Full wwPDB EM Validation Report (i)

Sep 28, 2024 – 07:39 AM EDT

PDB ID	:	5T0V
EMDB ID	:	EMD-8341
Title	:	Architecture of the Yeast Mitochondrial Iron-Sulfur Cluster Assembly Machinery: the Sub-Complex Formed by the Iron Donor, Yfh1, and the Scaffold, Isu1
Authors	:	Ranatunga, W.; Gakh, O.; Galeano, B.K.; Smith IV, D.Y.; Soderberg, C.A.; Al-Karadaghi, S.; Thompson, J.R.; Isaya, G.
Deposited on	:	2016-08-16
Resolution	:	17.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

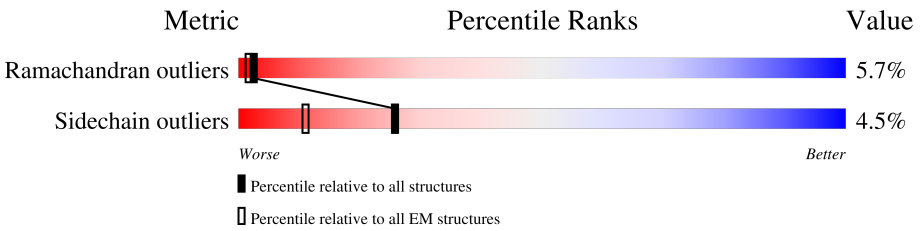
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 17.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	a	142	38% 92% 7% •
1	b	142	38% 92% 7% •
1	c	142	36% 90% 9% •
1	d	142	37% 97% •
1	e	142	38% 91% 8% •
1	f	142	37% 93% 6% •
1	g	142	36% 94% 6%
1	h	142	38% 92% 8%
1	i	142	42% 92% 8% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	j	142	38% 92% 8%
1	k	142	37% 90% 8% •
1	l	142	35% 89% 11%
1	m	142	38% 94% 6%
1	n	142	38% 93% 6% •
1	o	142	37% 94% 6%
1	p	142	37% 88% 12%
1	q	142	42% 91% 9%
1	r	142	37% 91% 8% •
1	s	142	37% 94% 6%
1	t	142	39% 91% 6% •
1	u	142	41% 94% 6%
1	v	142	35% 94% 6%
1	w	142	37% 94% 6%
1	x	142	37% 92% 7% •
2	A	121	37% 83% 14% •
2	B	121	33% 88% 12%
2	C	121	33% 87% 12% •
2	D	121	36% 81% 17% •
2	E	121	31% 85% 14% •
2	F	121	36% 86% 14%
2	G	121	35% 81% 18% •
2	H	121	31% 83% 16% •
2	I	121	34% 89% 11%
2	J	121	36% 84% 14% ••

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	K	121	31% 80% 20%
2	L	121	33% 90% 9% •
2	M	121	36% 90% 9% •
2	N	121	31% 83% 16% •
2	O	121	36% 92% 7% •
2	P	121	36% 86% 14%
2	Q	121	34% 86% 12% •
2	R	121	35% 92% 7% •
2	S	121	36% 87% 12% •
2	T	121	33% 88% 11% •
2	U	121	39% 80% 18% •
2	V	121	34% 86% 14%
2	W	121	35% 83% 16% •
2	X	121	33% 90% 9% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 48456 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 Iron sulfur cluster assembly protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	142	1072	672	186	205	9	0	0
1	b	142	1072	672	186	205	9	0	0
1	c	142	1072	672	186	205	9	0	0
1	d	142	1072	672	186	205	9	0	0
1	e	142	1072	672	186	205	9	0	0
1	f	142	1072	672	186	205	9	0	0
1	g	142	1072	672	186	205	9	0	0
1	h	142	1072	672	186	205	9	0	0
1	i	142	1072	672	186	205	9	0	0
1	j	142	1072	672	186	205	9	0	0
1	k	142	1072	672	186	205	9	0	0
1	l	142	1072	672	186	205	9	0	0
1	m	142	1072	672	186	205	9	0	0
1	n	142	1072	672	186	205	9	0	0
1	o	142	1072	672	186	205	9	0	0
1	p	142	1072	672	186	205	9	0	0
1	q	142	1072	672	186	205	9	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	r	142	1072	672	186	205	9	0	0
1	s	142	1072	672	186	205	9	0	0
1	t	142	1072	672	186	205	9	0	0
1	u	142	1072	672	186	205	9	0	0
1	v	142	1072	672	186	205	9	0	0
1	w	142	1072	672	186	205	9	0	0
1	x	142	1072	672	186	205	9	0	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	24	GLY	-	expression tag	UNP Q03020
a	25	SER	-	expression tag	UNP Q03020
a	26	HIS	-	expression tag	UNP Q03020
a	27	MET	-	expression tag	UNP Q03020
b	24	GLY	-	expression tag	UNP Q03020
b	25	SER	-	expression tag	UNP Q03020
b	26	HIS	-	expression tag	UNP Q03020
b	27	MET	-	expression tag	UNP Q03020
c	24	GLY	-	expression tag	UNP Q03020
c	25	SER	-	expression tag	UNP Q03020
c	26	HIS	-	expression tag	UNP Q03020
c	27	MET	-	expression tag	UNP Q03020
d	24	GLY	-	expression tag	UNP Q03020
d	25	SER	-	expression tag	UNP Q03020
d	26	HIS	-	expression tag	UNP Q03020
d	27	MET	-	expression tag	UNP Q03020
e	24	GLY	-	expression tag	UNP Q03020
e	25	SER	-	expression tag	UNP Q03020
e	26	HIS	-	expression tag	UNP Q03020
e	27	MET	-	expression tag	UNP Q03020
f	24	GLY	-	expression tag	UNP Q03020
f	25	SER	-	expression tag	UNP Q03020
f	26	HIS	-	expression tag	UNP Q03020
f	27	MET	-	expression tag	UNP Q03020
g	24	GLY	-	expression tag	UNP Q03020

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
g	25	SER	-	expression tag	UNP Q03020
g	26	HIS	-	expression tag	UNP Q03020
g	27	MET	-	expression tag	UNP Q03020
h	24	GLY	-	expression tag	UNP Q03020
h	25	SER	-	expression tag	UNP Q03020
h	26	HIS	-	expression tag	UNP Q03020
h	27	MET	-	expression tag	UNP Q03020
i	24	GLY	-	expression tag	UNP Q03020
i	25	SER	-	expression tag	UNP Q03020
i	26	HIS	-	expression tag	UNP Q03020
i	27	MET	-	expression tag	UNP Q03020
j	24	GLY	-	expression tag	UNP Q03020
j	25	SER	-	expression tag	UNP Q03020
j	26	HIS	-	expression tag	UNP Q03020
j	27	MET	-	expression tag	UNP Q03020
k	24	GLY	-	expression tag	UNP Q03020
k	25	SER	-	expression tag	UNP Q03020
k	26	HIS	-	expression tag	UNP Q03020
k	27	MET	-	expression tag	UNP Q03020
l	24	GLY	-	expression tag	UNP Q03020
l	25	SER	-	expression tag	UNP Q03020
l	26	HIS	-	expression tag	UNP Q03020
l	27	MET	-	expression tag	UNP Q03020
m	24	GLY	-	expression tag	UNP Q03020
m	25	SER	-	expression tag	UNP Q03020
m	26	HIS	-	expression tag	UNP Q03020
m	27	MET	-	expression tag	UNP Q03020
n	24	GLY	-	expression tag	UNP Q03020
n	25	SER	-	expression tag	UNP Q03020
n	26	HIS	-	expression tag	UNP Q03020
n	27	MET	-	expression tag	UNP Q03020
o	24	GLY	-	expression tag	UNP Q03020
o	25	SER	-	expression tag	UNP Q03020
o	26	HIS	-	expression tag	UNP Q03020
o	27	MET	-	expression tag	UNP Q03020
p	24	GLY	-	expression tag	UNP Q03020
p	25	SER	-	expression tag	UNP Q03020
p	26	HIS	-	expression tag	UNP Q03020
p	27	MET	-	expression tag	UNP Q03020
q	24	GLY	-	expression tag	UNP Q03020
q	25	SER	-	expression tag	UNP Q03020
q	26	HIS	-	expression tag	UNP Q03020

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
q	27	MET	-	expression tag	UNP Q03020
r	24	GLY	-	expression tag	UNP Q03020
r	25	SER	-	expression tag	UNP Q03020
r	26	HIS	-	expression tag	UNP Q03020
r	27	MET	-	expression tag	UNP Q03020
s	24	GLY	-	expression tag	UNP Q03020
s	25	SER	-	expression tag	UNP Q03020
s	26	HIS	-	expression tag	UNP Q03020
s	27	MET	-	expression tag	UNP Q03020
t	24	GLY	-	expression tag	UNP Q03020
t	25	SER	-	expression tag	UNP Q03020
t	26	HIS	-	expression tag	UNP Q03020
t	27	MET	-	expression tag	UNP Q03020
u	24	GLY	-	expression tag	UNP Q03020
u	25	SER	-	expression tag	UNP Q03020
u	26	HIS	-	expression tag	UNP Q03020
u	27	MET	-	expression tag	UNP Q03020
v	24	GLY	-	expression tag	UNP Q03020
v	25	SER	-	expression tag	UNP Q03020
v	26	HIS	-	expression tag	UNP Q03020
v	27	MET	-	expression tag	UNP Q03020
w	24	GLY	-	expression tag	UNP Q03020
w	25	SER	-	expression tag	UNP Q03020
w	26	HIS	-	expression tag	UNP Q03020
w	27	MET	-	expression tag	UNP Q03020
x	24	GLY	-	expression tag	UNP Q03020
x	25	SER	-	expression tag	UNP Q03020
x	26	HIS	-	expression tag	UNP Q03020
x	27	MET	-	expression tag	UNP Q03020

- Molecule 2 is a protein called Frataxin homolog, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	121	947	597	153	195	2	0	0
2	B	121	947	597	153	195	2	0	0
2	C	121	947	597	153	195	2	0	0
2	D	121	947	597	153	195	2	0	0
2	E	121	947	597	153	195	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	F	121	947	597	153	195	2	0	0
2	G	121	947	597	153	195	2	0	0
2	H	121	947	597	153	195	2	0	0
2	I	121	947	597	153	195	2	0	0
2	J	121	947	597	153	195	2	0	0
2	K	121	947	597	153	195	2	0	0
2	L	121	947	597	153	195	2	0	0
2	M	121	947	597	153	195	2	0	0
2	N	121	947	597	153	195	2	0	0
2	O	121	947	597	153	195	2	0	0
2	P	121	947	597	153	195	2	0	0
2	Q	121	947	597	153	195	2	0	0
2	R	121	947	597	153	195	2	0	0
2	S	121	947	597	153	195	2	0	0
2	T	121	947	597	153	195	2	0	0
2	U	121	947	597	153	195	2	0	0
2	V	121	947	597	153	195	2	0	0
2	W	121	947	597	153	195	2	0	0
2	X	121	947	597	153	195	2	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	ALA	TYR	conflict	UNP Q07540

Continued on next page...

Continued from previous page...

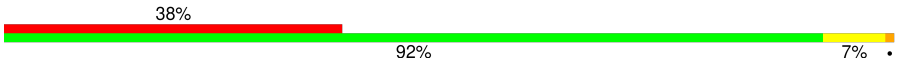
Chain	Residue	Modelled	Actual	Comment	Reference
B	73	ALA	TYR	conflict	UNP Q07540
C	73	ALA	TYR	conflict	UNP Q07540
D	73	ALA	TYR	conflict	UNP Q07540
E	73	ALA	TYR	conflict	UNP Q07540
F	73	ALA	TYR	conflict	UNP Q07540
G	73	ALA	TYR	conflict	UNP Q07540
H	73	ALA	TYR	conflict	UNP Q07540
I	73	ALA	TYR	conflict	UNP Q07540
J	73	ALA	TYR	conflict	UNP Q07540
K	73	ALA	TYR	conflict	UNP Q07540
L	73	ALA	TYR	conflict	UNP Q07540
M	73	ALA	TYR	conflict	UNP Q07540
N	73	ALA	TYR	conflict	UNP Q07540
O	73	ALA	TYR	conflict	UNP Q07540
P	73	ALA	TYR	conflict	UNP Q07540
Q	73	ALA	TYR	conflict	UNP Q07540
R	73	ALA	TYR	conflict	UNP Q07540
S	73	ALA	TYR	conflict	UNP Q07540
T	73	ALA	TYR	conflict	UNP Q07540
U	73	ALA	TYR	conflict	UNP Q07540
V	73	ALA	TYR	conflict	UNP Q07540
W	73	ALA	TYR	conflict	UNP Q07540
X	73	ALA	TYR	conflict	UNP Q07540

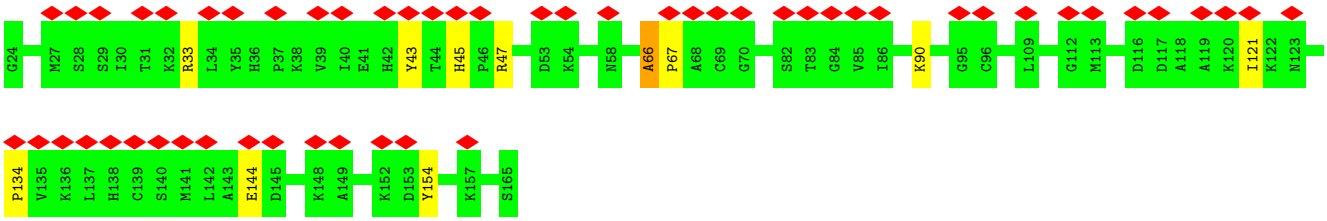
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

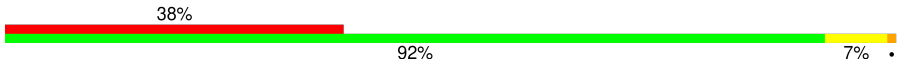
Chain a:

