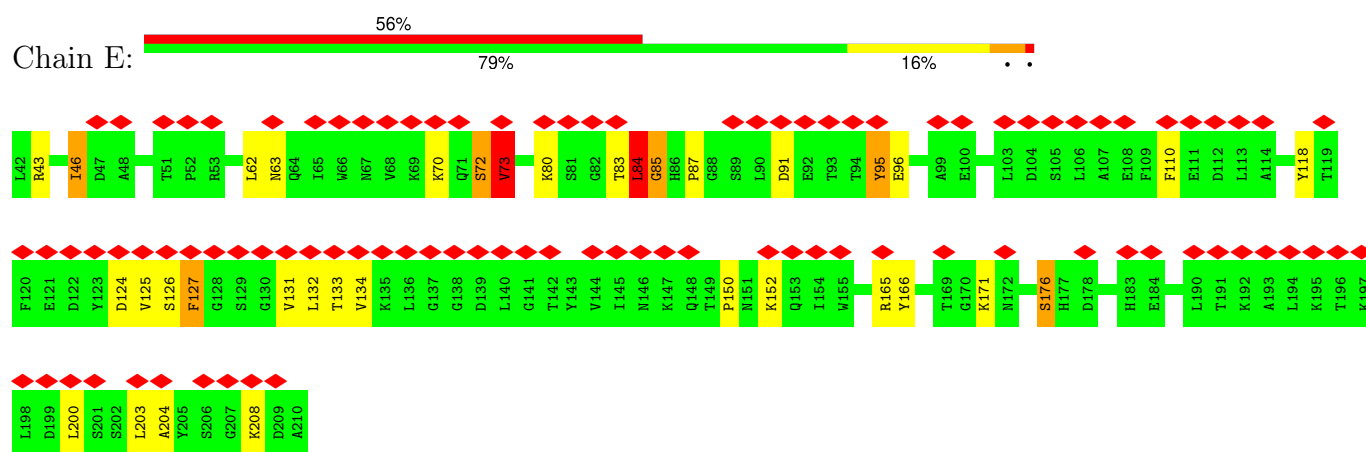
• Molecule 2: Frataxin, mitochondrial



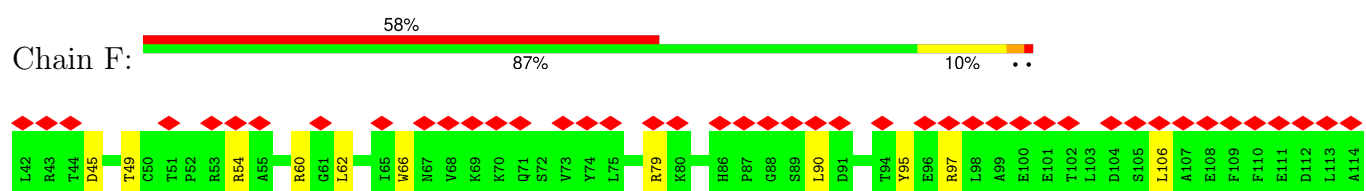
• Molecule 2: Frataxin, mitochondrial

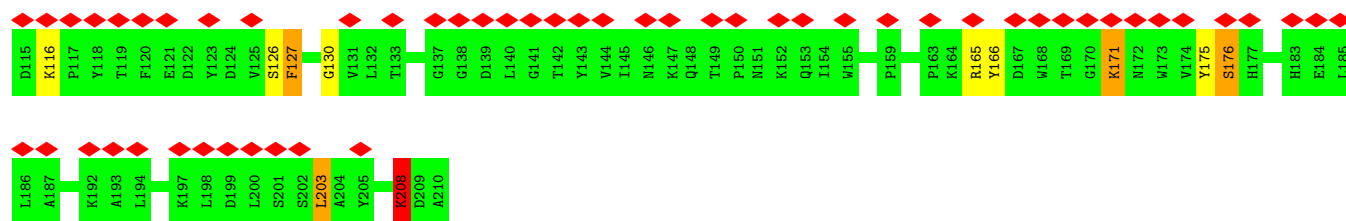


• Molecule 2: Frataxin, mitochondrial

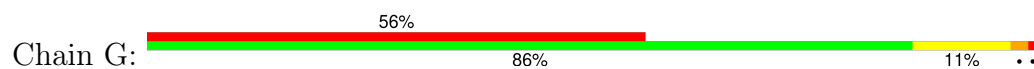


• Molecule 2: Frataxin, mitochondrial

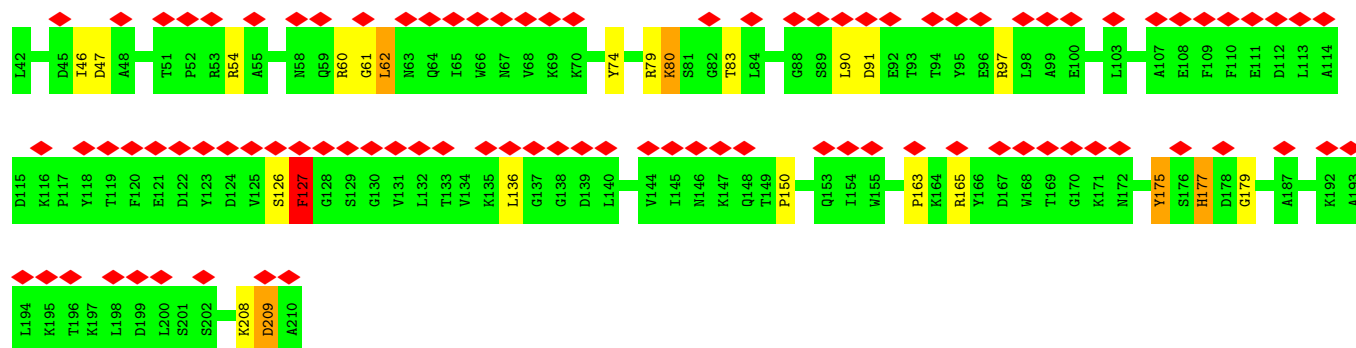
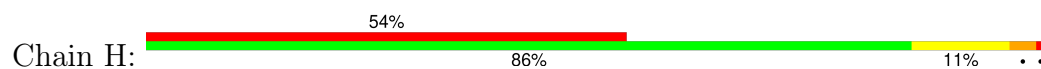




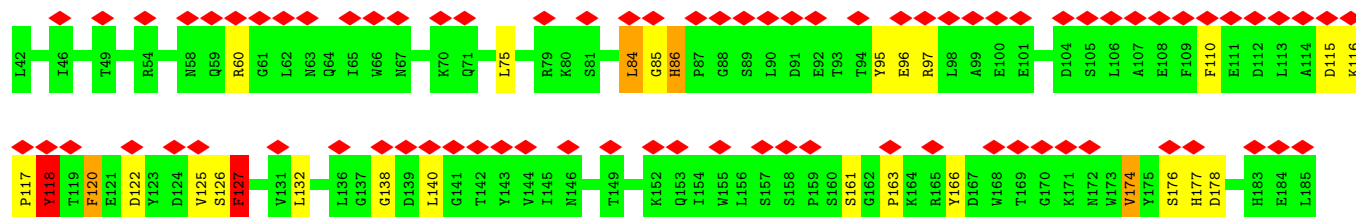
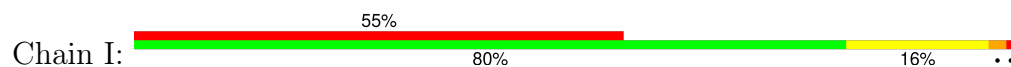
• Molecule 2: Frataxin, mitochondrial

