wwPDB EM Map/Model Validation Report (i)

Oct 10, 2016 – 02:06 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 Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

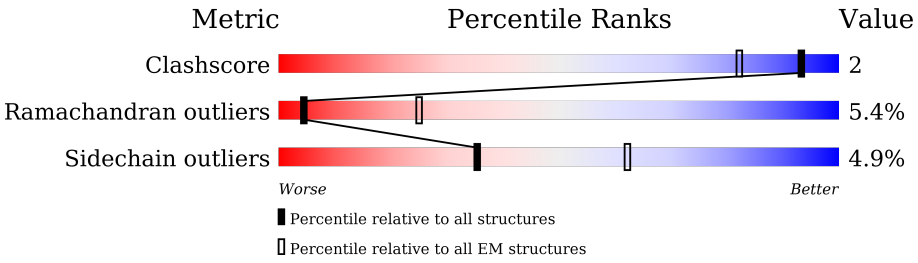
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	1	391	81% 15% •
1	2	391	87% 11% •
1	3	391	86% 10% •
1	4	391	86% 12% •
1	M	391	88% 11% •
1	N	391	91% 9% •
1	O	391	85% 13% •
1	P	391	88% 10% •
1	Q	391	90% 9% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	R	391	88% 11% •
1	S	391	90% 10%
1	T	391	89% 9% •
2	A	169	79% 18% •
2	B	169	88% 9% •
2	C	169	82% 15% •
2	D	169	85% 12% •
2	E	169	79% 16% • •
2	F	169	87% 10% • •
2	G	169	86% 11% • •
2	H	169	86% 11% • •
2	I	169	80% 16% • •
2	J	169	83% 16% •
2	K	169	80% 16% •
2	L	169	80% 17% • •
3	a	118	89% 10% •
3	b	118	93% 7%
3	c	118	95% • •
3	d	118	92% 8% •
3	e	118	92% 8% •
3	f	118	90% 10%
3	g	118	88% 12%
3	h	118	94% 5% •
3	i	118	91% 6% • •
3	j	118	83% 16% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	k	118	92% 7%
3	l	118	90% 9%

2 Entry composition

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	C	N	O	S	0	0
			3040	1905	540	576	19		
1	2	391	Total	C	N	O	S	0	0
			3040	1905	540	576	19		
1	3	391	Total	C	N	O	S	0	0
			3040	1905	540	576	19		
1	4	391	Total	C	N	O	S	0	0
			3040	1905	540	576	19		
1	M	391	Total	C	N	O	S	0	0
			3040	1905	540	576	19		
1	N	391	Total	C	N	O	S	0	0
			3040	1905	540	576	19		
1	O	391	Total	C	N	O	S	0	0
			3040	1905	540	576	19		
1	P	391	Total	C	N	O	S	0	0
			3040	1905	540	576	19		
1	Q	391	Total	C	N	O	S	0	0
			3040	1905	540	576	19		
1	R	391	Total	C	N	O	S	0	0
			3040	1905	540	576	19		
1	S	391	Total	C	N	O	S	0	0
			3040	1905	540	576	19		
1	T	391	Total	C	N	O	S	0	0
			3040	1905	540	576	19		

- Molecule 2 is a protein called Frataxin, mitochondrial.

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

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...