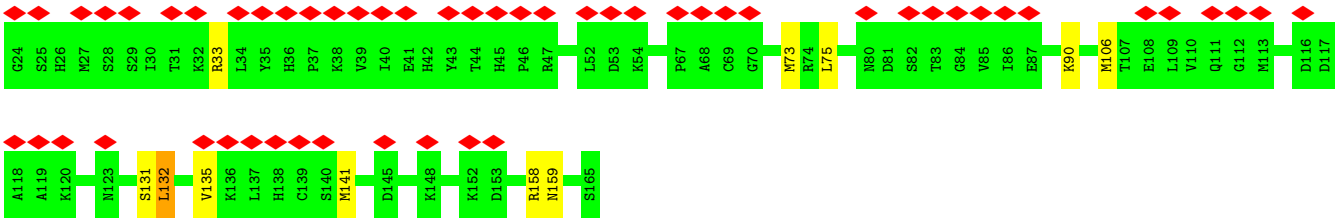




• Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

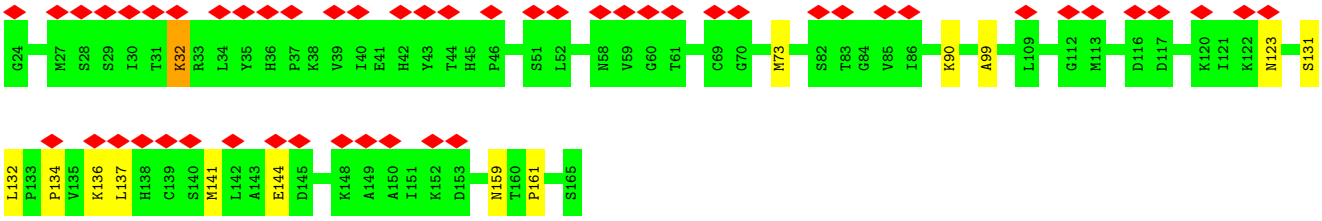
Chain b:





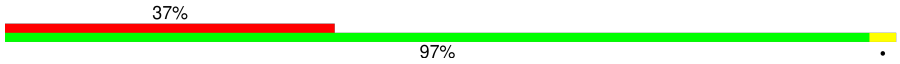
• Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

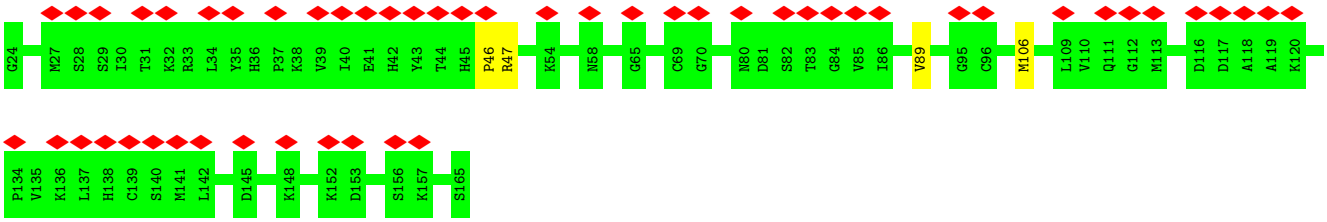
Chain c:



• Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

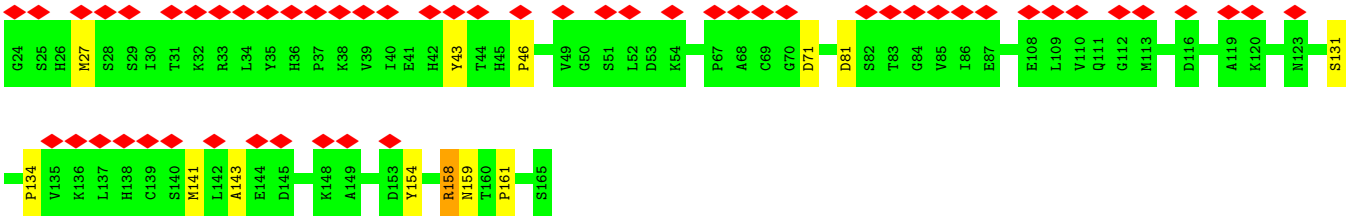
Chain d:





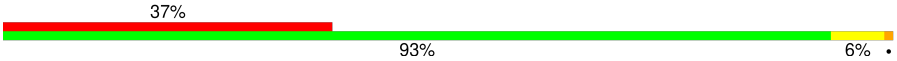
• Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

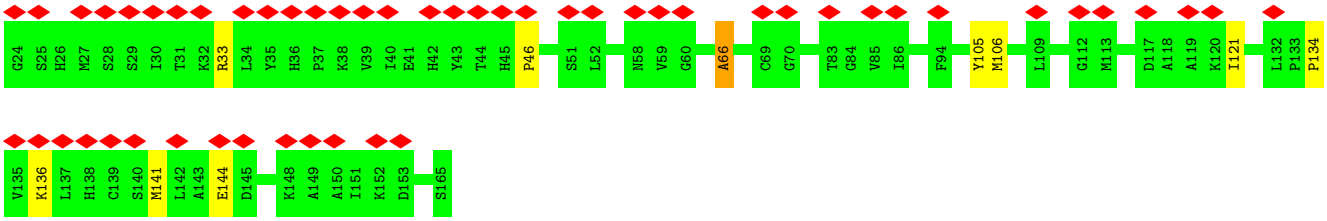
Chain e:



• Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

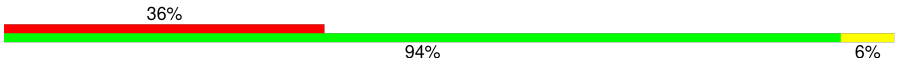
Chain f:

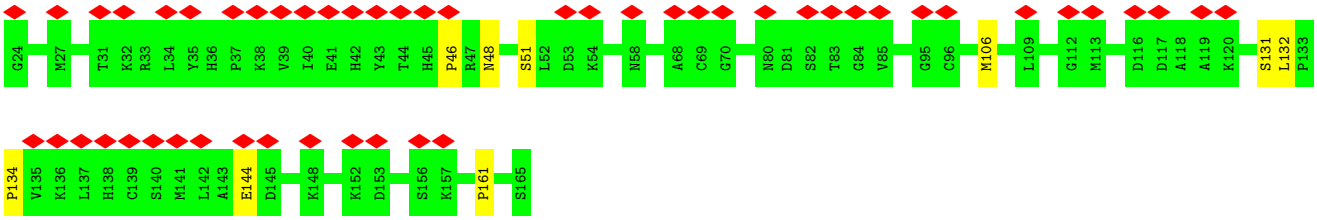




• Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

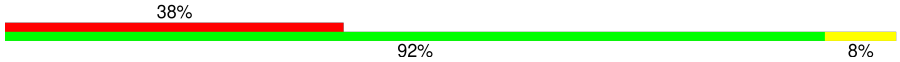
Chain g:

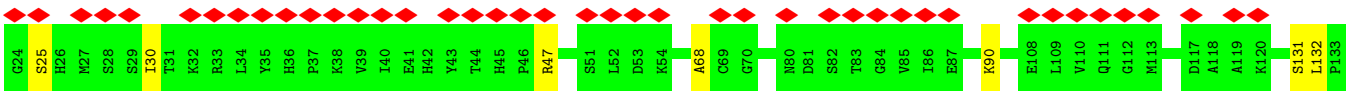


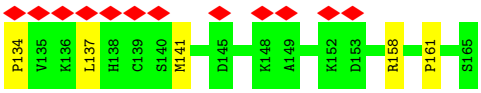


• Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain h:

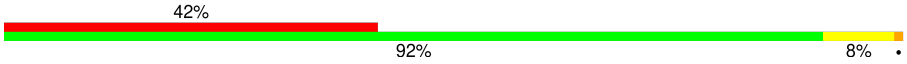


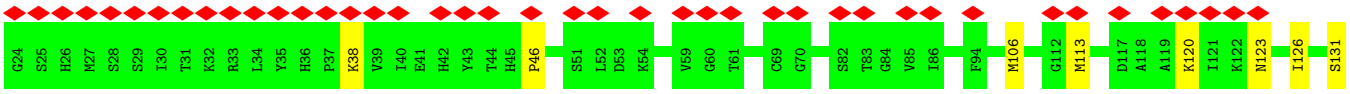


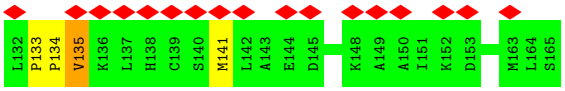


• Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain i:

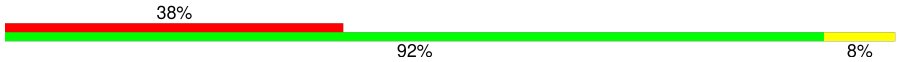


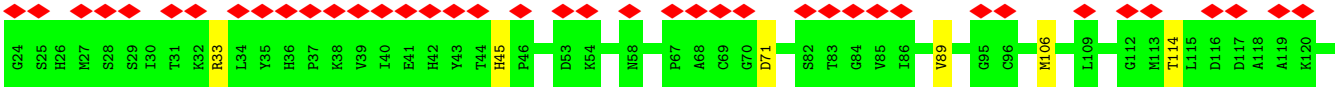


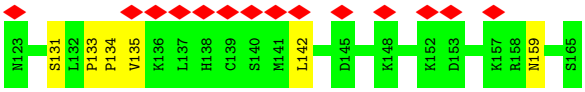


• Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain j:

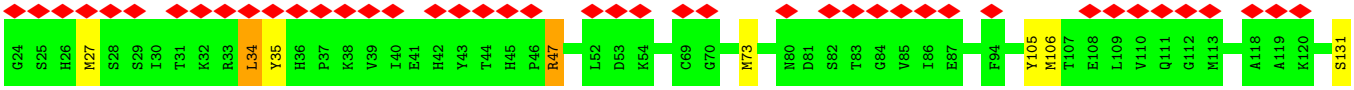


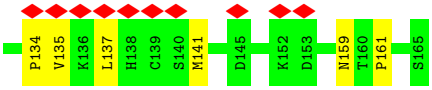




• Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

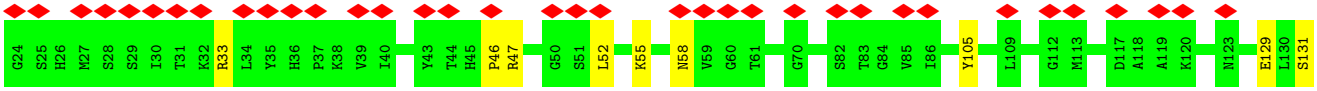
Chain k:

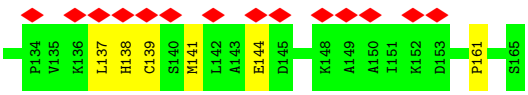




• Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

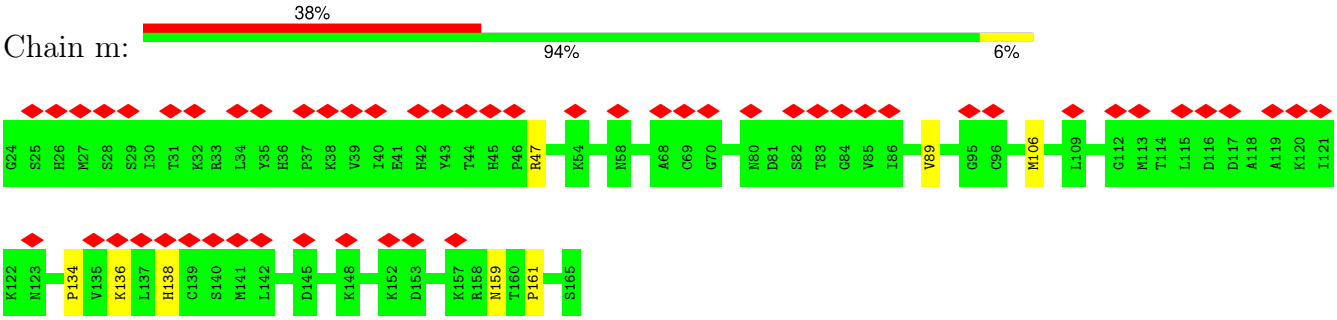
Chain l:





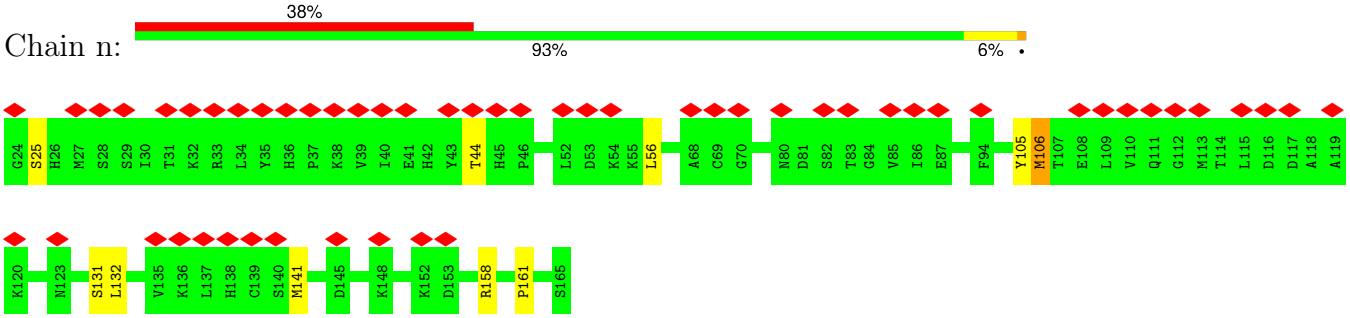
• Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain m:



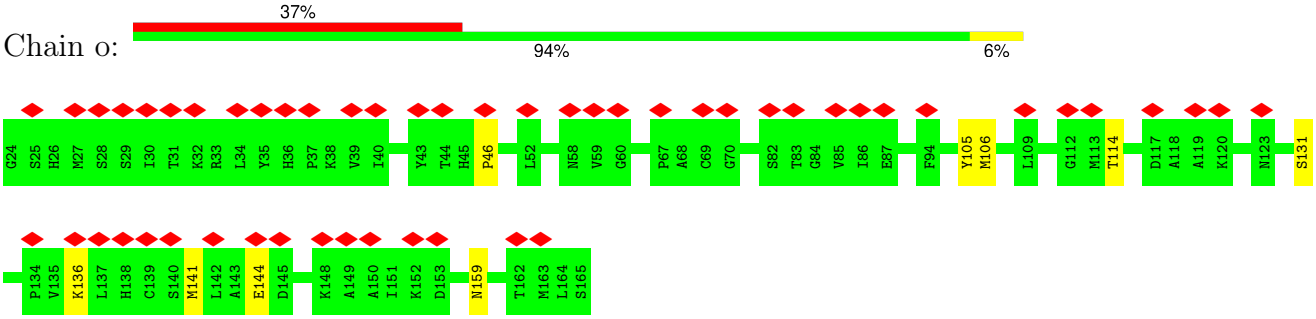
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain n:



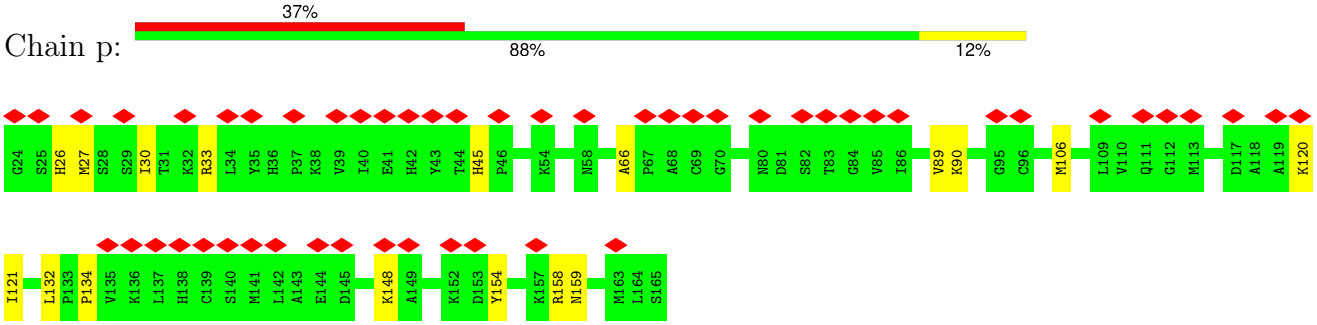
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain o:



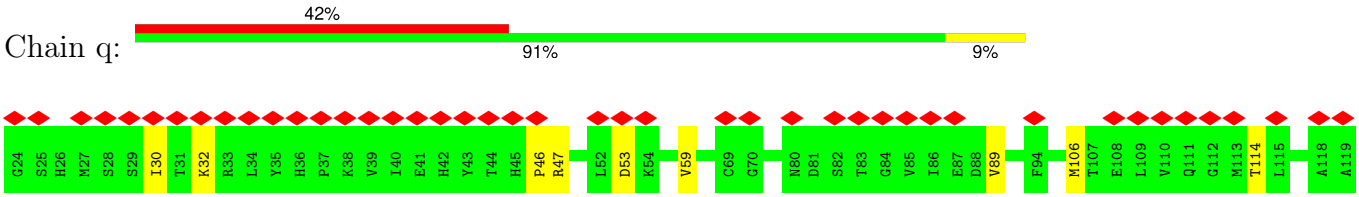
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

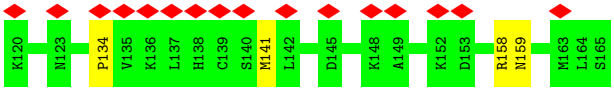
Chain p:



- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

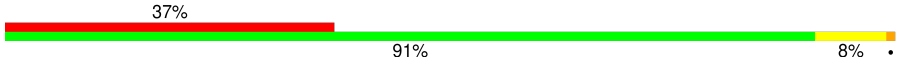
Chain q:

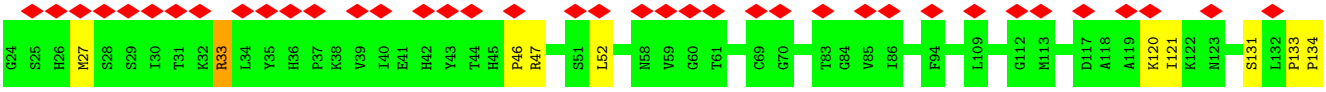


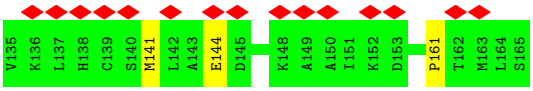


• Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain r:

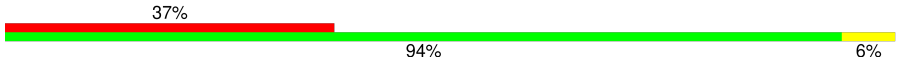


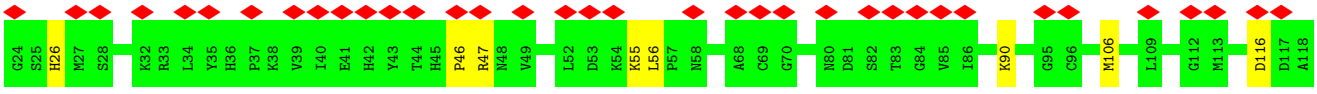


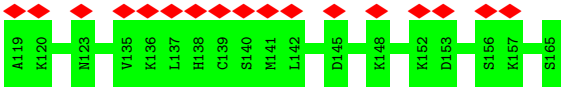


• Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain s:

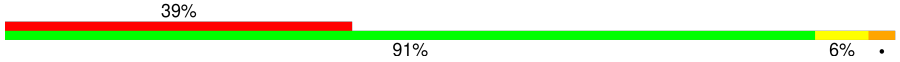


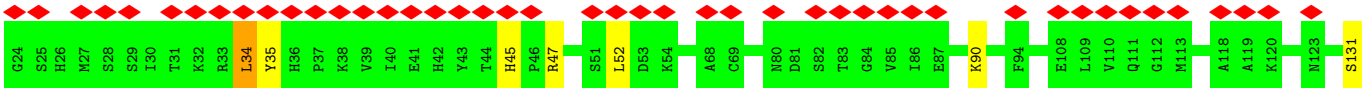


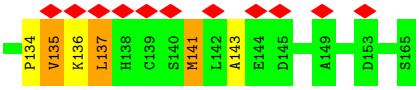


• Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain t:

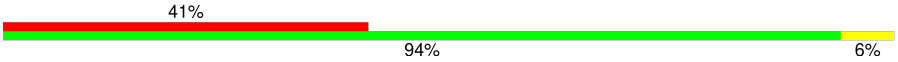


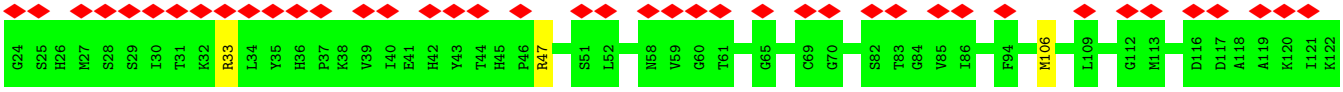


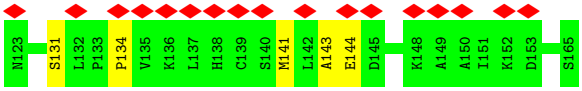


• Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain u:

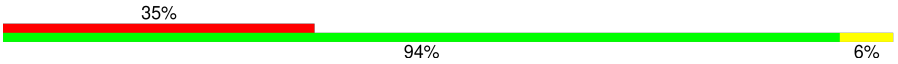


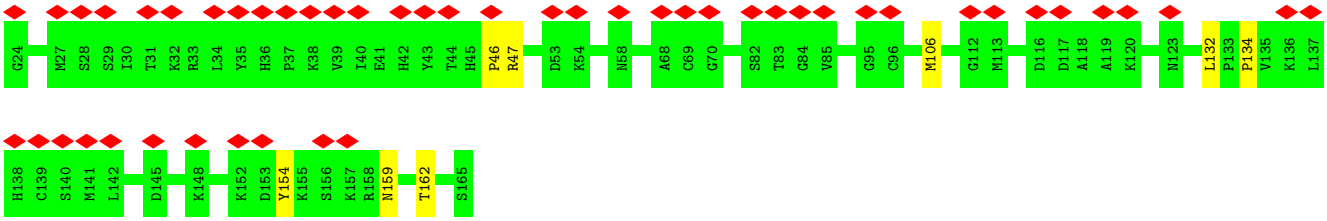




• Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

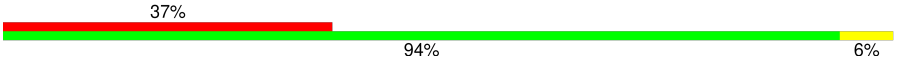
Chain v:

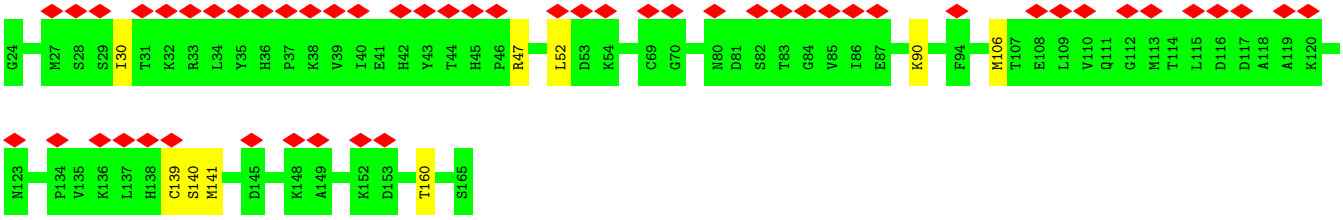




- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

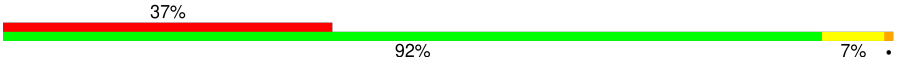
Chain w:

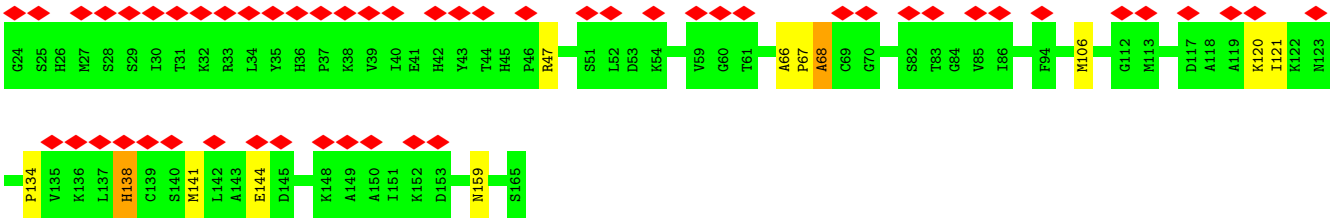




- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

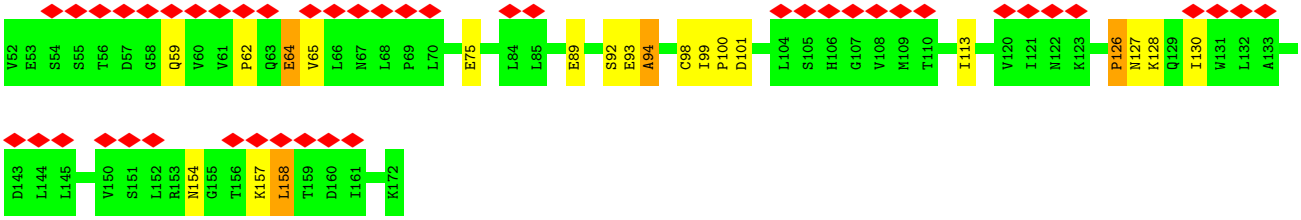
Chain x:





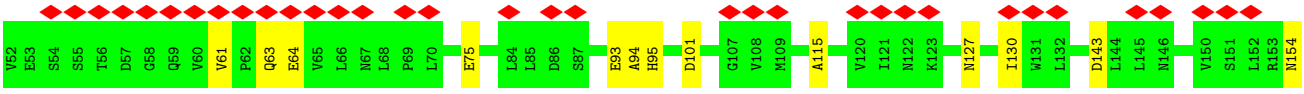
- Molecule 2: Frataxin homolog, mitochondrial

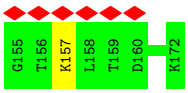
Chain A:



- Molecule 2: Frataxin homolog, mitochondrial

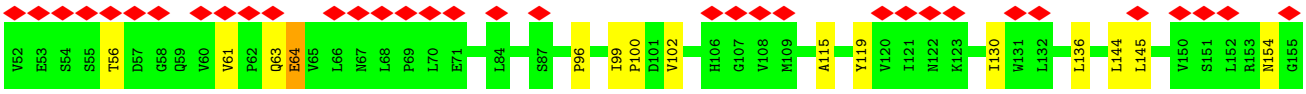
Chain B:

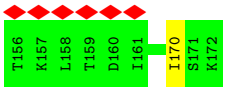




• Molecule 2: Frataxin homolog, mitochondrial

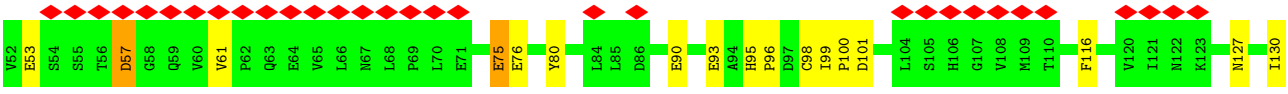
Chain C:

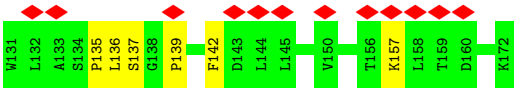




• Molecule 2: Frataxin homolog, mitochondrial

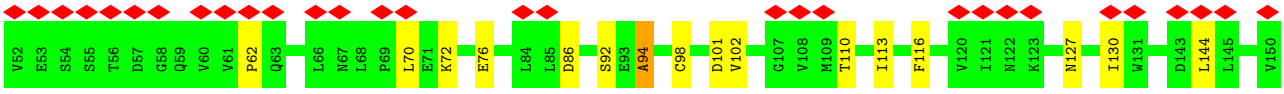
Chain D:

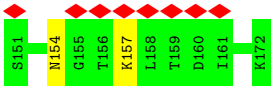




• Molecule 2: Frataxin homolog, mitochondrial

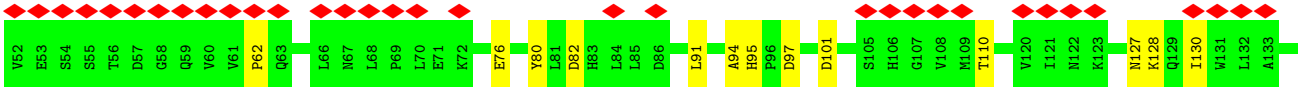
Chain E:

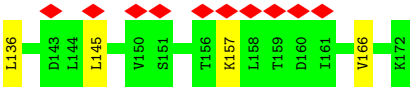




• Molecule 2: Frataxin homolog, mitochondrial

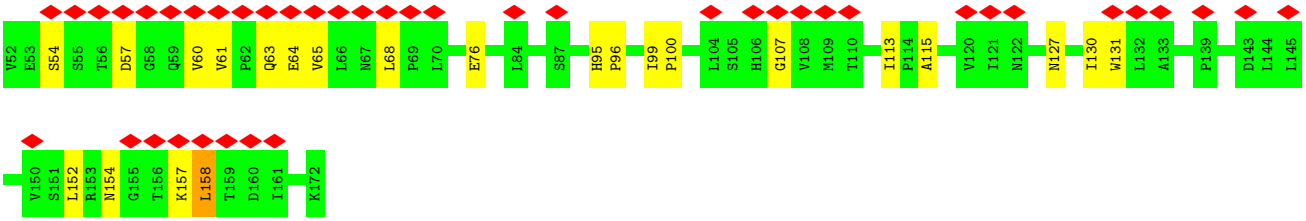
Chain F:





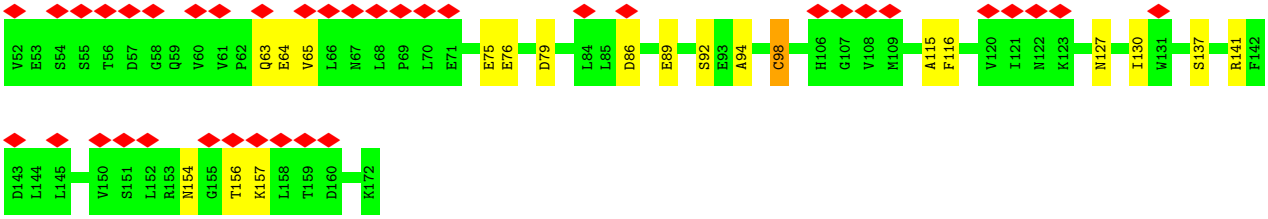
• Molecule 2: Frataxin homolog, mitochondrial

Chain G:



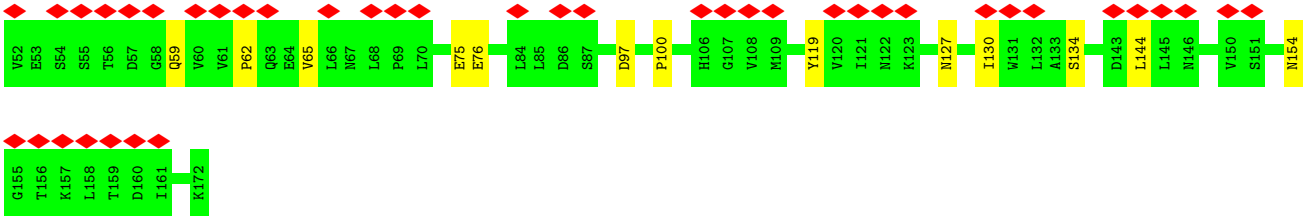
- Molecule 2: Frataxin homolog, mitochondrial

Chain H:



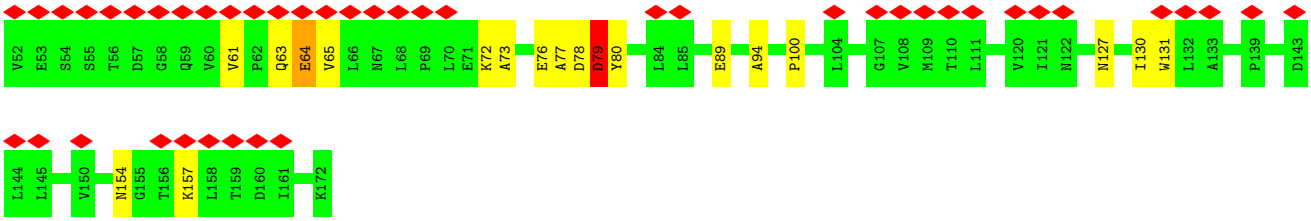
- Molecule 2: Frataxin homolog, mitochondrial

Chain I:



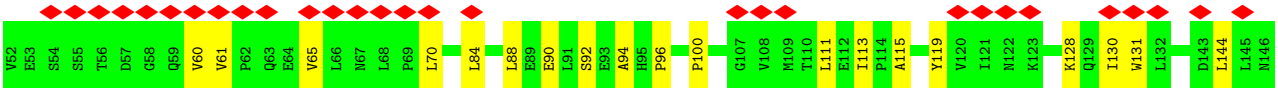
- Molecule 2: Frataxin homolog, mitochondrial

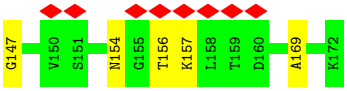
Chain J:



- Molecule 2: Frataxin homolog, mitochondrial

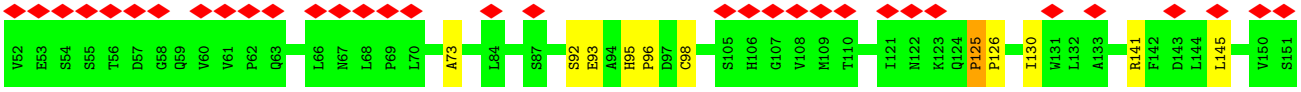
Chain K:

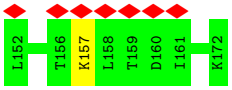




• Molecule 2: Frataxin homolog, mitochondrial

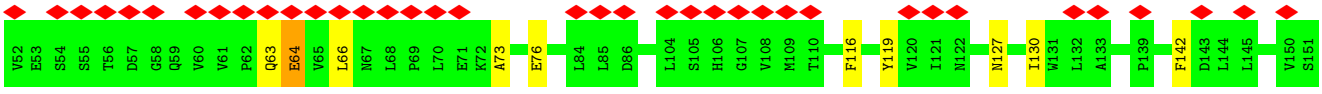
Chain L:

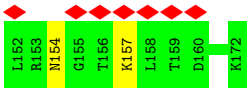




• Molecule 2: Frataxin homolog, mitochondrial

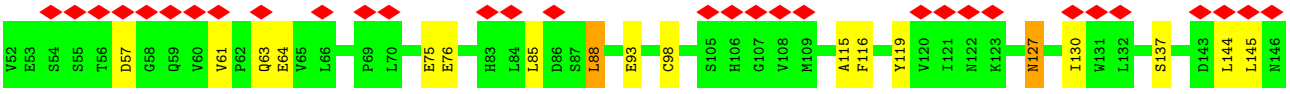
Chain M:

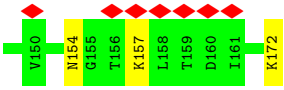




• Molecule 2: Frataxin homolog, mitochondrial

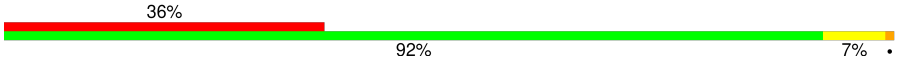
Chain N:

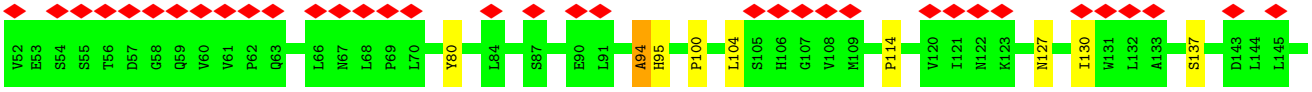


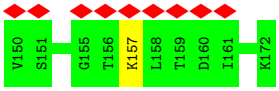


• Molecule 2: Frataxin homolog, mitochondrial

Chain O:

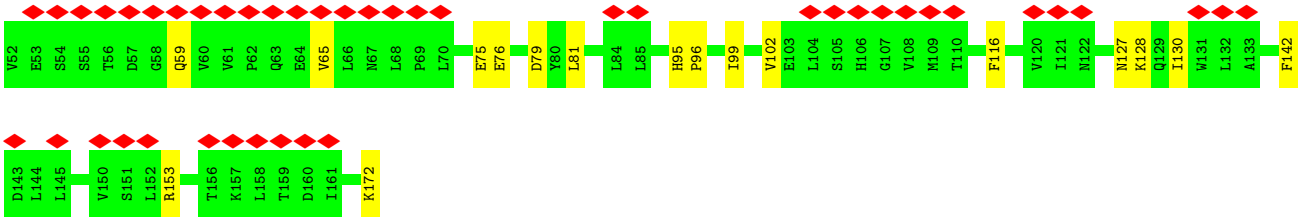






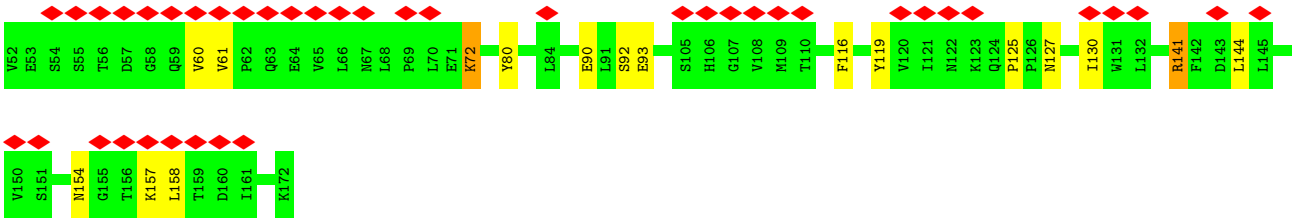
• Molecule 2: Frataxin homolog, mitochondrial

Chain P: 36% 86% 14%



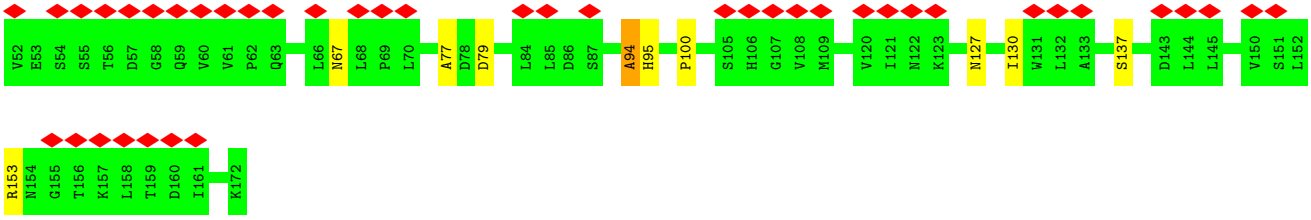
- Molecule 2: Frataxin homolog, mitochondrial

Chain Q: 34% 86% 12%



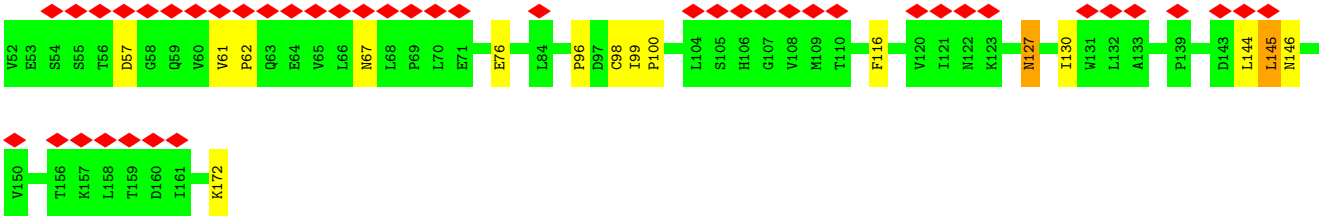
- Molecule 2: Frataxin homolog, mitochondrial

Chain R: 35% 92% 7%



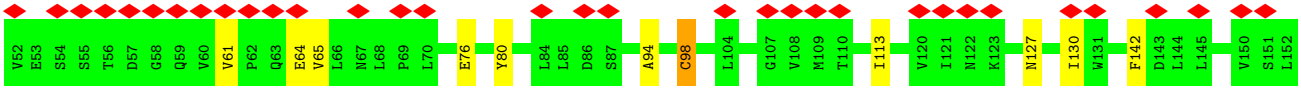
- Molecule 2: Frataxin homolog, mitochondrial

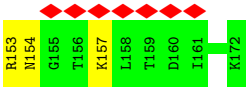
Chain S: 36% 87% 12%



- Molecule 2: Frataxin homolog, mitochondrial

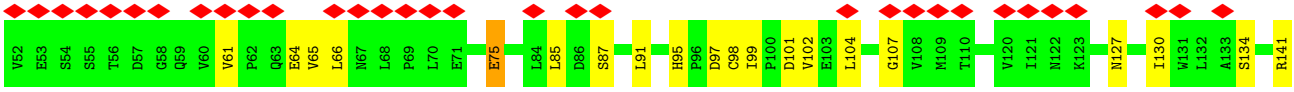
Chain T: 33% 88% 11%

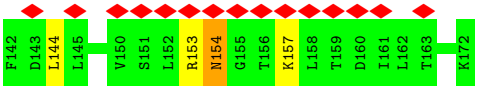




• Molecule 2: Frataxin homolog, mitochondrial

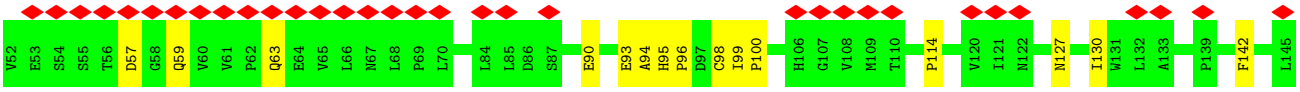
Chain U:

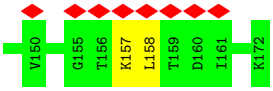




• Molecule 2: Frataxin homolog, mitochondrial

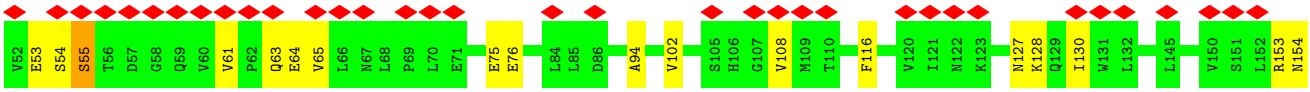
Chain V:

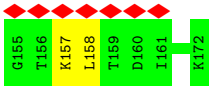




• Molecule 2: Frataxin homolog, mitochondrial

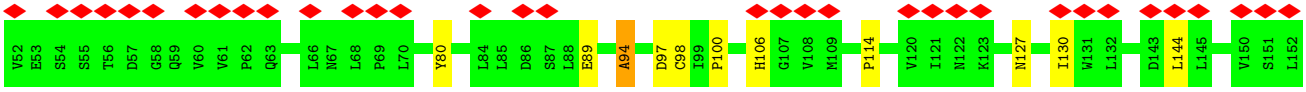
Chain W:

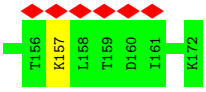




• Molecule 2: Frataxin homolog, mitochondrial

Chain X:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, O	Depositor
Number of particles used	4153	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 ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	210	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	115000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	12.440	Depositor
Minimum map value	-8.726	Depositor
Average map value	0.043	Depositor
Map value standard deviation	0.800	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	297.79202, 297.79202, 297.79202	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.034, 1.034, 1.034	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	a	1.04	0/1089	1.23	3/1466 (0.2%)
1	b	1.04	0/1089	1.28	6/1466 (0.4%)
1	c	1.02	0/1089	1.24	2/1466 (0.1%)
1	d	1.05	0/1089	1.18	0/1466
1	e	1.03	0/1089	1.29	5/1466 (0.3%)
1	f	1.06	0/1089	1.24	1/1466 (0.1%)
1	g	1.04	0/1089	1.18	1/1466 (0.1%)
1	h	1.00	0/1089	1.27	4/1466 (0.3%)
1	i	1.03	0/1089	1.19	1/1466 (0.1%)
1	j	1.02	0/1089	1.26	1/1466 (0.1%)
1	k	1.04	0/1089	1.27	6/1466 (0.4%)
1	l	1.04	0/1089	1.32	5/1466 (0.3%)
1	m	1.01	0/1089	1.17	0/1466
1	n	0.98	0/1089	1.22	3/1466 (0.2%)
1	o	0.98	0/1089	1.18	2/1466 (0.1%)
1	p	1.04	0/1089	1.27	5/1466 (0.3%)
1	q	1.04	0/1089	1.21	2/1466 (0.1%)
1	r	1.01	0/1089	1.24	1/1466 (0.1%)
1	s	1.05	0/1089	1.22	2/1466 (0.1%)
1	t	1.07	0/1089	1.24	2/1466 (0.1%)
1	u	1.05	0/1089	1.18	0/1466
1	v	1.04	0/1089	1.22	3/1466 (0.2%)
1	w	1.05	0/1089	1.22	0/1466
1	x	1.06	0/1089	1.25	3/1466 (0.2%)
2	A	0.99	0/967	1.21	2/1319 (0.2%)
2	B	1.02	0/967	1.24	0/1319
2	C	1.03	0/967	1.28	2/1319 (0.2%)
2	D	1.02	0/967	1.28	5/1319 (0.4%)
2	E	1.01	0/967	1.27	4/1319 (0.3%)
2	F	1.06	0/967	1.30	3/1319 (0.2%)
2	G	1.02	0/967	1.25	1/1319 (0.1%)
2	H	1.01	0/967	1.25	4/1319 (0.3%)
2	I	1.02	0/967	1.23	1/1319 (0.1%)
2	J	1.05	0/967	1.27	2/1319 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	K	0.98	0/967	1.27	3/1319 (0.2%)
2	L	1.01	0/967	1.23	1/1319 (0.1%)
2	M	1.02	0/967	1.26	3/1319 (0.2%)
2	N	1.00	0/967	1.32	7/1319 (0.5%)
2	O	1.01	0/967	1.19	1/1319 (0.1%)
2	P	1.03	0/967	1.31	4/1319 (0.3%)
2	Q	1.01	0/967	1.29	5/1319 (0.4%)
2	R	1.02	0/967	1.26	3/1319 (0.2%)
2	S	1.01	0/967	1.29	3/1319 (0.2%)
2	T	1.05	0/967	1.20	3/1319 (0.2%)
2	U	1.02	0/967	1.29	2/1319 (0.2%)
2	V	1.04	0/967	1.29	2/1319 (0.2%)
2	W	1.05	0/967	1.26	4/1319 (0.3%)
2	X	0.99	0/967	1.23	2/1319 (0.2%)
All	All	1.03	0/49344	1.25	125/66840 (0.2%)

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	a	0	1
1	n	0	1
1	r	0	2
1	t	0	1
2	I	0	1
2	M	0	1
All	All	0	7

There are no bond length outliers.

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	119	TYR	CB-CG-CD2	-10.14	114.91	121.00
2	C	119	TYR	CB-CG-CD1	10.11	127.07	121.00
1	l	105	TYR	CB-CG-CD2	-9.20	115.48	121.00
1	x	68	ALA	N-CA-CB	9.11	122.86	110.10
1	p	154	TYR	CB-CG-CD2	-8.95	115.63	121.00
1	c	131	SER	C-N-CA	8.26	142.36	121.70
1	b	158	ARG	NE-CZ-NH2	8.24	124.42	120.30
2	W	55	SER	N-CA-CB	8.24	122.86	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	119	TYR	CB-CG-CD2	-7.97	116.22	121.00
1	h	131	SER	C-N-CA	7.96	141.60	121.70
1	e	131	SER	C-N-CA	7.71	140.97	121.70
1	l	105	TYR	CB-CG-CD1	7.70	125.62	121.00
1	h	158	ARG	NE-CZ-NH2	7.69	124.15	120.30
1	k	47	ARG	NE-CZ-NH2	7.66	124.13	120.30
1	l	131	SER	C-N-CA	7.59	140.69	121.70
1	v	47	ARG	NE-CZ-NH2	7.46	124.03	120.30
2	M	142	PHE	CB-CG-CD1	7.30	125.91	120.80
2	K	119	TYR	CB-CG-CD1	7.29	125.38	121.00
2	X	94	ALA	N-CA-CB	7.28	120.29	110.10
2	D	80	TYR	CB-CG-CD2	-7.20	116.68	121.00
1	e	154	TYR	CB-CG-CD2	-7.17	116.70	121.00
2	N	119	TYR	CB-CG-CD2	-7.13	116.72	121.00
2	M	116	PHE	CB-CG-CD1	7.09	125.76	120.80
1	p	154	TYR	CB-CG-CD1	7.03	125.22	121.00
2	N	119	TYR	CB-CG-CD1	6.91	125.15	121.00
2	F	80	TYR	CB-CG-CD2	-6.91	116.85	121.00
2	Q	80	TYR	CB-CG-CD2	-6.91	116.86	121.00
2	T	80	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	q	46	PRO	C-N-CA	6.82	138.76	121.70
1	e	43	TYR	CB-CG-CD2	-6.81	116.91	121.00
1	l	33	ARG	NE-CZ-NH2	-6.72	116.94	120.30
2	D	80	TYR	CB-CG-CD1	6.67	125.00	121.00
1	x	67	PRO	C-N-CA	6.62	138.25	121.70
2	J	78	ASP	C-N-CA	6.61	138.22	121.70
2	N	116	PHE	CB-CG-CD2	-6.59	116.19	120.80
2	S	146	ASN	C-N-CA	6.57	136.10	122.30
1	k	73	MET	CG-SD-CE	-6.56	89.70	100.20
2	M	116	PHE	CB-CG-CD2	-6.53	116.23	120.80
2	N	116	PHE	CB-CG-CD1	6.41	125.29	120.80
2	J	79	ASP	N-CA-CB	6.37	122.07	110.60
2	R	94	ALA	N-CA-CB	6.35	118.99	110.10
2	H	141	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	v	154	TYR	CB-CG-CD1	6.27	124.76	121.00
1	b	158	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	t	131	SER	C-N-CA	6.14	137.06	121.70
1	a	66	ALA	N-CA-CB	6.09	118.63	110.10
2	L	141	ARG	NE-CZ-NH2	6.07	123.33	120.30
2	E	94	ALA	N-CA-CB	6.05	118.57	110.10
2	W	153	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	g	131	SER	C-N-CA	6.05	136.82	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	k	27	MET	C-N-CA	6.01	136.72	121.70
1	p	158	ARG	NE-CZ-NH2	5.99	123.29	120.30
2	I	75	GLU	C-N-CA	5.97	136.63	121.70
1	v	154	TYR	CB-CG-CD2	-5.97	117.42	121.00
2	Q	119	TYR	CB-CG-CD1	5.95	124.57	121.00
1	o	131	SER	C-N-CA	5.94	136.55	121.70
2	V	93	GLU	C-N-CA	5.90	136.44	121.70
2	E	110	THR	CA-CB-CG2	-5.83	104.24	112.40
1	b	33	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	R	153	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	j	131	SER	C-N-CA	5.82	136.24	121.70
2	V	57	ASP	N-CA-C	-5.81	95.30	111.00
2	U	75	GLU	C-N-CA	5.78	136.16	121.70
2	F	110	THR	CA-CB-CG2	-5.77	104.33	112.40
2	S	116	PHE	CB-CG-CD2	-5.75	116.78	120.80
1	f	66	ALA	N-CA-CB	5.74	118.14	110.10
2	H	75	GLU	C-N-CA	5.73	136.03	121.70
2	X	80	TYR	CA-CB-CG	-5.73	102.52	113.40
1	c	73	MET	CG-SD-CE	-5.71	91.06	100.20
1	e	158	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	b	132	LEU	N-CA-CB	5.68	121.75	110.40
2	Q	80	TYR	CB-CG-CD1	5.64	124.38	121.00
2	O	94	ALA	N-CA-CB	5.60	117.94	110.10
2	S	127	ASN	N-CA-CB	5.59	120.66	110.60
2	P	142	PHE	CB-CG-CD1	5.56	124.69	120.80
2	A	94	ALA	N-CA-CB	5.54	117.86	110.10
2	U	141	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	q	158	ARG	NE-CZ-NH2	5.50	123.05	120.30
2	A	75	GLU	C-N-CA	5.50	135.46	121.70
1	a	154	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	s	47	ARG	NE-CZ-NH2	5.48	123.04	120.30
2	P	153	ARG	NE-CZ-NH2	-5.47	117.57	120.30
2	H	98	CYS	N-CA-CB	5.46	120.44	110.60
2	T	98	CYS	N-CA-CB	5.43	120.38	110.60
2	P	116	PHE	CB-CG-CD1	5.43	124.60	120.80
1	x	66	ALA	N-CA-CB	5.43	117.70	110.10
2	F	80	TYR	CB-CG-CD1	5.42	124.25	121.00
1	e	27	MET	C-N-CA	5.41	135.22	121.70
1	b	73	MET	CG-SD-CE	-5.38	91.58	100.20
1	k	131	SER	C-N-CA	5.38	135.16	121.70
2	P	116	PHE	CB-CG-CD2	-5.38	117.03	120.80
1	l	131	SER	CA-C-N	5.38	129.03	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	b	131	SER	C-N-CA	5.37	135.12	121.70
2	N	137	SER	N-CA-CB	5.35	118.53	110.50
1	h	47	ARG	NE-CZ-NH1	-5.34	117.63	120.30
2	Q	119	TYR	N-CA-C	-5.33	96.60	111.00
1	t	35	TYR	CB-CG-CD2	-5.32	117.81	121.00
2	R	137	SER	N-CA-CB	5.32	118.47	110.50
1	p	33	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	E	116	PHE	CB-CG-CD2	-5.29	117.10	120.80
1	k	106	MET	CG-SD-CE	-5.29	91.73	100.20
2	D	57	ASP	N-CA-CB	5.29	120.12	110.60
2	W	116	PHE	CB-CG-CD1	5.28	124.49	120.80
1	s	47	ARG	NE-CZ-NH1	-5.25	117.67	120.30
2	D	142	PHE	CB-CA-C	-5.25	99.90	110.40
1	p	27	MET	C-N-CA	5.18	134.65	121.70
1	h	131	SER	CA-C-N	5.15	128.53	117.20
2	Q	141	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	a	43	TYR	CB-CG-CD1	-5.14	117.91	121.00
2	G	68	LEU	N-CA-C	-5.12	97.17	111.00
2	K	111	LEU	N-CA-C	-5.12	97.19	111.00
1	n	158	ARG	NE-CZ-NH2	5.12	122.86	120.30
2	W	102	VAL	N-CA-C	-5.11	97.21	111.00
1	n	131	SER	C-N-CA	5.09	134.44	121.70
2	N	127	ASN	N-CA-CB	5.07	119.72	110.60
1	k	34	LEU	N-CA-CB	5.06	120.52	110.40
2	H	116	PHE	CB-CG-CD1	5.06	124.34	120.80
2	N	88	LEU	CB-CG-CD1	5.04	119.57	111.00
2	T	94	ALA	N-CA-CB	5.04	117.15	110.10
1	n	106	MET	CG-SD-CE	-5.03	92.15	100.20
2	D	116	PHE	CB-CG-CD2	-5.03	117.28	120.80
1	i	113	MET	CG-SD-CE	-5.02	92.16	100.20
1	o	105	TYR	CB-CG-CD1	-5.02	117.99	121.00
2	E	101	ASP	C-N-CA	5.00	134.21	121.70
1	r	131	SER	O-C-N	-5.00	114.69	122.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	119	TYR	Sidechain
2	M	119	TYR	Sidechain
1	a	33	ARG	Sidechain
1	n	105	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	r	33	ARG	Sidechain
1	r	47	ARG	Sidechain
1	t	47	ARG	Sidechain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	140/142 (99%)	124 (89%)	11 (8%)	5 (4%)	3	20
1	b	140/142 (99%)	120 (86%)	17 (12%)	3 (2%)	5	30
1	c	140/142 (99%)	119 (85%)	15 (11%)	6 (4%)	2	17
1	d	140/142 (99%)	123 (88%)	16 (11%)	1 (1%)	19	57
1	e	140/142 (99%)	117 (84%)	18 (13%)	5 (4%)	3	20
1	f	140/142 (99%)	118 (84%)	18 (13%)	4 (3%)	3	23
1	g	140/142 (99%)	121 (86%)	13 (9%)	6 (4%)	2	17
1	h	140/142 (99%)	116 (83%)	19 (14%)	5 (4%)	3	20
1	i	140/142 (99%)	122 (87%)	12 (9%)	6 (4%)	2	17
1	j	140/142 (99%)	123 (88%)	12 (9%)	5 (4%)	3	20
1	k	140/142 (99%)	119 (85%)	14 (10%)	7 (5%)	1	16
1	l	140/142 (99%)	119 (85%)	13 (9%)	8 (6%)	1	14
1	m	140/142 (99%)	126 (90%)	10 (7%)	4 (3%)	3	23
1	n	140/142 (99%)	127 (91%)	9 (6%)	4 (3%)	3	23
1	o	140/142 (99%)	121 (86%)	16 (11%)	3 (2%)	5	30
1	p	140/142 (99%)	123 (88%)	10 (7%)	7 (5%)	1	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	q	140/142 (99%)	121 (86%)	12 (9%)	7 (5%)	1	16
1	r	140/142 (99%)	120 (86%)	15 (11%)	5 (4%)	3	20
1	s	140/142 (99%)	124 (89%)	13 (9%)	3 (2%)	5	30
1	t	140/142 (99%)	118 (84%)	16 (11%)	6 (4%)	2	17
1	u	140/142 (99%)	127 (91%)	10 (7%)	3 (2%)	5	30
1	v	140/142 (99%)	127 (91%)	8 (6%)	5 (4%)	3	20
1	w	140/142 (99%)	127 (91%)	11 (8%)	2 (1%)	9	41
1	x	140/142 (99%)	116 (83%)	19 (14%)	5 (4%)	3	20
2	A	119/121 (98%)	89 (75%)	15 (13%)	15 (13%)	0	4
2	B	119/121 (98%)	89 (75%)	21 (18%)	9 (8%)	1	10
2	C	119/121 (98%)	96 (81%)	12 (10%)	11 (9%)	0	8
2	D	119/121 (98%)	83 (70%)	21 (18%)	15 (13%)	0	4
2	E	119/121 (98%)	95 (80%)	14 (12%)	10 (8%)	0	9
2	F	119/121 (98%)	88 (74%)	23 (19%)	8 (7%)	1	12
2	G	119/121 (98%)	87 (73%)	15 (13%)	17 (14%)	0	3
2	H	119/121 (98%)	94 (79%)	13 (11%)	12 (10%)	0	7
2	I	119/121 (98%)	87 (73%)	24 (20%)	8 (7%)	1	12
2	J	119/121 (98%)	88 (74%)	18 (15%)	13 (11%)	0	6
2	K	119/121 (98%)	93 (78%)	13 (11%)	13 (11%)	0	6
2	L	119/121 (98%)	94 (79%)	16 (13%)	9 (8%)	1	10
2	M	119/121 (98%)	99 (83%)	14 (12%)	6 (5%)	1	16
2	N	119/121 (98%)	98 (82%)	14 (12%)	7 (6%)	1	13
2	O	119/121 (98%)	97 (82%)	17 (14%)	5 (4%)	2	17
2	P	119/121 (98%)	90 (76%)	20 (17%)	9 (8%)	1	10
2	Q	119/121 (98%)	98 (82%)	15 (13%)	6 (5%)	1	16
2	R	119/121 (98%)	93 (78%)	21 (18%)	5 (4%)	2	17
2	S	119/121 (98%)	98 (82%)	9 (8%)	12 (10%)	0	7
2	T	119/121 (98%)	98 (82%)	16 (13%)	5 (4%)	2	17
2	U	119/121 (98%)	85 (71%)	18 (15%)	16 (13%)	0	4
2	V	119/121 (98%)	90 (76%)	19 (16%)	10 (8%)	0	9
2	W	119/121 (98%)	89 (75%)	18 (15%)	12 (10%)	0	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	X	119/121 (98%)	95 (80%)	16 (13%)	8 (7%)	1 12
All	All	6216/6312 (98%)	5131 (82%)	729 (12%)	356 (6%)	2 14