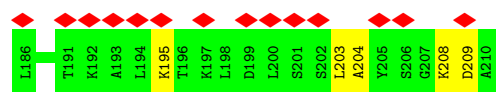


• Molecule 2: Frataxin, mitochondrial

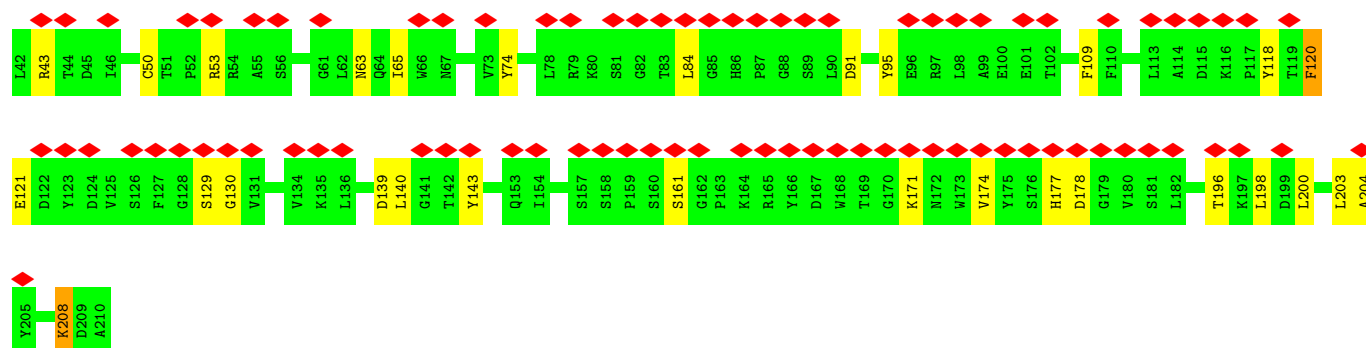
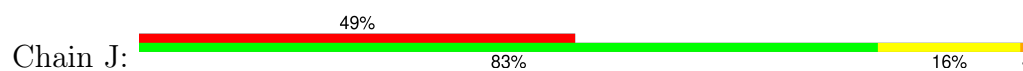


• Molecule 2: Frataxin, mitochondrial

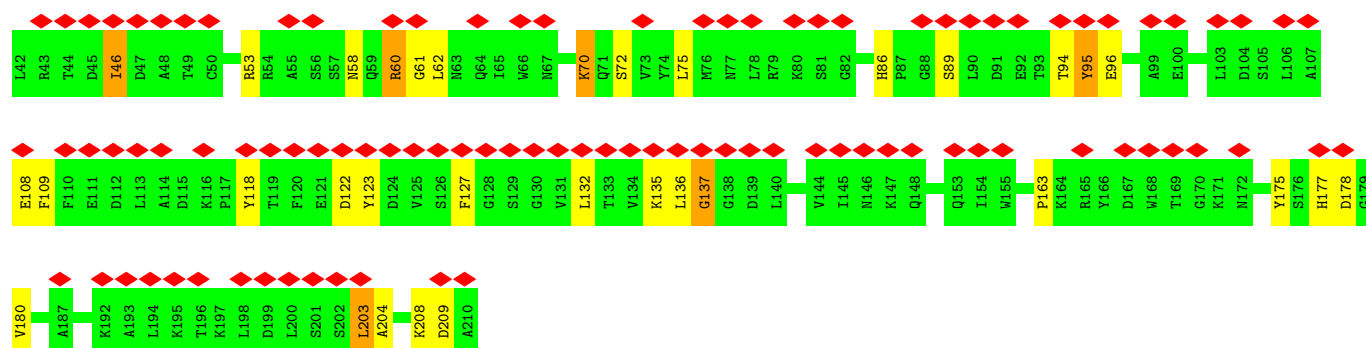
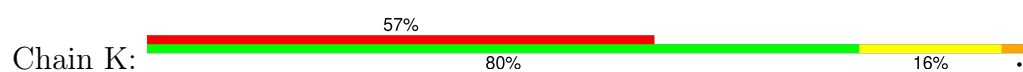




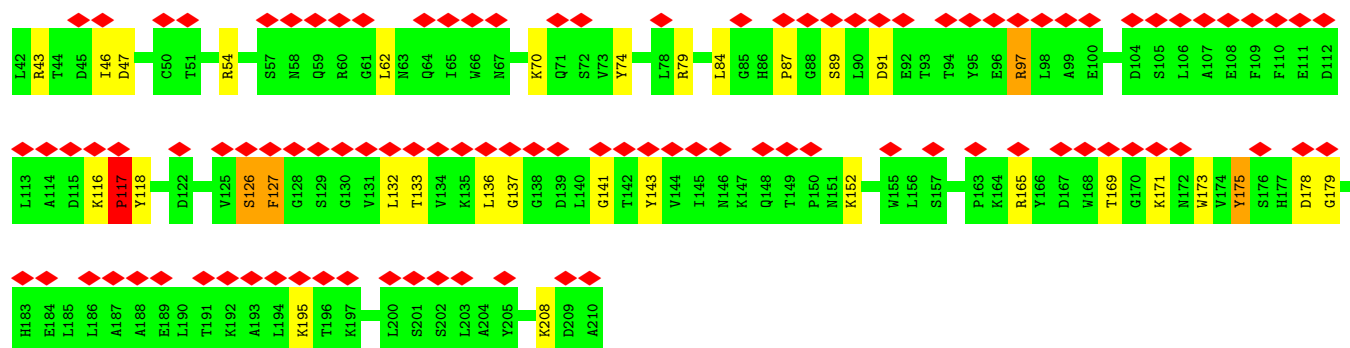
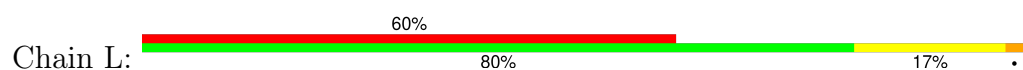
• Molecule 2: Frataxin, mitochondrial