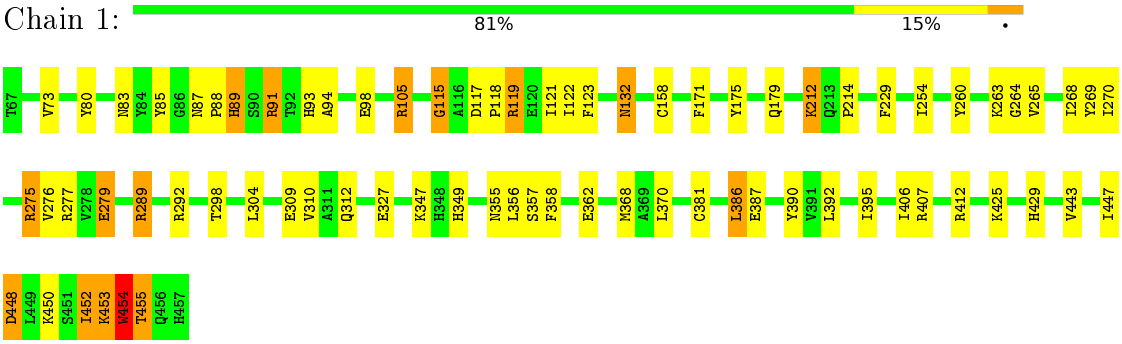
Mol	Chain	Residues	Atoms					AltConf	Trace
3	k	118	Total	C	N	O	S	0	0
			872	549	147	170	6		
3	l	118	Total	C	N	O	S	0	0
			872	549	147	170	6		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

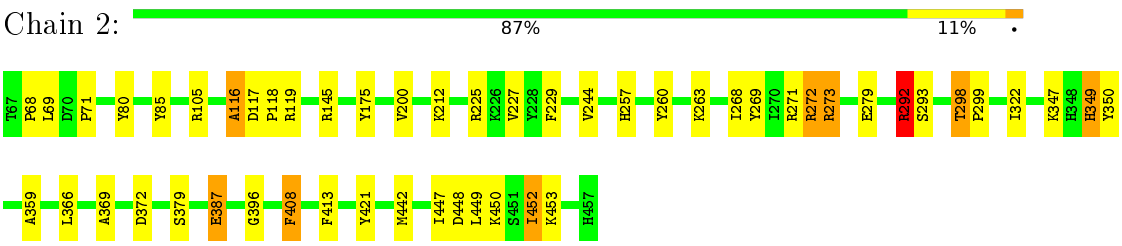
- Molecule 1: Cysteine desulfurase, mitochondrial

Chain 1:



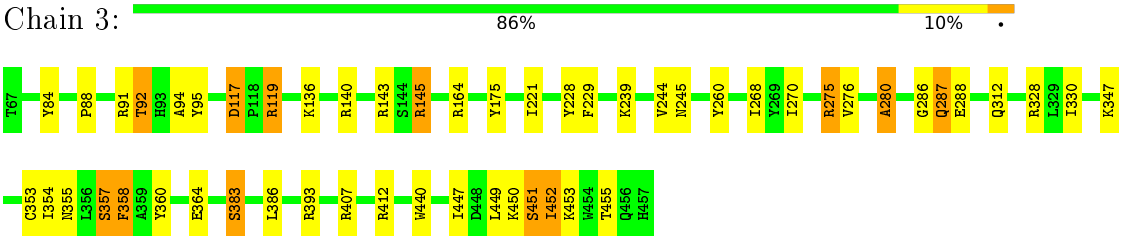
- Molecule 1: Cysteine desulfurase, mitochondrial

Chain 2:



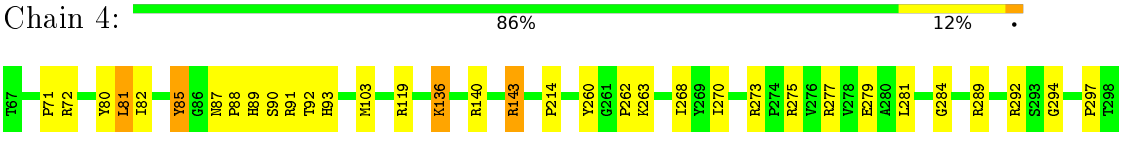
- Molecule 1: Cysteine desulfurase, mitochondrial

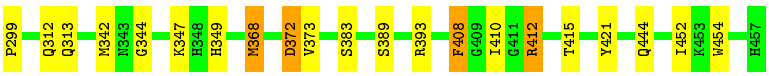
Chain 3:



- Molecule 1: Cysteine desulfurase, mitochondrial

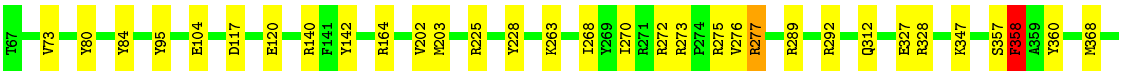
Chain 4:





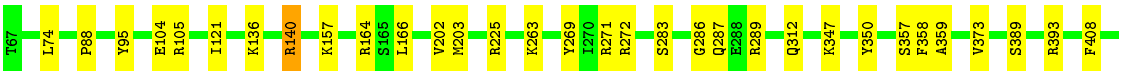
• Molecule 1: Cysteine desulfurase, mitochondrial

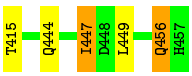
Chain M:



• Molecule 1: Cysteine desulfurase, mitochondrial

Chain N:





• Molecule 1: Cysteine desulfurase, mitochondrial

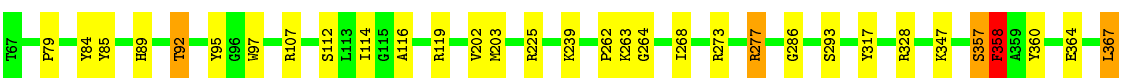
Chain O:

• Molecule 1: Cysteine desulfurase, mitochondrial

Chain P:

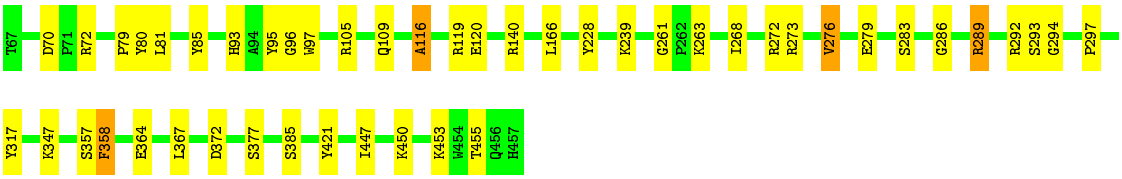
• Molecule 1: Cysteine desulfurase, mitochondrial

Chain Q:



• Molecule 1: Cysteine desulfurase, mitochondrial

Chain R:

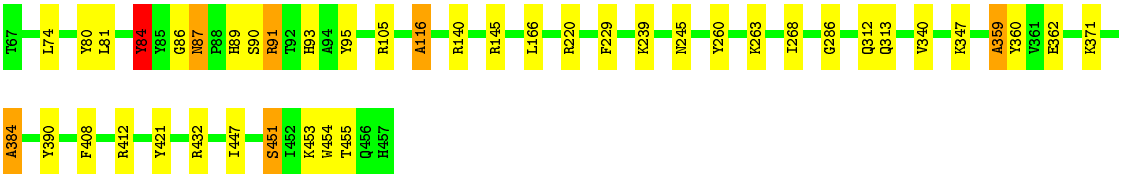


• Molecule 1: Cysteine desulfurase, mitochondrial

Chain S:

• Molecule 1: Cysteine desulfurase, mitochondrial

Chain T:



• Molecule 2: Frataxin, mitochondrial

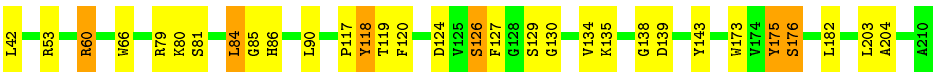
Chain A:

• Molecule 2: Frataxin, mitochondrial

Chain B:

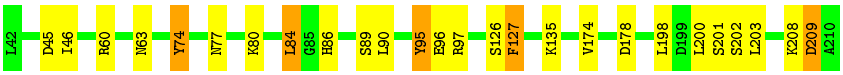
• Molecule 2: Frataxin, mitochondrial

Chain C:



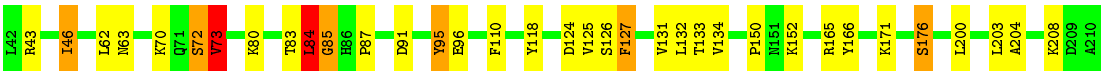
• Molecule 2: Frataxin, mitochondrial

Chain D:



• Molecule 2: Frataxin, mitochondrial

Chain E:



• Molecule 2: Frataxin, mitochondrial

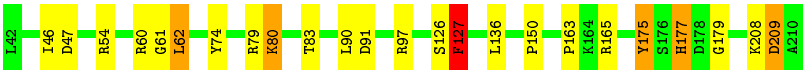
Chain F:

• Molecule 2: Frataxin, mitochondrial

Chain G:

• Molecule 2: Frataxin, mitochondrial

Chain H:

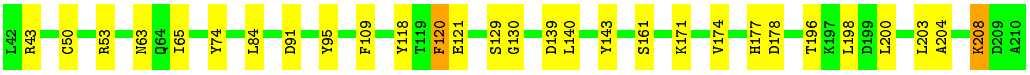


• Molecule 2: Frataxin, mitochondrial

Chain I:

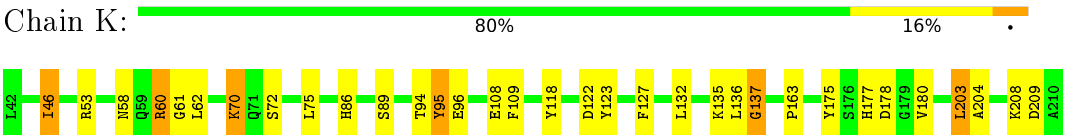
• Molecule 2: Frataxin, mitochondrial

Chain J:



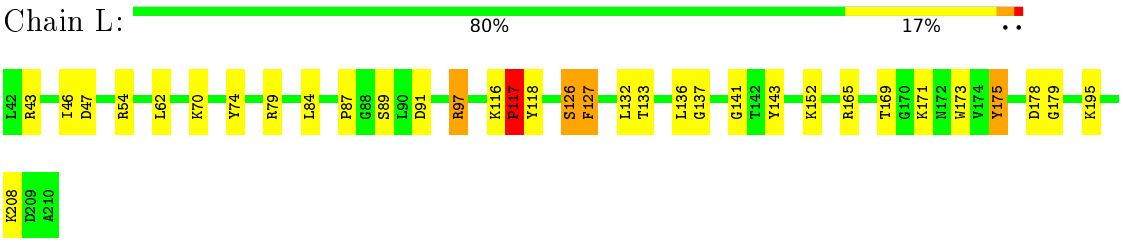
• Molecule 2: Frataxin, mitochondrial

Chain K:



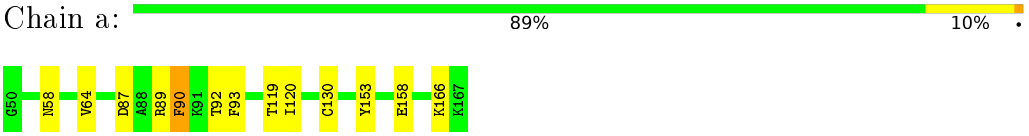
• Molecule 2: Frataxin, mitochondrial

Chain L:



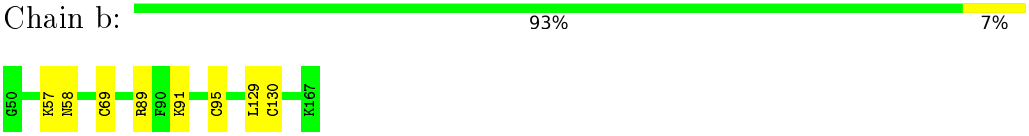
• Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial

Chain a:



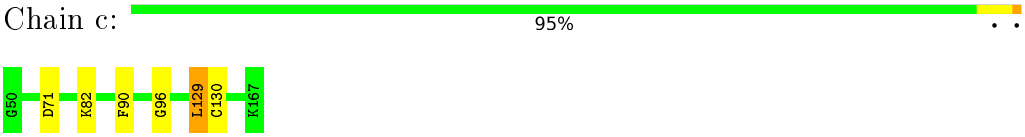
• Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial

Chain b:



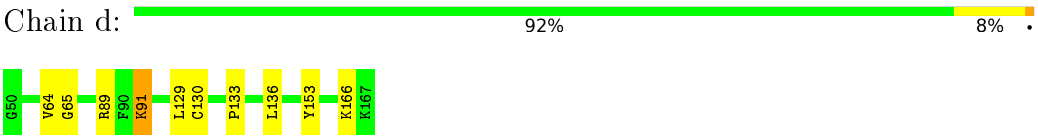
• Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial

Chain c:



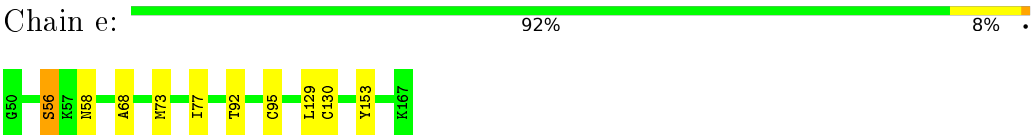
• Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial

Chain d:



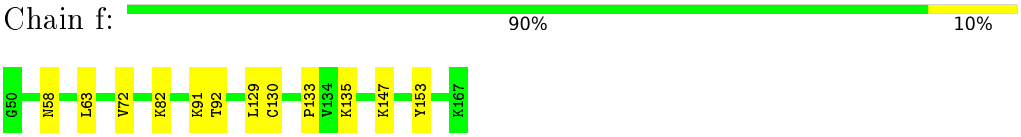
• Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial

Chain e:



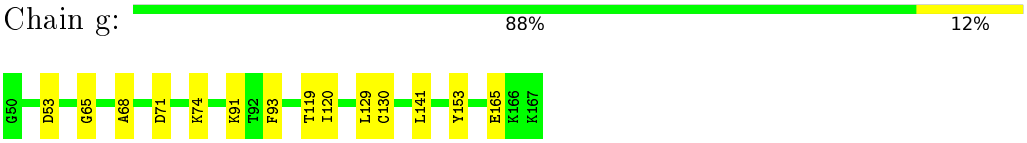
• Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial

Chain f:



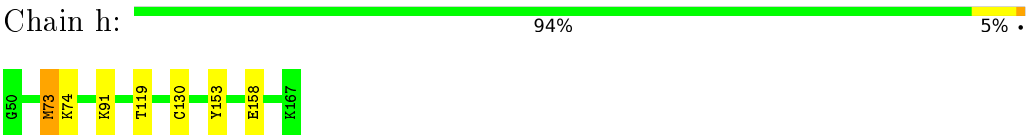
• Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial

Chain g:



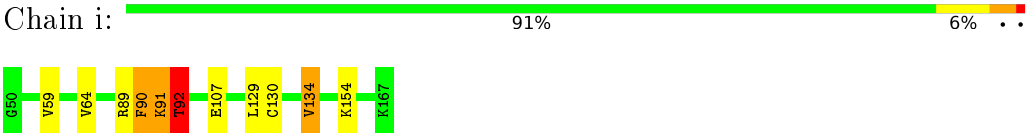
• Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial

Chain h:



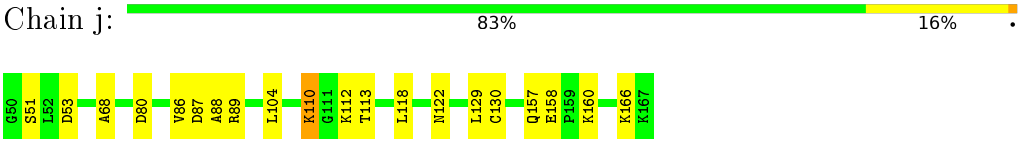
• Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial

Chain i:



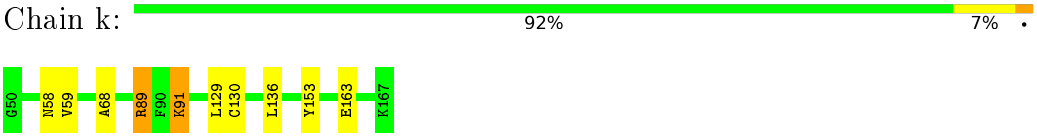
• Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial

Chain j:



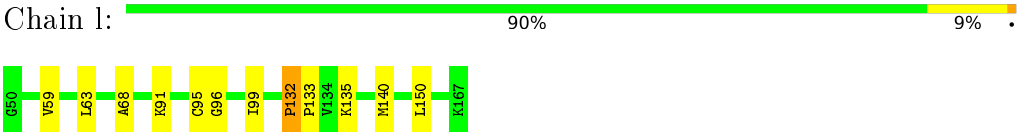
• Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial

Chain k:



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

Chain l:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	4124	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	210	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	115000	Depositor
Image detector	Not provided	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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
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	$\#\|Z\|>2$	RMSZ	$\#\|Z\|>2$
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(^{o})	Ideal(^{o})
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 (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	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	24
1	2	389/391 (100%)	341 (88%)	27 (7%)	21 (5%)	2	29
1	3	389/391 (100%)	334 (86%)	37 (10%)	18 (5%)	3	33
1	4	389/391 (100%)	332 (85%)	34 (9%)	23 (6%)	2	27
1	M	389/391 (100%)	346 (89%)	30 (8%)	13 (3%)	5	40
1	N	389/391 (100%)	340 (87%)	40 (10%)	9 (2%)	8	48
1	O	389/391 (100%)	332 (85%)	35 (9%)	22 (6%)	2	28
1	P	389/391 (100%)	345 (89%)	29 (8%)	15 (4%)	4	36
1	Q	389/391 (100%)	343 (88%)	32 (8%)	14 (4%)	4	38
1	R	389/391 (100%)	342 (88%)	31 (8%)	16 (4%)	3	35
1	S	389/391 (100%)	335 (86%)	36 (9%)	18 (5%)	3	33
1	T	389/391 (100%)	341 (88%)	34 (9%)	14 (4%)	4	38
2	A	167/169 (99%)	124 (74%)	28 (17%)	15 (9%)	1	17
2	B	167/169 (99%)	140 (84%)	18 (11%)	9 (5%)	2	29
2	C	167/169 (99%)	125 (75%)	27 (16%)	15 (9%)	1	17
2	D	167/169 (99%)	126 (75%)	33 (20%)	8 (5%)	3	32
2	E	167/169 (99%)	133 (80%)	20 (12%)	14 (8%)	1	18
2	F	167/169 (99%)	134 (80%)	23 (14%)	10 (6%)	2	26
2	G	167/169 (99%)	135 (81%)	23 (14%)	9 (5%)	2	29
2	H	167/169 (99%)	133 (80%)	25 (15%)	9 (5%)	2	29
2	I	167/169 (99%)	130 (78%)	21 (13%)	16 (10%)	1	15
2	J	167/169 (99%)	132 (79%)	17 (10%)	18 (11%)	0	11
2	K	167/169 (99%)	137 (82%)	22 (13%)	8 (5%)	3	32
2	L	167/169 (99%)	125 (75%)	27 (16%)	15 (9%)	1	17
3	a	116/118 (98%)	94 (81%)	16 (14%)	6 (5%)	2	30
3	b	116/118 (98%)	102 (88%)	9 (8%)	5 (4%)	3	34
3	c	116/118 (98%)	97 (84%)	16 (14%)	3 (3%)	7	45
3	d	116/118 (98%)	97 (84%)	12 (10%)	7 (6%)	2	26
3	e	116/118 (98%)	97 (84%)	12 (10%)	7 (6%)	2	26
3	f	116/118 (98%)	98 (84%)	13 (11%)	5 (4%)	3	34