All (356) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	47	ARG
1	a	66	ALA
2	A	59	GLN
2	A	93	GLU
2	A	94	ALA
1	b	132	LEU
2	C	100	PRO
2	C	102	VAL
2	D	75	GLU
2	D	98	CYS
2	E	94	ALA
2	E	98	CYS
1	f	121	ILE
2	F	82	ASP
2	F	97	ASP
2	F	127	ASN
1	g	51	SER
2	G	99	ILE
2	G	100	PRO
2	G	127	ASN
2	G	154	ASN
1	h	25	SER
1	h	68	ALA
2	H	92	SER
2	H	98	CYS
1	i	120	LYS
1	i	134	PRO
2	I	127	ASN
2	J	64	GLU
2	J	127	ASN
2	K	96	PRO
2	K	100	PRO
2	K	115	ALA
2	K	154	ASN
2	L	125	PRO
2	L	130	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	M	63	GLN
1	n	132	LEU
2	N	61	VAL
2	N	98	CYS
1	o	46	PRO
2	O	94	ALA
2	O	127	ASN
2	P	59	GLN
2	P	75	GLU
2	P	127	ASN
1	q	47	ARG
2	Q	72	LYS
1	r	46	PRO
2	R	77	ALA
2	R	94	ALA
2	S	127	ASN
1	t	137	LEU
1	t	143	ALA
2	T	98	CYS
2	T	127	ASN
2	U	102	VAL
2	U	154	ASN
1	v	162	THR
2	V	94	ALA
2	V	98	CYS
2	V	127	ASN
2	V	130	ILE
1	w	140	SER
2	W	55	SER
2	W	127	ASN
2	X	94	ALA
2	X	100	PRO
2	X	127	ASN
2	A	62	PRO
2	A	92	SER
2	A	98	CYS
2	A	127	ASN
1	b	159	ASN
2	B	101	ASP
2	B	115	ALA
2	B	154	ASN
1	c	137	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	56	THR
2	C	130	ILE
2	D	57	ASP
2	D	101	ASP
2	D	127	ASN
2	D	130	ILE
1	e	143	ALA
2	E	62	PRO
2	E	92	SER
2	E	127	ASN
1	f	134	PRO
2	F	94	ALA
2	F	130	ILE
2	G	60	VAL
2	G	95	HIS
2	G	115	ALA
2	H	65	VAL
2	H	86	ASP
2	H	94	ALA
2	H	127	ASN
2	H	154	ASN
2	I	59	GLN
2	I	65	VAL
2	I	130	ILE
1	j	133	PRO
1	j	142	LEU
2	J	65	VAL
2	J	73	ALA
2	J	77	ALA
2	J	79	ASP
2	J	80	TYR
2	J	94	ALA
1	k	34	LEU
1	k	35	TYR
1	k	134	PRO
1	k	137	LEU
1	k	159	ASN
2	K	130	ILE
1	l	47	ARG
2	L	98	CYS
2	L	145	LEU
1	m	134	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	M	73	ALA
2	M	127	ASN
2	M	130	ILE
1	n	44	THR
2	N	63	GLN
2	N	127	ASN
2	N	130	ILE
1	o	159	ASN
1	p	30	ILE
1	p	120	LYS
2	P	65	VAL
2	P	79	ASP
2	P	130	ILE
1	q	32	LYS
1	q	159	ASN
2	Q	127	ASN
2	Q	154	ASN
2	R	127	ASN
2	R	130	ILE
1	s	116	ASP
2	S	130	ILE
2	S	145	LEU
1	t	34	LEU
1	t	134	PRO
2	T	65	VAL
2	T	154	ASN
1	u	134	PRO
1	u	143	ALA
2	U	104	LEU
2	U	127	ASN
1	v	159	ASN
2	W	63	GLN
2	W	65	VAL
2	W	76	GLU
2	W	130	ILE
1	x	68	ALA
1	x	159	ASN
2	X	98	CYS
2	X	130	ILE
1	a	134	PRO
2	A	64	GLU
2	A	100	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	158	LEU
1	b	135	VAL
2	B	127	ASN
2	B	143	ASP
1	c	159	ASN
2	C	64	GLU
2	D	90	GLU
1	e	46	PRO
1	e	159	ASN
1	e	161	PRO
1	f	46	PRO
1	g	48	ASN
1	g	134	PRO
2	G	57	ASP
2	G	63	GLN
2	G	96	PRO
2	G	107	GLY
2	G	130	ILE
2	H	63	GLN
2	H	115	ALA
1	i	131	SER
1	i	135	VAL
2	I	62	PRO
2	I	97	ASP
2	I	100	PRO
2	I	154	ASN
1	j	114	THR
1	j	159	ASN
2	J	130	ILE
2	J	154	ASN
2	K	70	LEU
2	K	92	SER
2	K	94	ALA
2	K	147	GLY
2	K	169	ALA
1	l	46	PRO
1	l	55	LYS
1	l	137	LEU
2	L	73	ALA
1	m	159	ASN
1	n	161	PRO
2	N	115	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	145	LEU
2	O	130	ILE
1	p	121	ILE
1	p	134	PRO
1	p	159	ASN
2	P	81	LEU
1	q	114	THR
2	Q	92	SER
1	r	120	LYS
1	s	55	LYS
2	S	57	ASP
2	S	67	ASN
2	S	98	CYS
1	t	135	VAL
1	t	141	MET
2	T	130	ILE
2	U	98	CYS
2	U	101	ASP
2	U	107	GLY
2	U	130	ILE
2	V	90	GLU
2	V	114	PRO
2	W	61	VAL
2	W	75	GLU
1	x	134	PRO
1	x	138	HIS
2	X	97	ASP
2	A	130	ILE
2	B	63	GLN
2	B	94	ALA
2	B	130	ILE
2	C	96	PRO
2	C	115	ALA
2	C	145	LEU
2	D	100	PRO
2	D	135	PRO
2	E	70	LEU
2	E	72	LYS
2	E	130	ILE
1	f	66	ALA
2	F	62	PRO
2	G	113	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	h	137	LEU
2	H	130	ILE
1	j	134	PRO
1	l	129	GLU
1	l	161	PRO
1	m	138	HIS
2	M	64	GLU
2	M	66	LEU
2	P	96	PRO
2	Q	90	GLU
1	r	161	PRO
2	S	99	ILE
2	S	144	LEU
2	U	66	LEU
2	U	75	GLU
2	U	97	ASP
2	U	144	LEU
1	v	134	PRO
2	V	99	ILE
2	V	100	PRO
2	W	54	SER
2	W	154	ASN
1	a	121	ILE
2	A	101	ASP
1	c	99	ALA
1	c	134	PRO
2	C	99	ILE
2	C	154	ASN
2	D	61	VAL
2	D	99	ILE
2	D	136	LEU
2	E	154	ASN
2	F	101	ASP
1	g	161	PRO
1	h	134	PRO
1	h	161	PRO
2	H	89	GLU
2	H	137	SER
2	J	63	GLN
1	k	161	PRO
2	K	65	VAL
2	L	92	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	95	HIS
1	n	25	SER
1	o	114	THR
2	O	100	PRO
2	P	99	ILE
2	Q	130	ILE
1	r	134	PRO
1	s	46	PRO
2	S	100	PRO
1	u	131	SER
2	U	61	VAL
2	U	85	LEU
2	U	87	SER
1	v	46	PRO
1	v	132	LEU
2	V	63	GLN
2	W	94	ALA
1	x	120	LYS
2	X	106	HIS
2	A	65	VAL
2	A	126	PRO
2	A	154	ASN
1	c	32	LYS
2	C	63	GLN
2	D	96	PRO
2	D	137	SER
1	e	134	PRO
2	F	136	LEU
2	G	54	SER
2	G	158	LEU
1	l	138	HIS
1	l	139	CYS
1	q	30	ILE
1	q	59	VAL
2	S	61	VAL
2	S	62	PRO
2	S	96	PRO
2	W	53	GLU
2	X	89	GLU
1	d	46	PRO
1	g	46	PRO
2	K	61	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	r	133	PRO
2	U	134	SER
2	E	102	VAL
1	i	46	PRO
2	J	100	PRO
2	K	60	VAL
2	L	126	PRO
1	m	161	PRO
2	V	96	PRO
1	a	67	PRO
1	c	161	PRO
1	g	132	LEU
2	G	65	VAL
2	J	61	VAL
2	O	114	PRO
1	p	66	ALA
1	q	134	PRO
1	w	160	THR
2	D	139	PRO
1	p	132	LEU
2	R	100	PRO
2	B	61	VAL
2	G	61	VAL
1	i	133	PRO
1	k	135	VAL
2	L	96	PRO

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	a	121/121 (100%)	118 (98%)	3 (2%)	42	61
1	b	121/121 (100%)	117 (97%)	4 (3%)	33	52
1	c	121/121 (100%)	114 (94%)	7 (6%)	17	38
1	d	121/121 (100%)	118 (98%)	3 (2%)	42	61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	e	121/121 (100%)	117 (97%)	4 (3%)	33	52
1	f	121/121 (100%)	115 (95%)	6 (5%)	20	41
1	g	121/121 (100%)	119 (98%)	2 (2%)	56	72
1	h	121/121 (100%)	117 (97%)	4 (3%)	33	52
1	i	121/121 (100%)	115 (95%)	6 (5%)	20	41
1	j	121/121 (100%)	115 (95%)	6 (5%)	20	41
1	k	121/121 (100%)	118 (98%)	3 (2%)	42	61
1	l	121/121 (100%)	117 (97%)	4 (3%)	33	52
1	m	121/121 (100%)	117 (97%)	4 (3%)	33	52
1	n	121/121 (100%)	118 (98%)	3 (2%)	42	61
1	o	121/121 (100%)	117 (97%)	4 (3%)	33	52
1	p	121/121 (100%)	115 (95%)	6 (5%)	20	41
1	q	121/121 (100%)	117 (97%)	4 (3%)	33	52
1	r	121/121 (100%)	115 (95%)	6 (5%)	20	41
1	s	121/121 (100%)	117 (97%)	4 (3%)	33	52
1	t	121/121 (100%)	113 (93%)	8 (7%)	14	34
1	u	121/121 (100%)	116 (96%)	5 (4%)	26	47
1	v	121/121 (100%)	120 (99%)	1 (1%)	79	85
1	w	121/121 (100%)	114 (94%)	7 (6%)	17	38
1	x	121/121 (100%)	115 (95%)	6 (5%)	20	41
2	A	109/109 (100%)	101 (93%)	8 (7%)	11	31
2	B	109/109 (100%)	104 (95%)	5 (5%)	23	44
2	C	109/109 (100%)	104 (95%)	5 (5%)	23	44
2	D	109/109 (100%)	103 (94%)	6 (6%)	18	39
2	E	109/109 (100%)	104 (95%)	5 (5%)	23	44
2	F	109/109 (100%)	102 (94%)	7 (6%)	14	35
2	G	109/109 (100%)	103 (94%)	6 (6%)	18	39
2	H	109/109 (100%)	104 (95%)	5 (5%)	23	44
2	I	109/109 (100%)	106 (97%)	3 (3%)	38	57
2	J	109/109 (100%)	102 (94%)	7 (6%)	14	35
2	K	109/109 (100%)	100 (92%)	9 (8%)	9	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	109/109 (100%)	106 (97%)	3 (3%)	38	57
2	M	109/109 (100%)	105 (96%)	4 (4%)	29	49
2	N	109/109 (100%)	98 (90%)	11 (10%)	6	20
2	O	109/109 (100%)	104 (95%)	5 (5%)	23	44
2	P	109/109 (100%)	104 (95%)	5 (5%)	23	44
2	Q	109/109 (100%)	99 (91%)	10 (9%)	7	23
2	R	109/109 (100%)	106 (97%)	3 (3%)	38	57
2	S	109/109 (100%)	106 (97%)	3 (3%)	38	57
2	T	109/109 (100%)	102 (94%)	7 (6%)	14	35
2	U	109/109 (100%)	101 (93%)	8 (7%)	11	31
2	V	109/109 (100%)	104 (95%)	5 (5%)	23	44
2	W	109/109 (100%)	104 (95%)	5 (5%)	23	44
2	X	109/109 (100%)	106 (97%)	3 (3%)	38	57
All	All	5520/5520 (100%)	5272 (96%)	248 (4%)	26	45