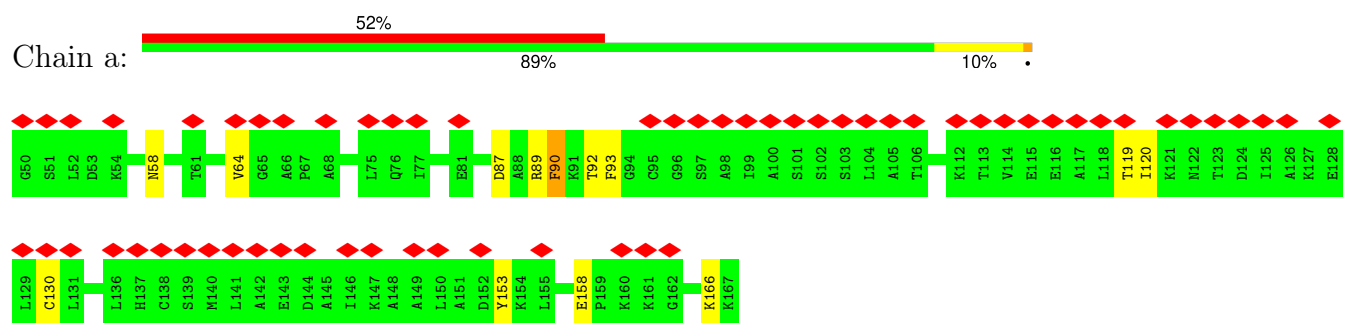
• Molecule 2: Frataxin, mitochondrial



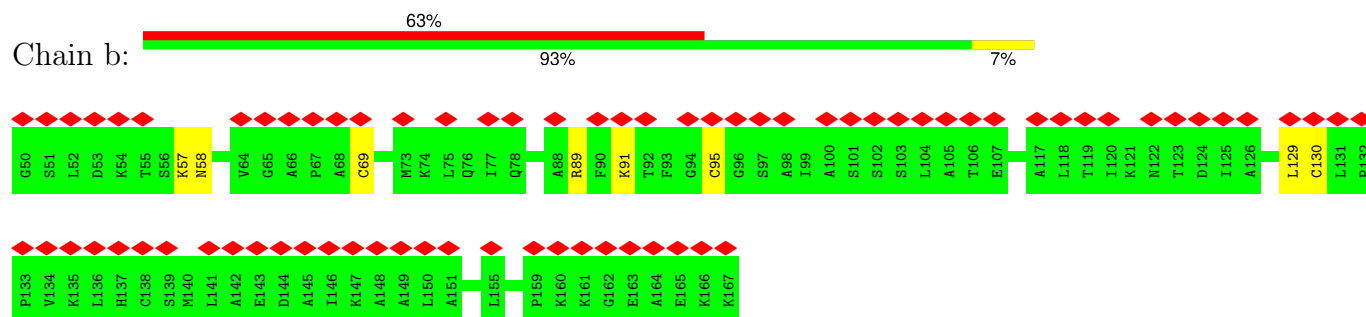
• Molecule 2: Frataxin, mitochondrial



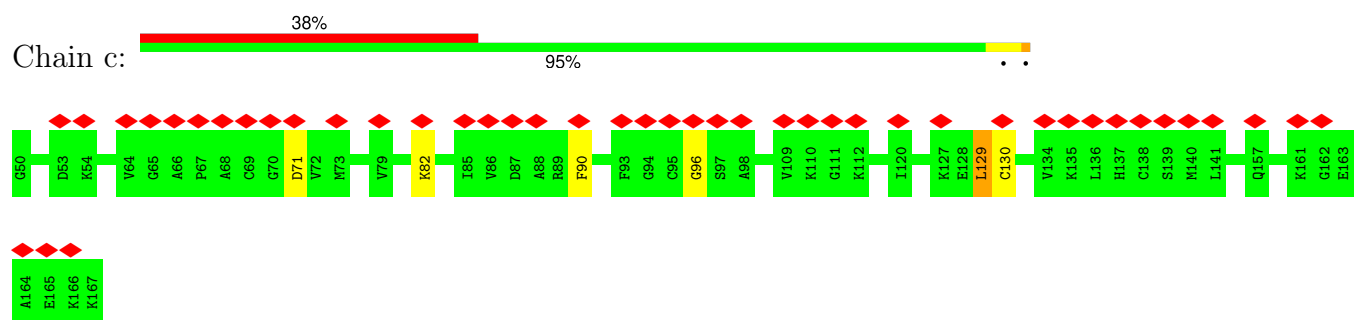
• Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



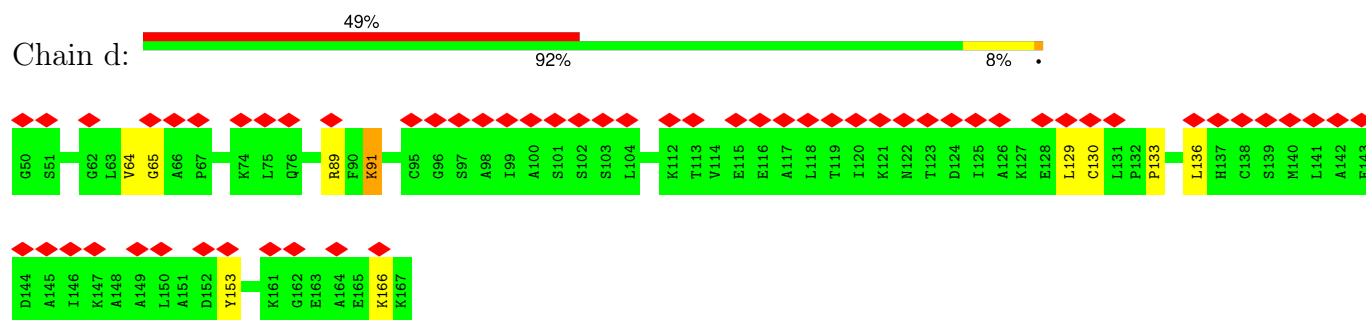
- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



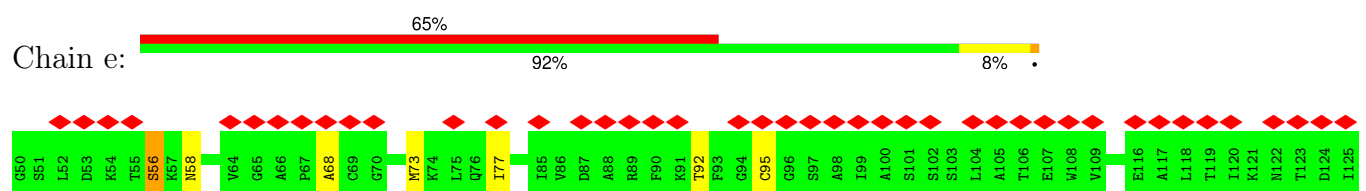
- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial

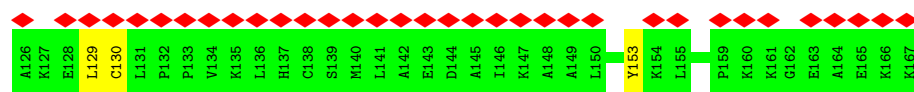


- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial

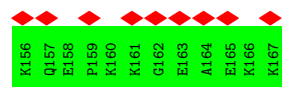
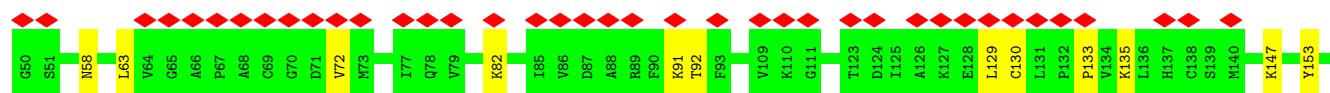
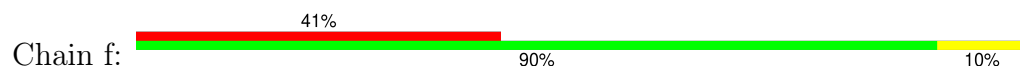


- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial

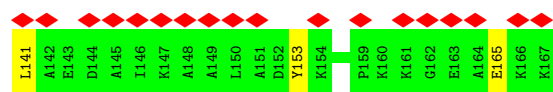
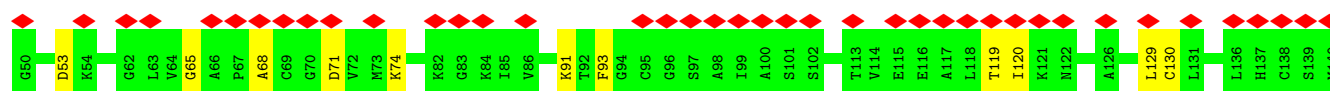
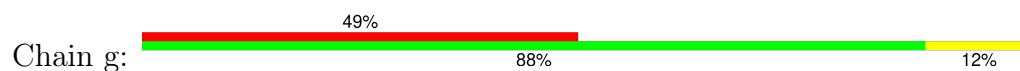




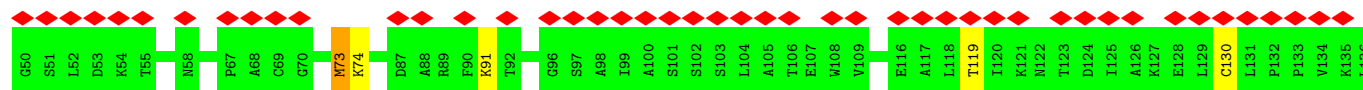
- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



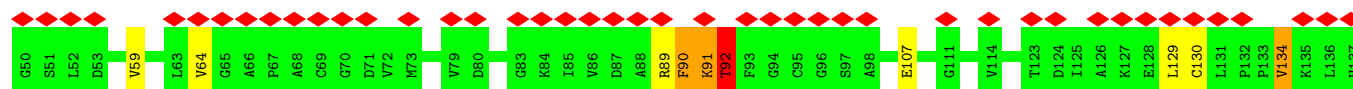
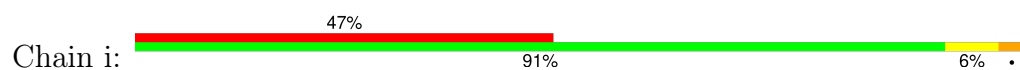
- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



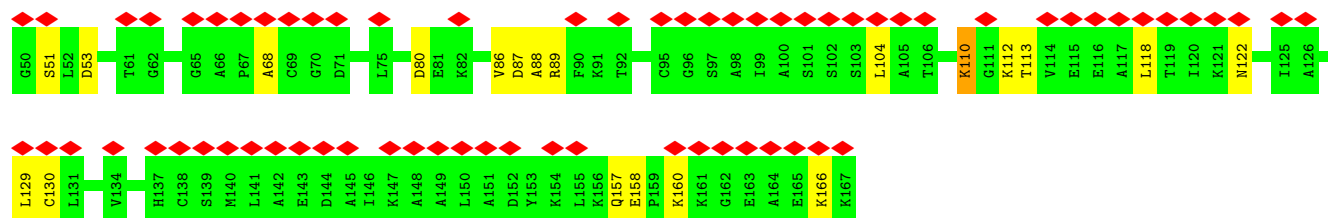
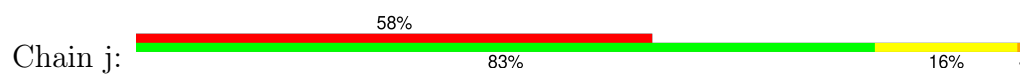
- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