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 20
3	h	116/118 (98%)	100 (86%)	14 (12%)	2 (2%)	11 55
3	i	116/118 (98%)	96 (83%)	13 (11%)	7 (6%)	2 26
3	j	116/118 (98%)	86 (74%)	16 (14%)	14 (12%)	0 8
3	k	116/118 (98%)	99 (85%)	10 (9%)	7 (6%)	2 26
3	l	116/118 (98%)	99 (85%)	12 (10%)	5 (4%)	3 34
All	All	8064/8136 (99%)	6798 (84%)	834 (10%)	432 (5%)	4 29

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 (i)

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%)	21 57
1	2	333/333 (100%)	319 (96%)	14 (4%)	36 70
1	3	333/333 (100%)	318 (96%)	15 (4%)	34 69
1	4	333/333 (100%)	314 (94%)	19 (6%)	25 62
1	M	333/333 (100%)	320 (96%)	13 (4%)	39 72
1	N	333/333 (100%)	316 (95%)	17 (5%)	29 66
1	O	333/333 (100%)	318 (96%)	15 (4%)	34 69
1	P	333/333 (100%)	319 (96%)	14 (4%)	36 70
1	Q	333/333 (100%)	323 (97%)	10 (3%)	48 77
1	R	333/333 (100%)	314 (94%)	19 (6%)	25 62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	S	333/333 (100%)	320 (96%)	13 (4%)	39 72
1	T	333/333 (100%)	318 (96%)	15 (4%)	34 69
2	A	146/146 (100%)	134 (92%)	12 (8%)	14 49
2	B	146/146 (100%)	140 (96%)	6 (4%)	37 71
2	C	146/146 (100%)	140 (96%)	6 (4%)	37 71
2	D	146/146 (100%)	140 (96%)	6 (4%)	37 71
2	E	146/146 (100%)	137 (94%)	9 (6%)	23 60
2	F	146/146 (100%)	138 (94%)	8 (6%)	27 63
2	G	146/146 (100%)	138 (94%)	8 (6%)	27 63
2	H	146/146 (100%)	138 (94%)	8 (6%)	27 63
2	I	146/146 (100%)	135 (92%)	11 (8%)	17 53
2	J	146/146 (100%)	142 (97%)	4 (3%)	52 79
2	K	146/146 (100%)	135 (92%)	11 (8%)	17 53
2	L	146/146 (100%)	133 (91%)	13 (9%)	12 44
3	a	94/94 (100%)	89 (95%)	5 (5%)	28 64
3	b	94/94 (100%)	91 (97%)	3 (3%)	46 76
3	c	94/94 (100%)	90 (96%)	4 (4%)	35 70
3	d	94/94 (100%)	92 (98%)	2 (2%)	61 84
3	e	94/94 (100%)	93 (99%)	1 (1%)	80 91
3	f	94/94 (100%)	89 (95%)	5 (5%)	28 64
3	g	94/94 (100%)	91 (97%)	3 (3%)	46 76
3	h	94/94 (100%)	89 (95%)	5 (5%)	28 64
3	i	94/94 (100%)	87 (93%)	7 (7%)	17 54
3	j	94/94 (100%)	89 (95%)	5 (5%)	28 64
3	k	94/94 (100%)	91 (97%)	3 (3%)	46 76
3	l	94/94 (100%)	87 (93%)	7 (7%)	17 54
All	All	6876/6876 (100%)	6538 (95%)	338 (5%)	35 67

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

Mol	Chain	Res	Type
1	R	276	VAL
2	A	70	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	132	LEU
1	R	453	LYS
1	T	74	LEU

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

Mol	Chain	Res	Type
1	P	156	HIS
1	R	83	ASN
3	i	122	ASN
1	P	355	ASN
1	Q	108	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.