All (248) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	45	HIS
1	a	90	LYS
1	a	144	GLU
2	A	64	GLU
2	A	89	GLU
2	A	99	ILE
2	A	113	ILE
2	A	126	PRO
2	A	128	LYS
2	A	157	LYS
2	A	158	LEU
1	b	75	LEU
1	b	90	LYS
1	b	106	MET
1	b	141	MET
2	B	64	GLU
2	B	75	GLU
2	B	93	GLU
2	B	95	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	157	LYS
1	c	32	LYS
1	c	90	LYS
1	c	123	ASN
1	c	132	LEU
1	c	136	LYS
1	c	141	MET
1	c	144	GLU
2	C	61	VAL
2	C	64	GLU
2	C	136	LEU
2	C	144	LEU
2	C	170	ILE
1	d	47	ARG
1	d	89	VAL
1	d	106	MET
2	D	53	GLU
2	D	75	GLU
2	D	76	GLU
2	D	93	GLU
2	D	95	HIS
2	D	157	LYS
1	e	71	ASP
1	e	81	ASP
1	e	141	MET
1	e	158	ARG
2	E	76	GLU
2	E	86	ASP
2	E	113	ILE
2	E	144	LEU
2	E	157	LYS
1	f	33	ARG
1	f	105	TYR
1	f	106	MET
1	f	136	LYS
1	f	141	MET
1	f	144	GLU
2	F	76	GLU
2	F	91	LEU
2	F	95	HIS
2	F	128	LYS
2	F	145	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	157	LYS
2	F	166	VAL
1	g	106	MET
1	g	144	GLU
2	G	64	GLU
2	G	76	GLU
2	G	131	TRP
2	G	152	LEU
2	G	157	LYS
2	G	158	LEU
1	h	30	ILE
1	h	90	LYS
1	h	132	LEU
1	h	141	MET
2	H	64	GLU
2	H	76	GLU
2	H	79	ASP
2	H	156	THR
2	H	157	LYS
1	i	38	LYS
1	i	106	MET
1	i	123	ASN
1	i	126	ILE
1	i	135	VAL
1	i	141	MET
2	I	76	GLU
2	I	134	SER
2	I	144	LEU
1	j	33	ARG
1	j	45	HIS
1	j	71	ASP
1	j	89	VAL
1	j	106	MET
1	j	135	VAL
2	J	64	GLU
2	J	72	LYS
2	J	76	GLU
2	J	79	ASP
2	J	89	GLU
2	J	131	TRP
2	J	157	LYS
1	k	47	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	k	105	TYR
1	k	141	MET
2	K	84	LEU
2	K	88	LEU
2	K	90	GLU
2	K	113	ILE
2	K	128	LYS
2	K	131	TRP
2	K	144	LEU
2	K	156	THR
2	K	157	LYS
1	l	52	LEU
1	l	58	ASN
1	l	141	MET
1	l	144	GLU
2	L	93	GLU
2	L	125	PRO
2	L	157	LYS
1	m	47	ARG
1	m	89	VAL
1	m	106	MET
1	m	136	LYS
2	M	64	GLU
2	M	76	GLU
2	M	154	ASN
2	M	157	LYS
1	n	56	LEU
1	n	106	MET
1	n	141	MET
2	N	57	ASP
2	N	64	GLU
2	N	75	GLU
2	N	76	GLU
2	N	85	LEU
2	N	88	LEU
2	N	93	GLU
2	N	144	LEU
2	N	154	ASN
2	N	157	LYS
2	N	172	LYS
1	o	106	MET
1	o	136	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	o	141	MET
1	o	144	GLU
2	O	80	TYR
2	O	95	HIS
2	O	104	LEU
2	O	137	SER
2	O	157	LYS
1	p	26	HIS
1	p	45	HIS
1	p	89	VAL
1	p	90	LYS
1	p	106	MET
1	p	148	LYS
2	P	76	GLU
2	P	95	HIS
2	P	102	VAL
2	P	128	LYS
2	P	172	LYS
1	q	53	ASP
1	q	89	VAL
1	q	106	MET
1	q	141	MET
2	Q	60	VAL
2	Q	61	VAL
2	Q	72	LYS
2	Q	93	GLU
2	Q	116	PHE
2	Q	125	PRO
2	Q	141	ARG
2	Q	144	LEU
2	Q	157	LYS
2	Q	158	LEU
1	r	27	MET
1	r	33	ARG
1	r	52	LEU
1	r	121	ILE
1	r	141	MET
1	r	144	GLU
2	R	67	ASN
2	R	79	ASP
2	R	95	HIS
1	s	26	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	s	56	LEU
1	s	90	LYS
1	s	106	MET
2	S	76	GLU
2	S	145	LEU
2	S	172	LYS
1	t	34	LEU
1	t	45	HIS
1	t	52	LEU
1	t	90	LYS
1	t	135	VAL
1	t	136	LYS
1	t	137	LEU
1	t	141	MET
2	T	61	VAL
2	T	64	GLU
2	T	76	GLU
2	T	113	ILE
2	T	142	PHE
2	T	153	ARG
2	T	157	LYS
1	u	33	ARG
1	u	47	ARG
1	u	106	MET
1	u	141	MET
1	u	144	GLU
2	U	64	GLU
2	U	65	VAL
2	U	91	LEU
2	U	95	HIS
2	U	99	ILE
2	U	153	ARG
2	U	154	ASN
2	U	157	LYS
1	v	106	MET
2	V	59	GLN
2	V	95	HIS
2	V	142	PHE
2	V	157	LYS
2	V	158	LEU
1	w	30	ILE
1	w	47	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	w	52	LEU
1	w	90	LYS
1	w	106	MET
1	w	139	CYS
1	w	141	MET
2	W	64	GLU
2	W	108	VAL
2	W	128	LYS
2	W	157	LYS
2	W	158	LEU
1	x	47	ARG
1	x	106	MET
1	x	121	ILE
1	x	138	HIS
1	x	141	MET
1	x	144	GLU
2	X	114	PRO
2	X	144	LEU
2	X	157	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	138	HIS
2	A	59	GLN
2	A	140	ASN
1	b	26	HIS
1	b	42	HIS
2	B	95	HIS
2	B	124	GLN
2	B	146	ASN
2	C	83	HIS
1	d	26	HIS
2	D	59	GLN
2	D	140	ASN
1	e	45	HIS
1	e	111	GLN
1	f	123	ASN
2	F	95	HIS
2	F	106	HIS
1	g	36	HIS
1	g	42	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	g	48	ASN
1	g	138	HIS
1	h	42	HIS
2	H	95	HIS
1	i	26	HIS
1	i	42	HIS
2	I	95	HIS
2	J	74	HIS
1	l	45	HIS
1	l	111	GLN
1	l	138	HIS
2	L	74	HIS
1	m	45	HIS
1	m	111	GLN
2	M	59	GLN
2	M	63	GLN
2	M	95	HIS
2	M	106	HIS
1	n	42	HIS
2	N	95	HIS
1	o	45	HIS
2	O	95	HIS
1	q	42	HIS
2	Q	95	HIS
1	r	26	HIS
1	r	138	HIS
2	R	106	HIS
2	S	83	HIS
2	T	95	HIS
1	u	123	ASN
1	u	138	HIS
1	v	45	HIS
1	v	159	ASN
2	V	63	GLN
2	V	74	HIS
2	V	83	HIS
2	V	95	HIS
2	V	154	ASN
1	w	111	GLN
1	w	159	ASN
2	X	63	GLN

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-8341. 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: 144

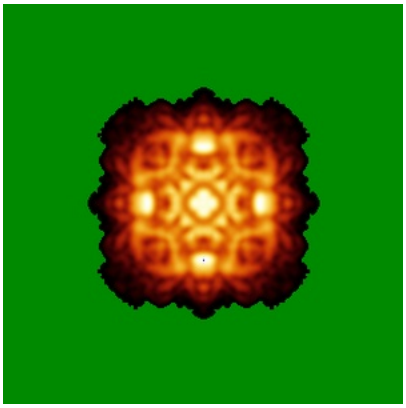
Y Index: 144

Z Index: 144

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

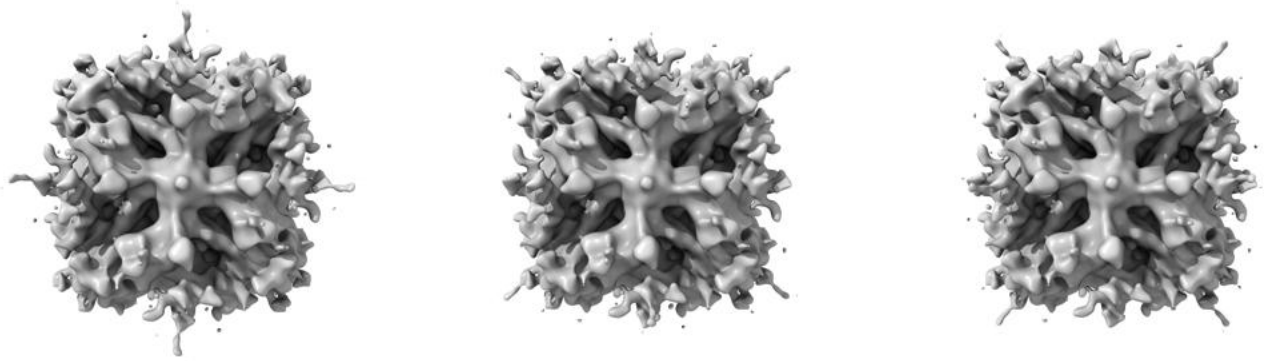
Y

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



X Y Z

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.

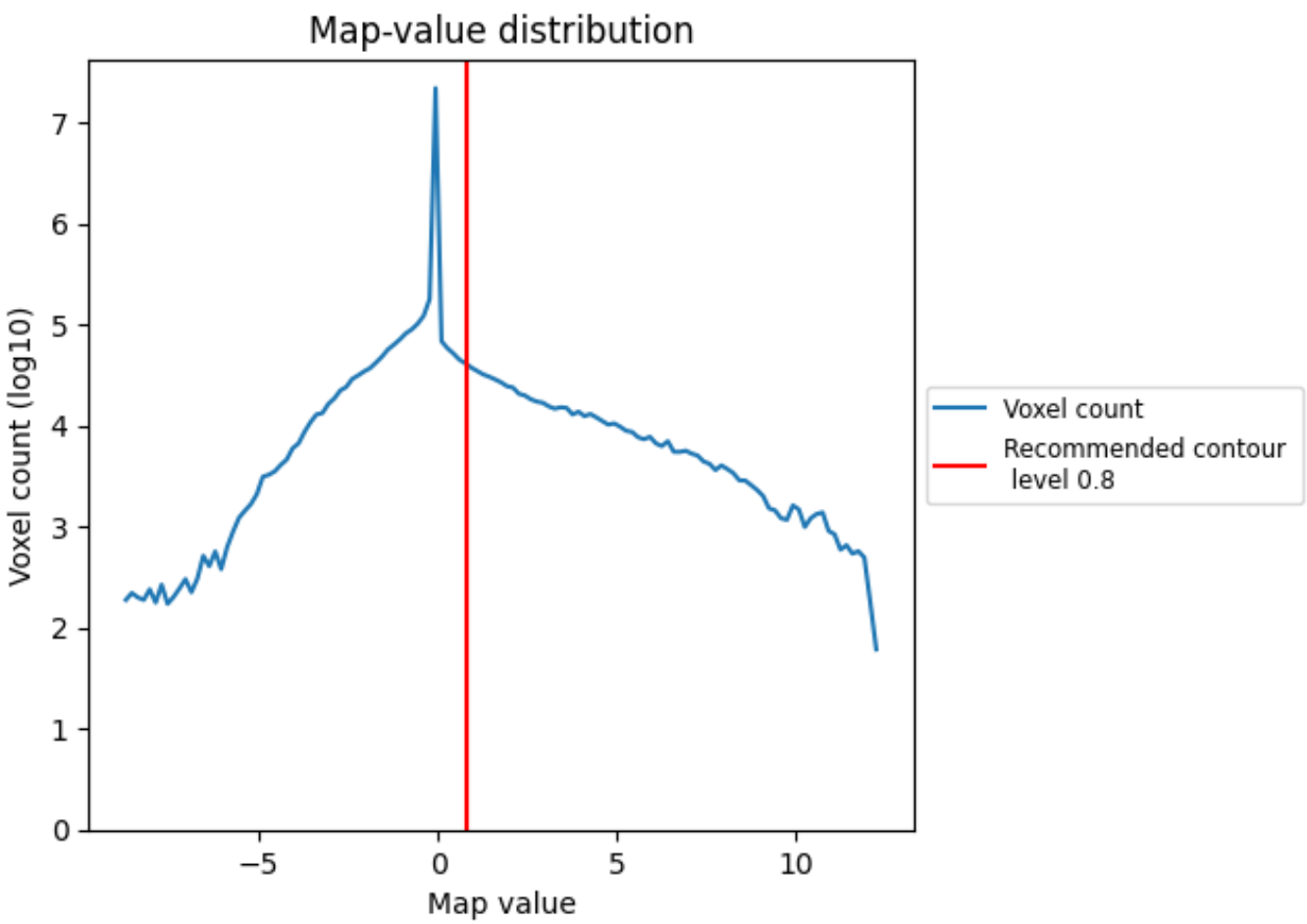
6.6 Mask visualisation (i)