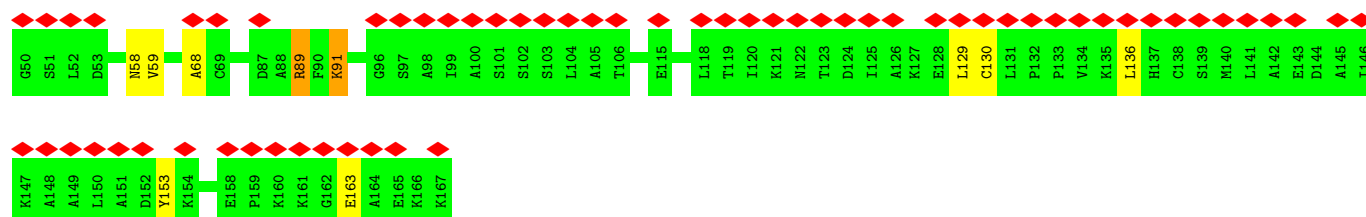
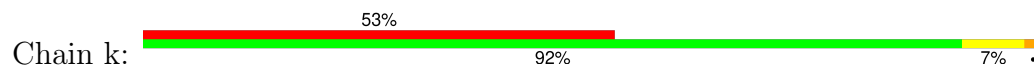
- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



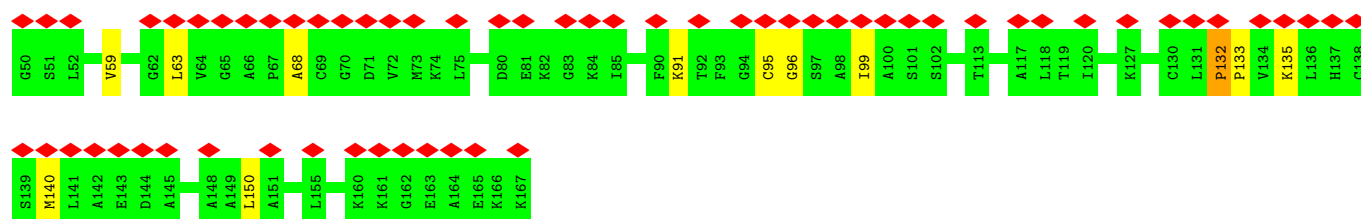
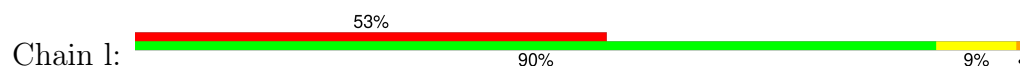
- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, O	Depositor
Number of particles used	4124	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; The ctf.auto function from EMAN2 was applied.	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	210	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	115000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	8.552	Depositor
Minimum map value	0.000	Depositor
Average map value	0.316	Depositor
Map value standard deviation	0.812	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	124.3, 181.5, 181.5	wwPDB
Map dimensions	113, 165, 165	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	1	1.09	0/3096	1.27	10/4185 (0.2%)
1	2	1.10	0/3096	1.31	21/4185 (0.5%)
1	3	1.13	1/3096 (0.0%)	1.31	27/4185 (0.6%)
1	4	1.09	0/3096	1.28	11/4185 (0.3%)
1	M	1.12	0/3096	1.27	18/4185 (0.4%)
1	N	1.11	0/3096	1.24	12/4185 (0.3%)
1	O	1.12	1/3096 (0.0%)	1.32	16/4185 (0.4%)
1	P	1.12	0/3096	1.26	13/4185 (0.3%)
1	Q	1.10	0/3096	1.25	15/4185 (0.4%)
1	R	1.13	2/3096 (0.1%)	1.28	13/4185 (0.3%)
1	S	1.13	0/3096	1.24	8/4185 (0.2%)
1	T	1.14	1/3096 (0.0%)	1.25	18/4185 (0.4%)
2	A	1.08	0/1356	1.35	11/1838 (0.6%)
2	B	1.09	0/1356	1.32	7/1838 (0.4%)
2	C	1.11	2/1356 (0.1%)	1.41	12/1838 (0.7%)
2	D	1.10	0/1356	1.34	9/1838 (0.5%)
2	E	1.11	0/1356	1.33	11/1838 (0.6%)
2	F	1.12	0/1356	1.37	10/1838 (0.5%)
2	G	1.12	1/1356 (0.1%)	1.36	10/1838 (0.5%)
2	H	1.11	0/1356	1.36	9/1838 (0.5%)
2	I	1.08	0/1356	1.35	13/1838 (0.7%)
2	J	1.08	0/1356	1.34	8/1838 (0.4%)
2	K	1.09	0/1356	1.35	7/1838 (0.4%)
2	L	1.05	0/1356	1.32	8/1838 (0.4%)
3	a	0.99	0/881	1.27	4/1181 (0.3%)
3	b	0.96	0/881	1.13	0/1181
3	c	0.98	0/881	1.18	0/1181
3	d	1.00	0/881	1.22	1/1181 (0.1%)
3	e	0.96	0/881	1.20	3/1181 (0.3%)
3	f	0.97	0/881	1.20	2/1181 (0.2%)
3	g	0.99	0/881	1.22	1/1181 (0.1%)
3	h	0.99	0/881	1.19	0/1181
3	i	0.99	0/881	1.22	3/1181 (0.3%)
3	j	0.98	0/881	1.24	2/1181 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	k	1.00	0/881	1.19	1/1181 (0.1%)
3	l	0.97	0/881	1.18	1/1181 (0.1%)
All	All	1.09	8/63996 (0.0%)	1.28	315/86448 (0.4%)

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	1	0	3
1	2	0	3
1	3	0	2
1	4	0	2
1	M	0	1
1	P	0	1
1	Q	0	2
1	R	0	1
1	T	0	3
2	G	0	1
2	H	0	1
2	I	0	1
2	J	0	1
3	a	0	1
3	d	0	1
3	g	0	1
3	h	0	1
3	k	0	1
All	All	0	27

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	53	ARG	NE-CZ	5.92	1.40	1.33
1	3	275	ARG	NE-CZ	5.59	1.40	1.33
1	T	105	ARG	NE-CZ	5.42	1.40	1.33
1	R	289	ARG	NE-CZ	5.40	1.40	1.33
2	G	79	ARG	CD-NE	5.28	1.55	1.46

The worst 5 of 315 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	95	TYR	CB-CG-CD2	-13.02	113.19	121.00
1	R	95	TYR	CB-CG-CD1	11.22	127.73	121.00
1	R	95	TYR	CB-CG-CD2	-11.09	114.35	121.00
2	K	95	TYR	CB-CG-CD1	10.23	127.14	121.00
1	R	85	TYR	CB-CG-CD2	-10.20	114.88	121.00

There are no chirality outliers.

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	121	ILE	Mainchain
1	1	260	TYR	Sidechain
1	1	269	TYR	Sidechain
1	2	175	TYR	Sidechain
1	2	269	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3040	0	3058	26	0
1	2	3040	0	3058	5	0
1	3	3040	0	3057	10	0
1	4	3040	0	3058	8	0
1	M	3040	0	3058	7	0
1	N	3040	0	3058	3	0
1	O	3040	0	3057	19	0
1	P	3040	0	3058	11	0
1	Q	3040	0	3057	14	0
1	R	3040	0	3058	4	0
1	S	3040	0	3058	2	0
1	T	3040	0	3058	8	0
2	A	1328	0	1302	2	0
2	B	1328	0	1302	2	0
2	C	1328	0	1302	9	0
2	D	1328	0	1302	9	0
2	E	1328	0	1302	39	0
2	F	1328	0	1302	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1328	0	1302	2	0
2	H	1328	0	1302	4	0
2	I	1328	0	1302	2	0
2	J	1328	0	1302	2	0
2	K	1328	0	1301	25	0
2	L	1328	0	1302	11	0
3	a	872	0	917	0	0
3	b	872	0	917	0	0
3	c	872	0	917	0	0
3	d	872	0	917	0	0
3	e	872	0	917	0	0
3	f	872	0	916	0	0
3	g	872	0	917	0	0
3	h	872	0	917	0	0
3	i	872	0	917	0	0
3	j	872	0	917	0	0
3	k	872	0	917	0	0
3	l	872	0	917	0	0
All	All	62880	0	63319	188	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 2.

The worst 5 of 188 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)
2:E:126:SER:N	2:E:127:PHE:CD1	1.78	1.50
1:Q:95:TYR:OH	2:C:134:VAL:CG1	1.63	1.45
2:E:126:SER:N	2:E:127:PHE:HD1	1.01	1.43
2:E:126:SER:CA	2:E:127:PHE:HB2	1.71	1.20
2:E:126:SER:HA	2:E:127:PHE:CB	1.63	1.18

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	1	389/391 (100%)	333 (86%)	30 (8%)	26 (7%)	1	12
1	2	389/391 (100%)	341 (88%)	27 (7%)	21 (5%)	1	15
1	3	389/391 (100%)	334 (86%)	37 (10%)	18 (5%)	2	17
1	4	389/391 (100%)	332 (85%)	34 (9%)	23 (6%)	1	13
1	M	389/391 (100%)	346 (89%)	30 (8%)	13 (3%)	3	21
1	N	389/391 (100%)	340 (87%)	40 (10%)	9 (2%)	5	28
1	O	389/391 (100%)	332 (85%)	35 (9%)	22 (6%)	1	14
1	P	389/391 (100%)	345 (89%)	29 (8%)	15 (4%)	2	19
1	Q	389/391 (100%)	343 (88%)	32 (8%)	14 (4%)	3	20
1	R	389/391 (100%)	342 (88%)	31 (8%)	16 (4%)	2	18
1	S	389/391 (100%)	335 (86%)	36 (9%)	18 (5%)	2	17
1	T	389/391 (100%)	341 (88%)	34 (9%)	14 (4%)	3	20
2	A	167/169 (99%)	124 (74%)	28 (17%)	15 (9%)	0	8
2	B	167/169 (99%)	140 (84%)	18 (11%)	9 (5%)	1	15
2	C	167/169 (99%)	125 (75%)	27 (16%)	15 (9%)	0	8
2	D	167/169 (99%)	126 (75%)	33 (20%)	8 (5%)	2	16
2	E	167/169 (99%)	133 (80%)	20 (12%)	14 (8%)	0	9
2	F	167/169 (99%)	134 (80%)	23 (14%)	10 (6%)	1	13
2	G	167/169 (99%)	135 (81%)	23 (14%)	9 (5%)	1	15
2	H	167/169 (99%)	133 (80%)	25 (15%)	9 (5%)	1	15
2	I	167/169 (99%)	130 (78%)	21 (13%)	16 (10%)	0	7
2	J	167/169 (99%)	132 (79%)	17 (10%)	18 (11%)	0	6
2	K	167/169 (99%)	137 (82%)	22 (13%)	8 (5%)	2	16
2	L	167/169 (99%)	125 (75%)	27 (16%)	15 (9%)	0	8
3	a	116/118 (98%)	94 (81%)	16 (14%)	6 (5%)	1	15
3	b	116/118 (98%)	102 (88%)	9 (8%)	5 (4%)	2	17
3	c	116/118 (98%)	97 (84%)	16 (14%)	3 (3%)	4	26
3	d	116/118 (98%)	97 (84%)	12 (10%)	7 (6%)	1	13
3	e	116/118 (98%)	97 (84%)	12 (10%)	7 (6%)	1	13
3	f	116/118 (98%)	98 (84%)	13 (11%)	5 (4%)	2	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	g	116/118 (98%)	95 (82%)	12 (10%)	9 (8%)	1	10
3	h	116/118 (98%)	100 (86%)	14 (12%)	2 (2%)	7	37
3	i	116/118 (98%)	96 (83%)	13 (11%)	7 (6%)	1	13
3	j	116/118 (98%)	86 (74%)	16 (14%)	14 (12%)	0	4
3	k	116/118 (98%)	99 (85%)	10 (9%)	7 (6%)	1	13
3	l	116/118 (98%)	99 (85%)	12 (10%)	5 (4%)	2	17
All	All	8064/8136 (99%)	6798 (84%)	834 (10%)	432 (5%)	3	15

5 of 432 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	88	PRO
1	1	89	HIS
1	1	98	GLU
1	1	119	ARG
1	1	298	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	333/333 (100%)	311 (93%)	22 (7%)	14	34
1	2	333/333 (100%)	319 (96%)	14 (4%)	25	46
1	3	333/333 (100%)	318 (96%)	15 (4%)	23	45
1	4	333/333 (100%)	314 (94%)	19 (6%)	17	38
1	M	333/333 (100%)	320 (96%)	13 (4%)	27	48
1	N	333/333 (100%)	316 (95%)	17 (5%)	20	41
1	O	333/333 (100%)	318 (96%)	15 (4%)	23	45
1	P	333/333 (100%)	319 (96%)	14 (4%)	25	46
1	Q	333/333 (100%)	323 (97%)	10 (3%)	36	55
1	R	333/333 (100%)	314 (94%)	19 (6%)	17	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	333/333 (100%)	320 (96%)	13 (4%)	27	48
1	T	333/333 (100%)	318 (96%)	15 (4%)	23	45
2	A	146/146 (100%)	134 (92%)	12 (8%)	9	28
2	B	146/146 (100%)	140 (96%)	6 (4%)	26	47
2	C	146/146 (100%)	140 (96%)	6 (4%)	26	47
2	D	146/146 (100%)	140 (96%)	6 (4%)	26	47
2	E	146/146 (100%)	137 (94%)	9 (6%)	15	36
2	F	146/146 (100%)	138 (94%)	8 (6%)	18	39
2	G	146/146 (100%)	138 (94%)	8 (6%)	18	39
2	H	146/146 (100%)	138 (94%)	8 (6%)	18	39
2	I	146/146 (100%)	135 (92%)	11 (8%)	11	31
2	J	146/146 (100%)	142 (97%)	4 (3%)	40	58
2	K	146/146 (100%)	135 (92%)	11 (8%)	11	31
2	L	146/146 (100%)	133 (91%)	13 (9%)	8	25
3	a	94/94 (100%)	89 (95%)	5 (5%)	19	40
3	b	94/94 (100%)	91 (97%)	3 (3%)	34	53
3	c	94/94 (100%)	90 (96%)	4 (4%)	25	46
3	d	94/94 (100%)	92 (98%)	2 (2%)	48	66
3	e	94/94 (100%)	93 (99%)	1 (1%)	70	80
3	f	94/94 (100%)	89 (95%)	5 (5%)	19	40
3	g	94/94 (100%)	91 (97%)	3 (3%)	34	53
3	h	94/94 (100%)	89 (95%)	5 (5%)	19	40
3	i	94/94 (100%)	87 (93%)	7 (7%)	11	31
3	j	94/94 (100%)	89 (95%)	5 (5%)	19	40
3	k	94/94 (100%)	91 (97%)	3 (3%)	34	53
3	l	94/94 (100%)	87 (93%)	7 (7%)	11	31
All	All	6876/6876 (100%)	6538 (95%)	338 (5%)	23	42

5 of 338 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	70	LYS
2	I	174	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	200	LEU
2	G	175	TYR
3	j	110	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	177	HIS
3	i	122	ASN
1	O	148	HIS
1	N	349	HIS
3	j	122	ASN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

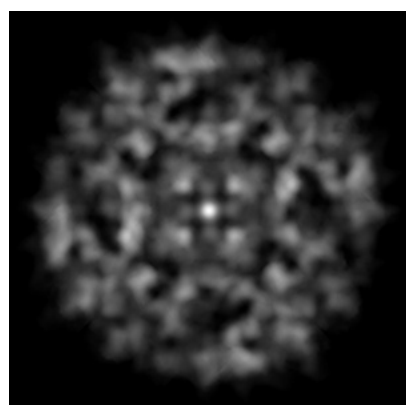
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8301. 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](#)

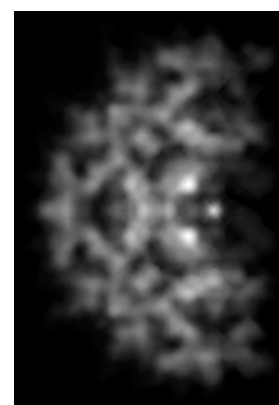
6.1.1 Primary map



X



Y

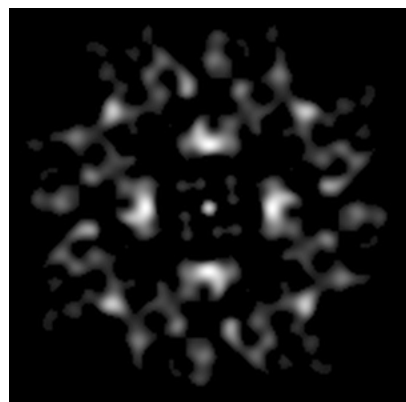


Z

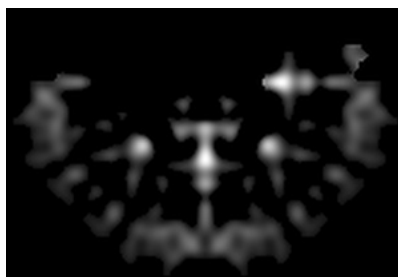
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

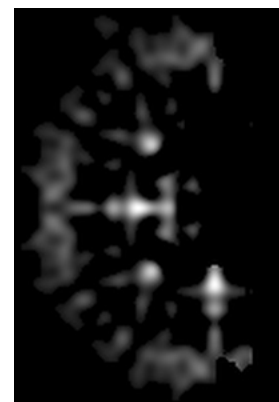
6.2.1 Primary map



X Index: 56



Y Index: 82

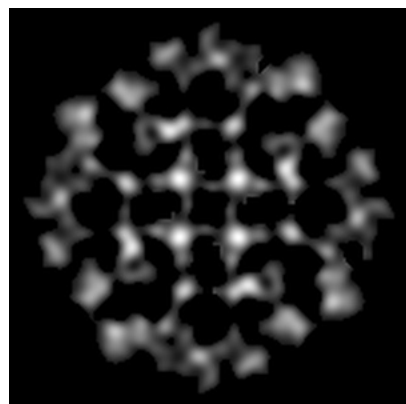


Z Index: 82

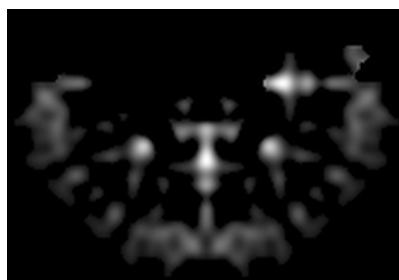
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

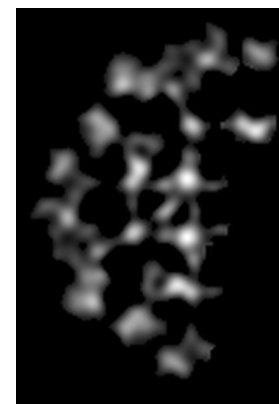
6.3.1 Primary map



X Index: 71



Y Index: 82

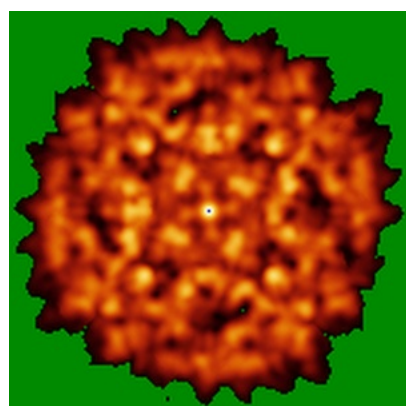


Z Index: 93

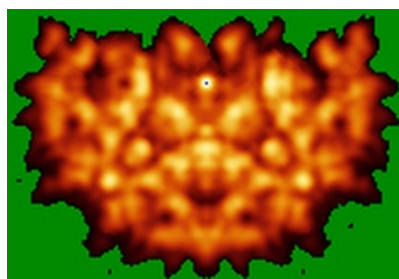
The images above show the largest variance slices of the map in three orthogonal directions.

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

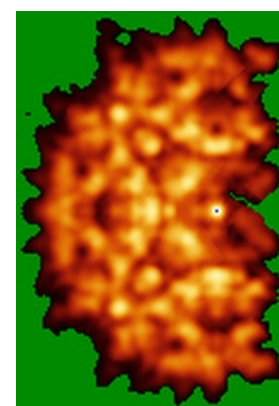
6.4.1 Primary map



X



Y

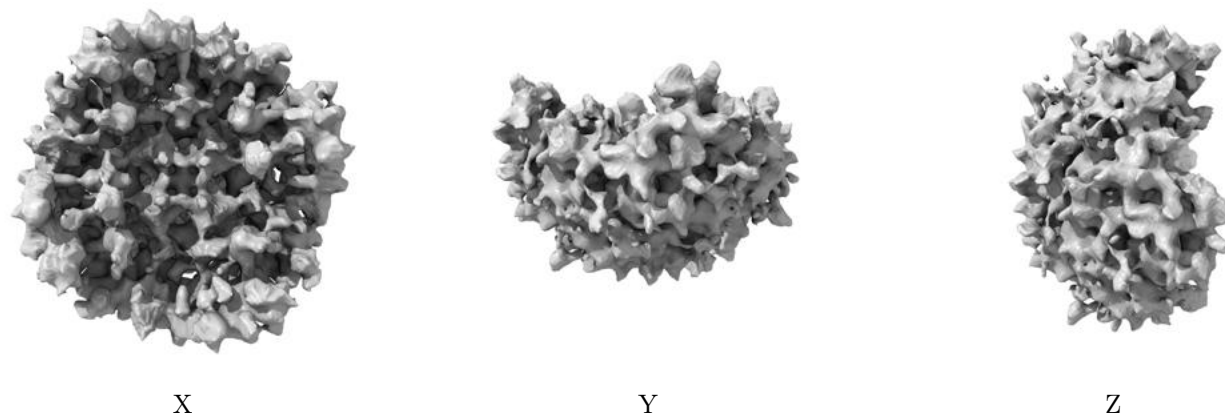


Z

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

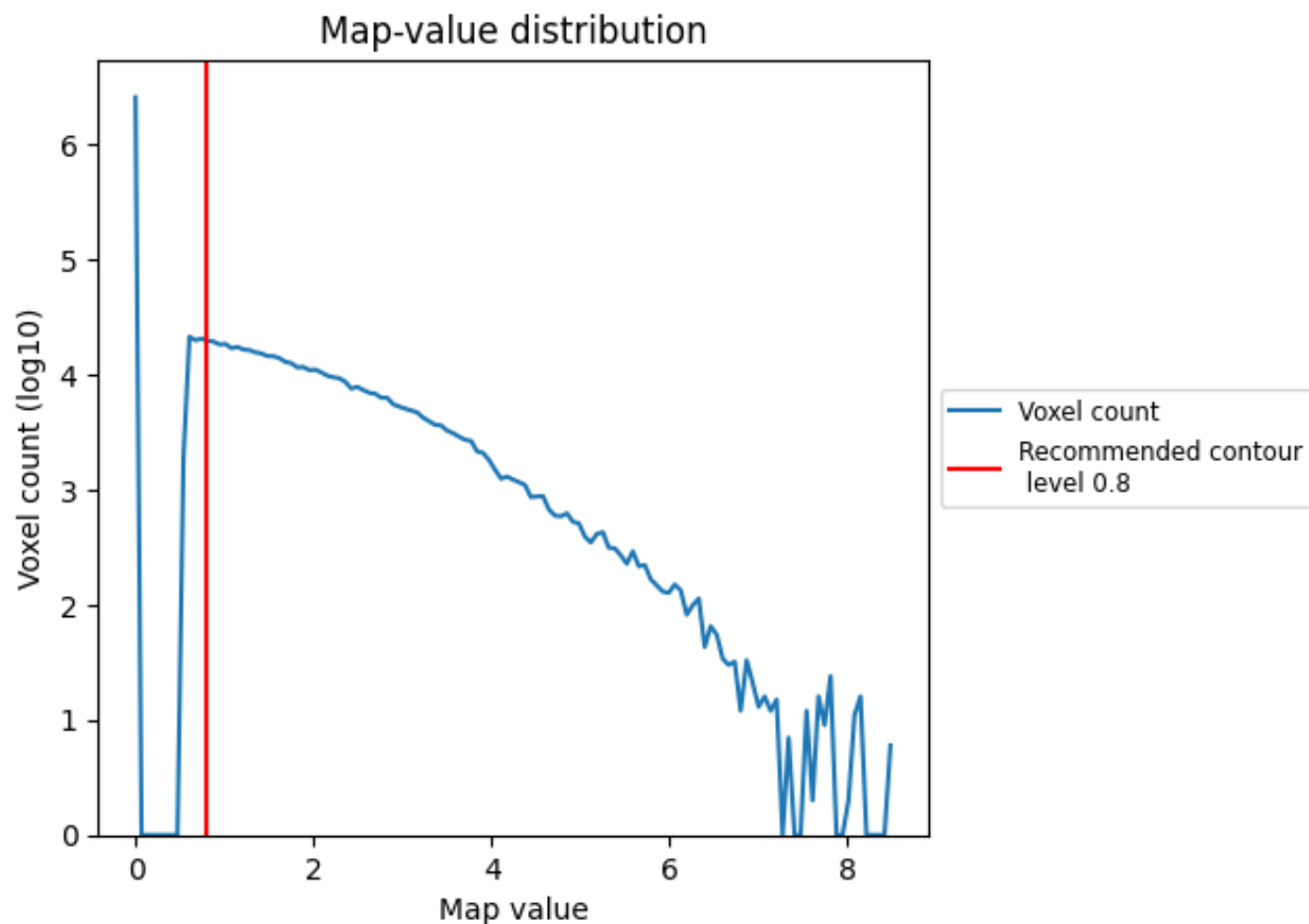
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

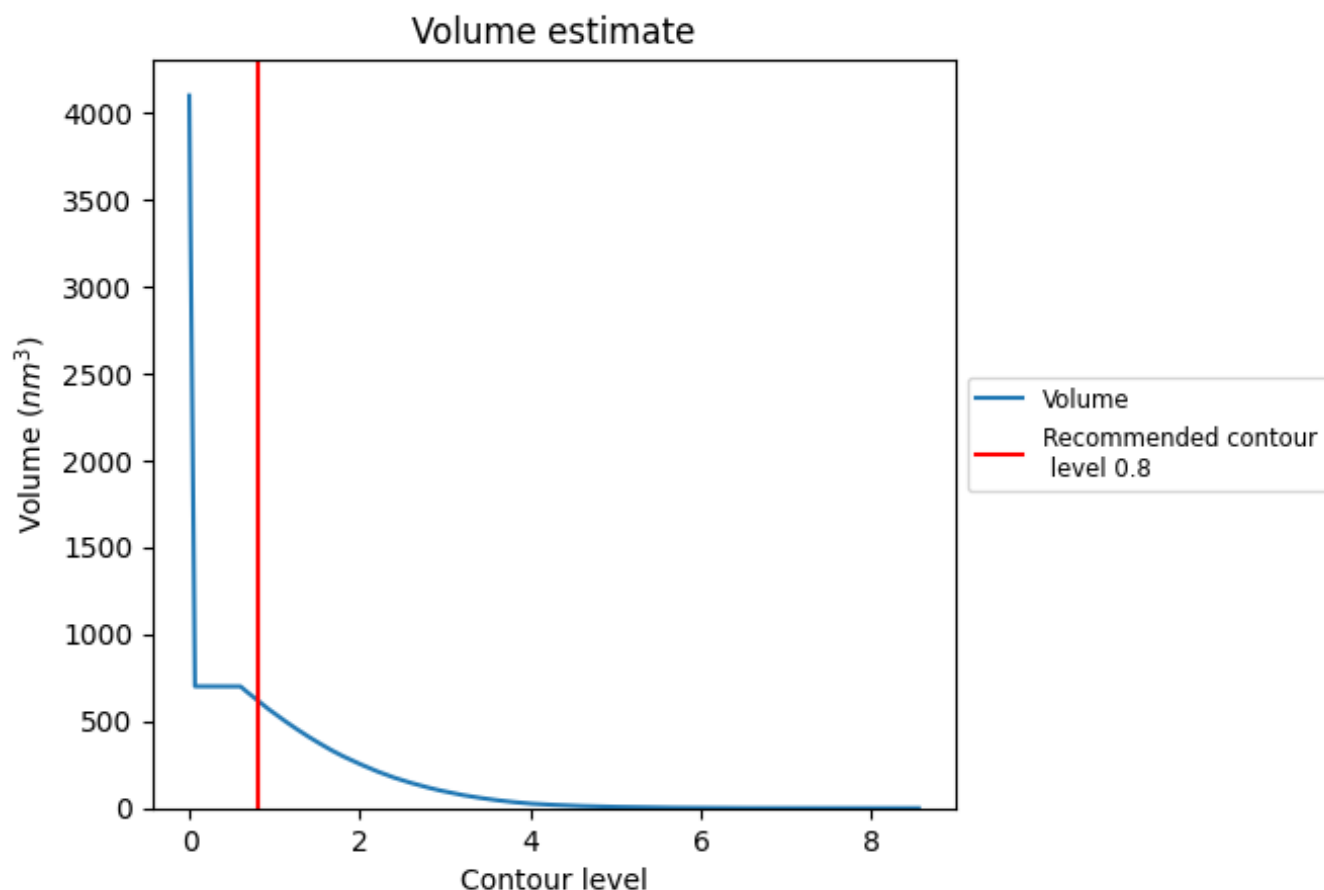
This section contains the results of statistical analysis of the map.

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 619 nm³; this corresponds to an approximate mass of 559 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 [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

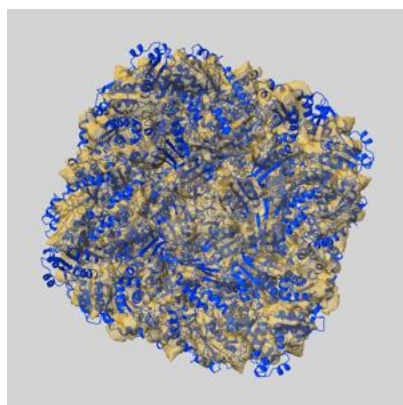
8 Fourier-Shell correlation ⓘ

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

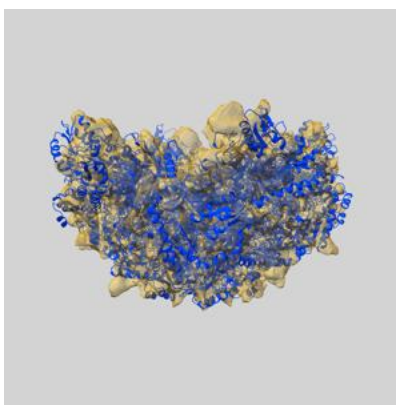
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8301 and PDB model 5KZ5. Per-residue inclusion information can be found in section [3](#) on page [8](#).

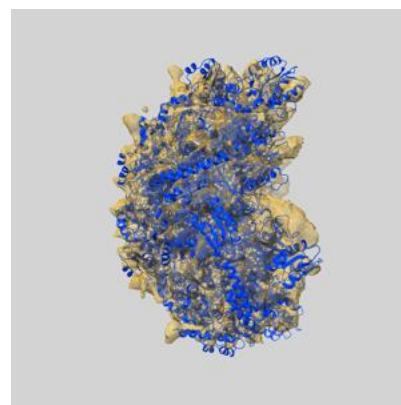
9.1 Map-model overlay [i](#)



X



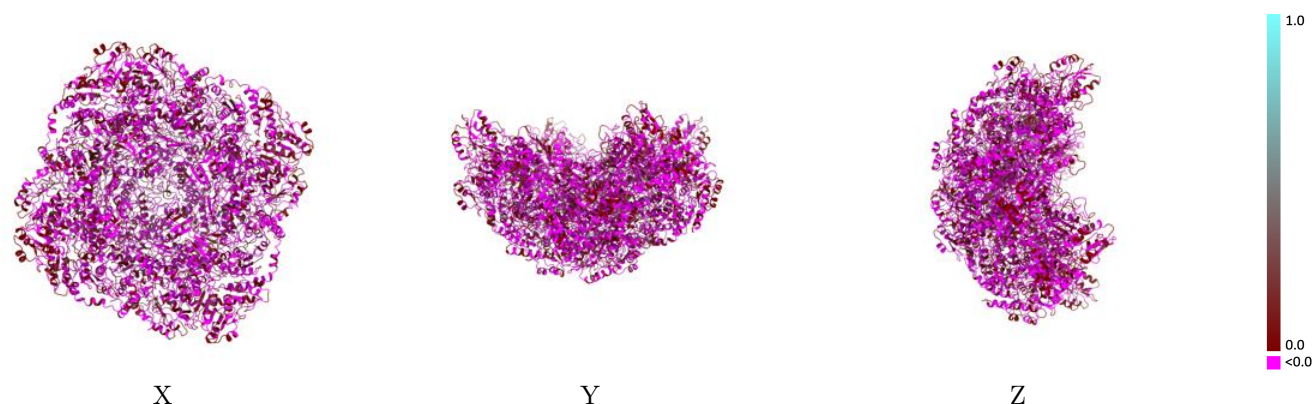
Y



Z

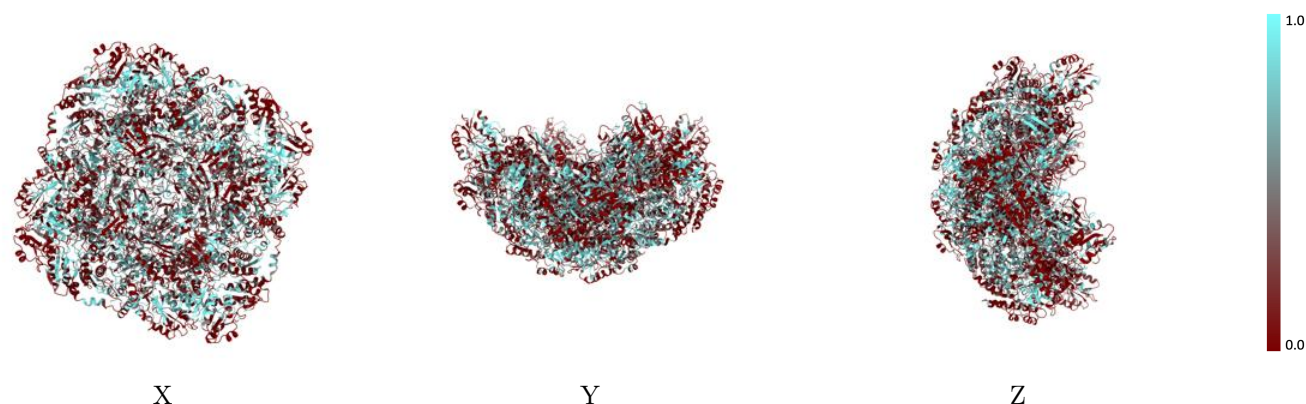
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



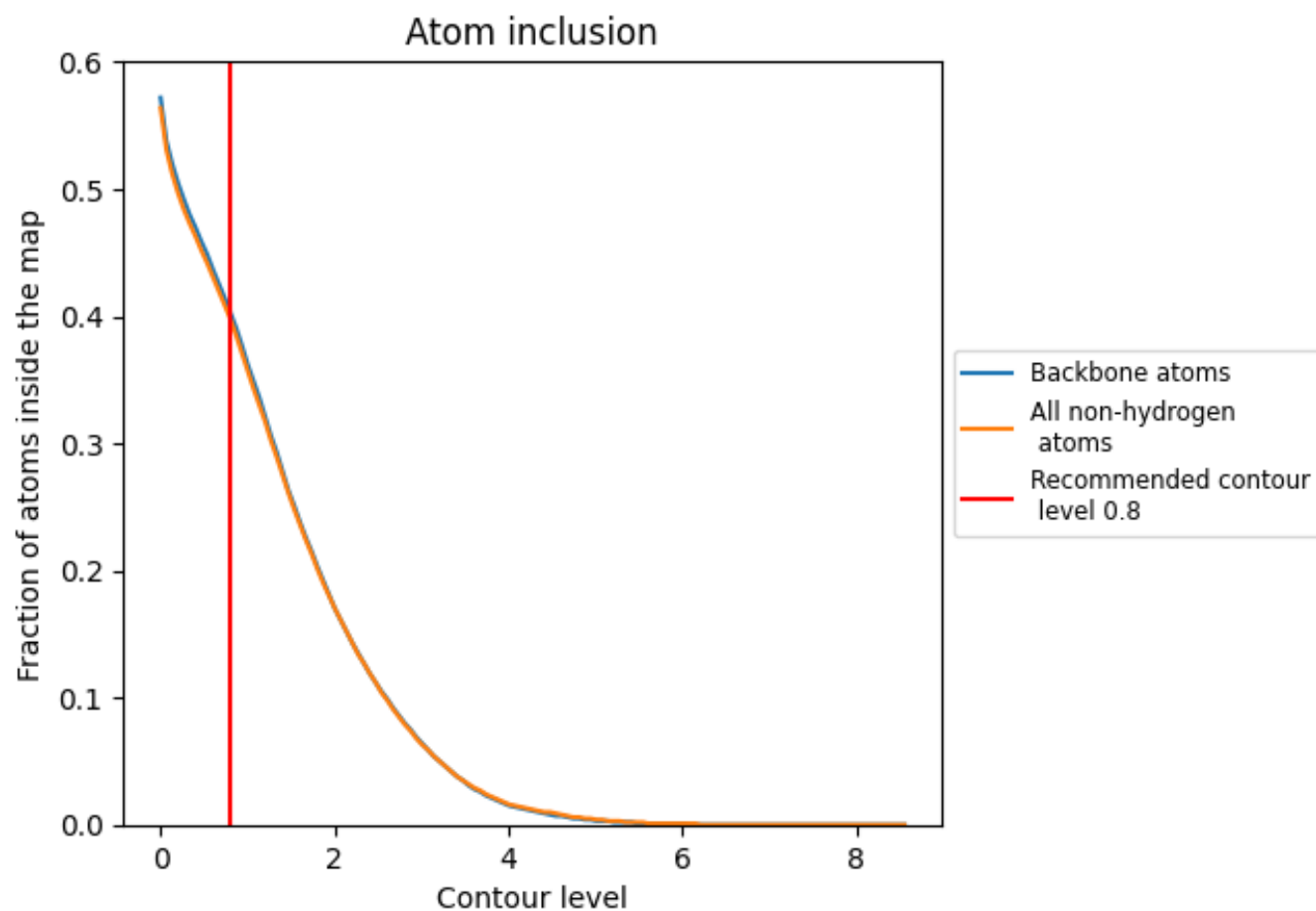
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 40% of all backbone atoms, 40% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3980	 -0.0210
1	 0.4510	 -0.0190
2	 0.4320	 -0.0260
3	 0.3890	 -0.0290
4	 0.4560	 -0.0170
A	 0.3990	 -0.0250
B	 0.4460	 -0.0130
C	 0.3460	 -0.0420
D	 0.4090	 -0.0230
E	 0.4230	 -0.0110
F	 0.3770	 -0.0470
G	 0.4240	 -0.0240
H	 0.4230	 -0.0290
I	 0.3990	 -0.0400
J	 0.4470	 -0.0230
K	 0.3990	 -0.0220
L	 0.3530	 -0.0460
M	 0.3810	 -0.0150
N	 0.3550	 -0.0190
O	 0.3420	 -0.0220
P	 0.3630	 -0.0040
Q	 0.3610	 -0.0150
R	 0.3530	 -0.0110
S	 0.3650	 -0.0080
T	 0.3330	 -0.0120
a	 0.4510	 -0.0180
b	 0.3490	 -0.0370
c	 0.5370	 -0.0160
d	 0.4720	 -0.0030
e	 0.3310	 -0.0300
f	 0.5320	 -0.0150
g	 0.4540	 -0.0380
h	 0.3920	 -0.0240
i	 0.4640	 -0.0270
j	 0.4410	 -0.0390



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	 0.4390	 -0.0140
l	 0.4750	 -0.0210