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

7 Map analysis (i)

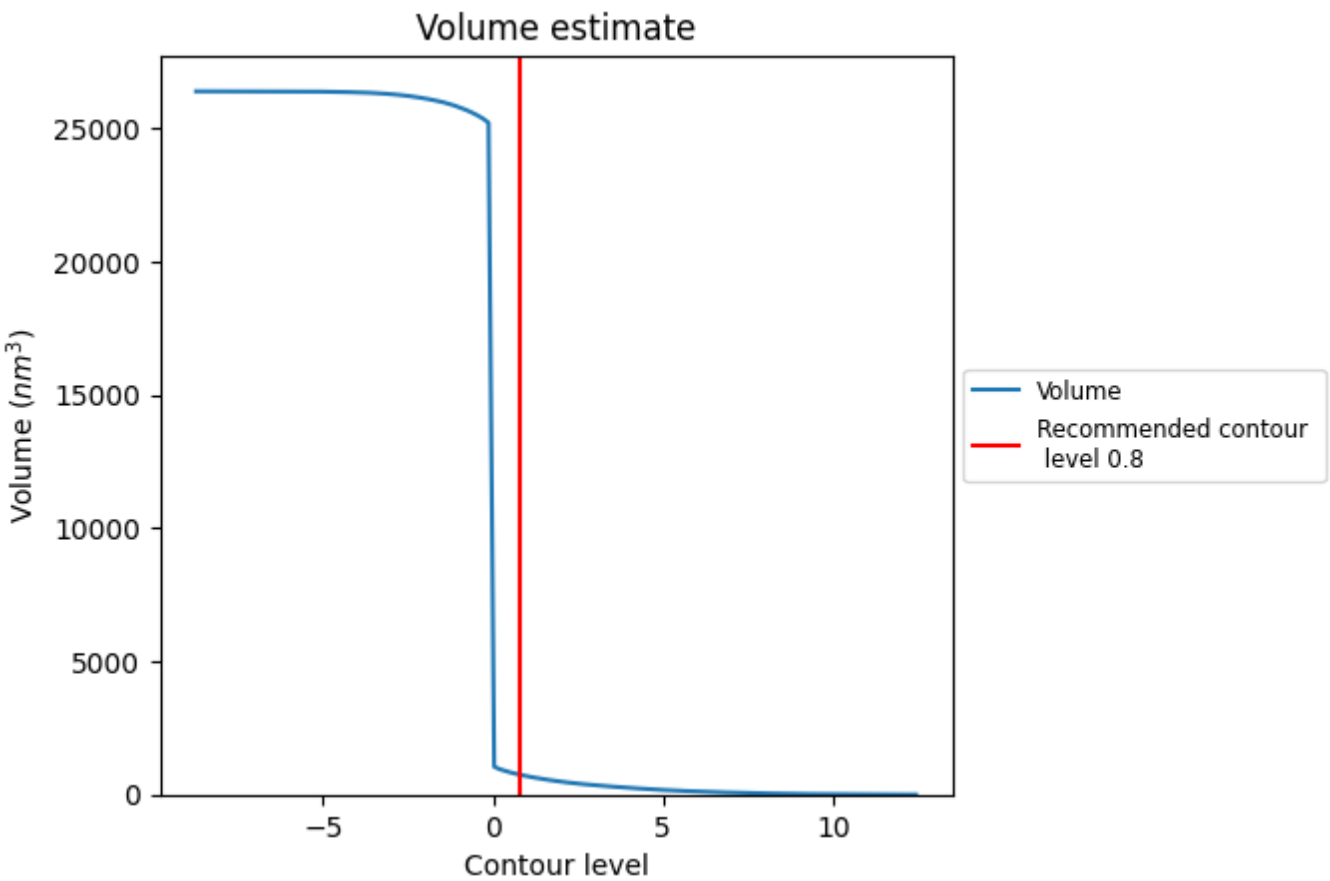
This section contains the results of statistical analysis of the map.

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.

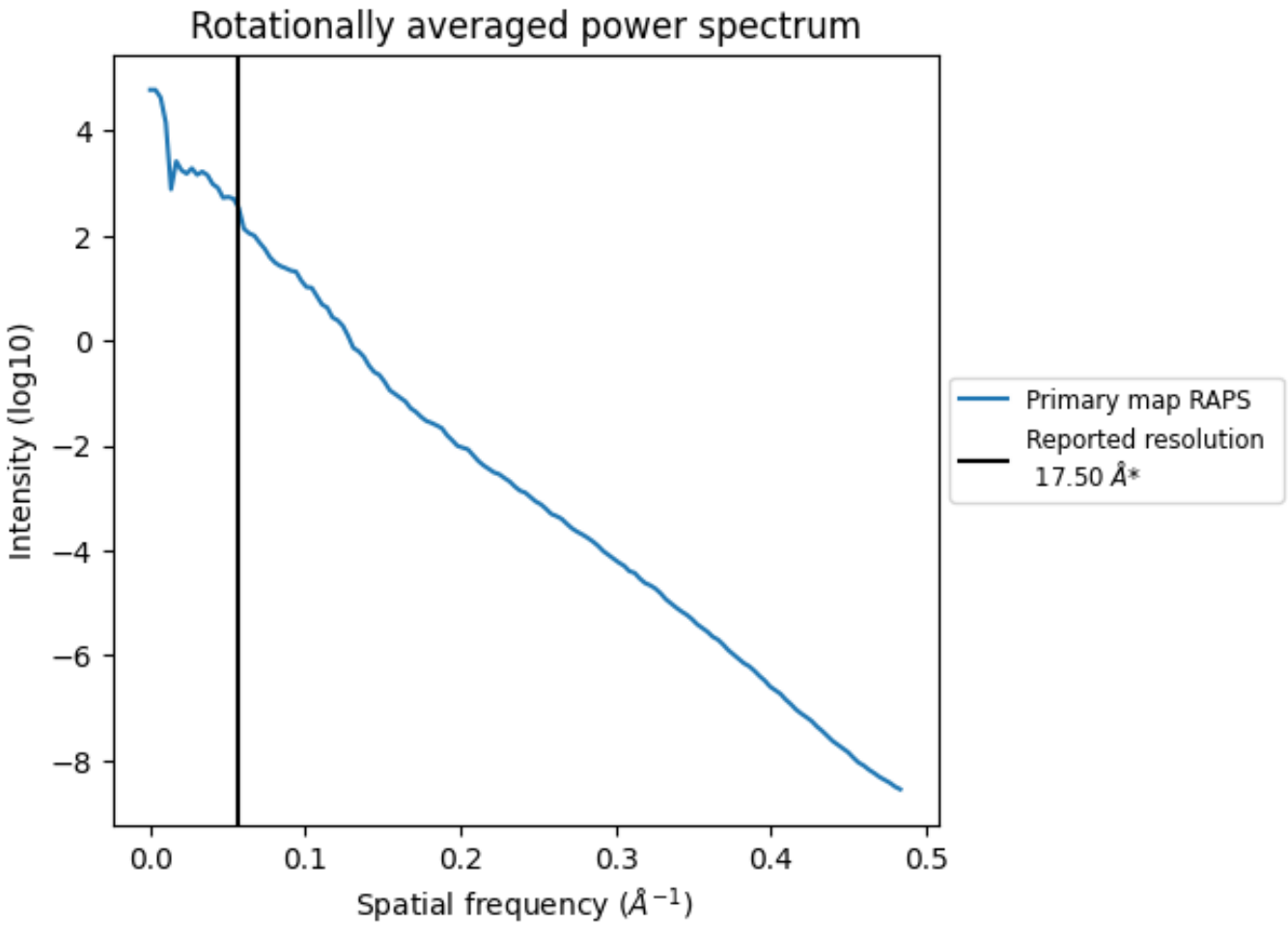
7.2 Volume estimate (i)



The volume at the recommended contour level is 743 nm^3; this corresponds to an approximate mass of 672 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)

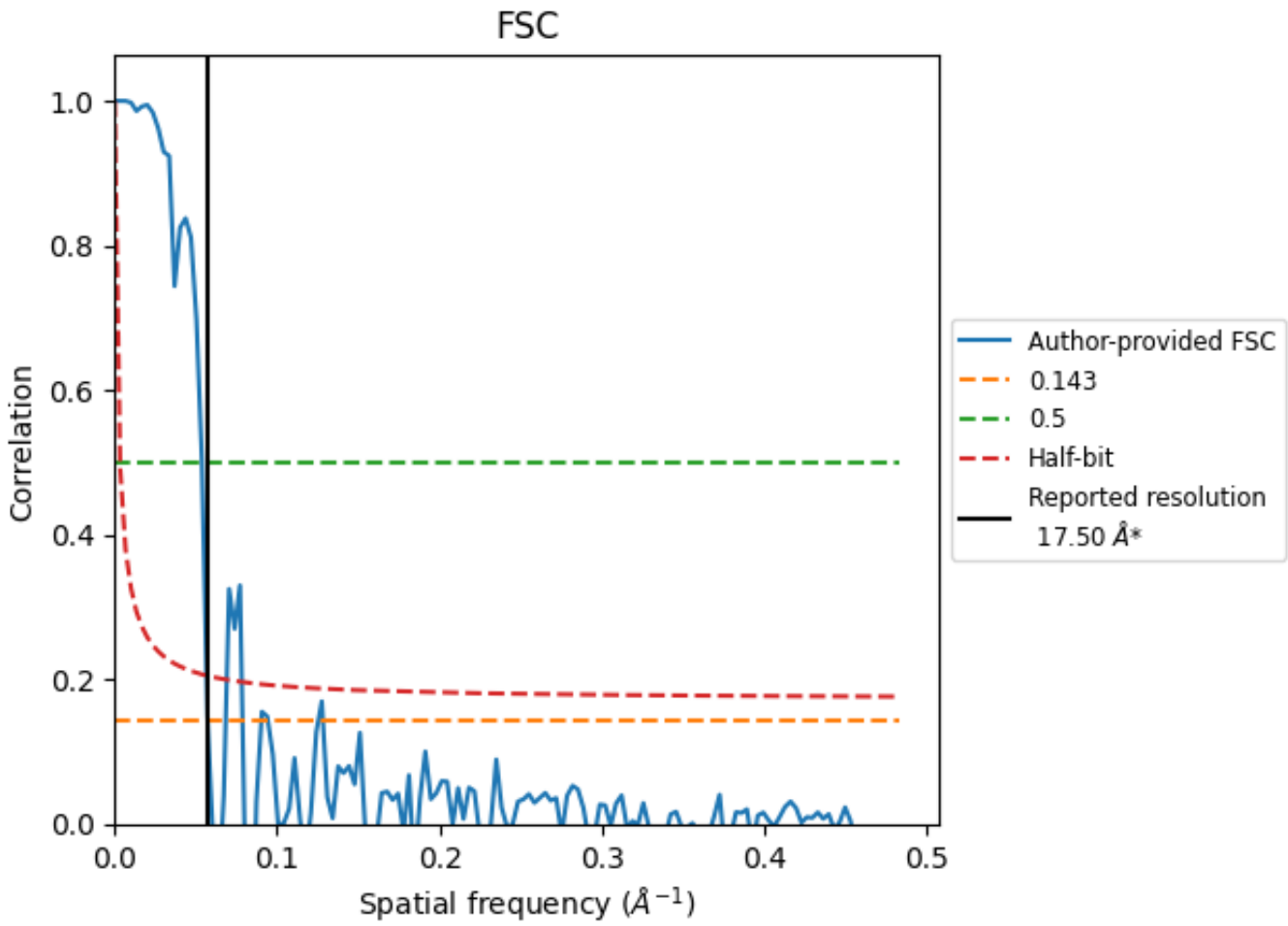


*Reported resolution corresponds to spatial frequency of 0.057 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.057 Å^{-1}

8.2 Resolution estimates (i)

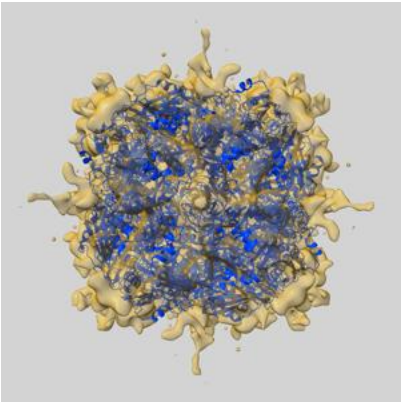
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	17.50	-	-
Author-provided FSC curve	17.45	18.59	17.67
Unmasked-calculated*	-	-	-

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

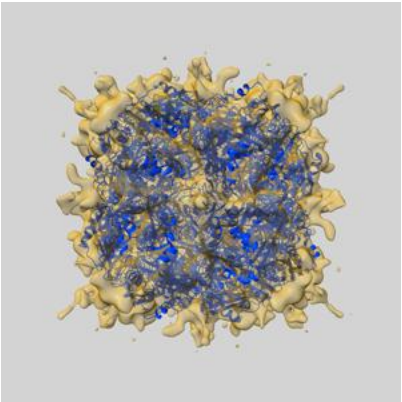
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8341 and PDB model 5T0V. Per-residue inclusion information can be found in section 3 on page 11.

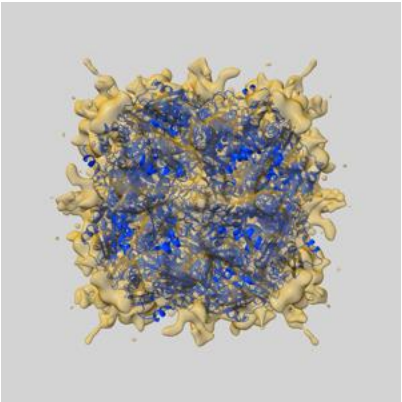
9.1 Map-model overlay (i)



X



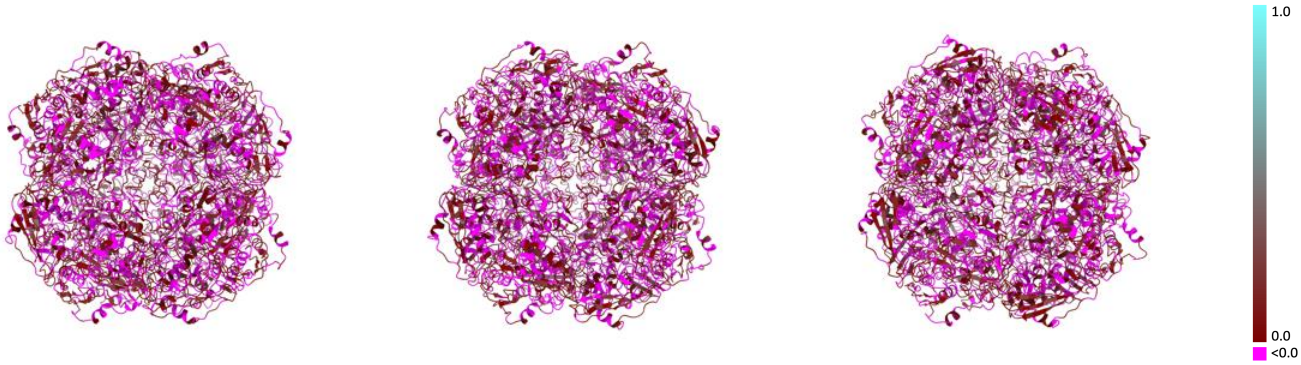
Y



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.

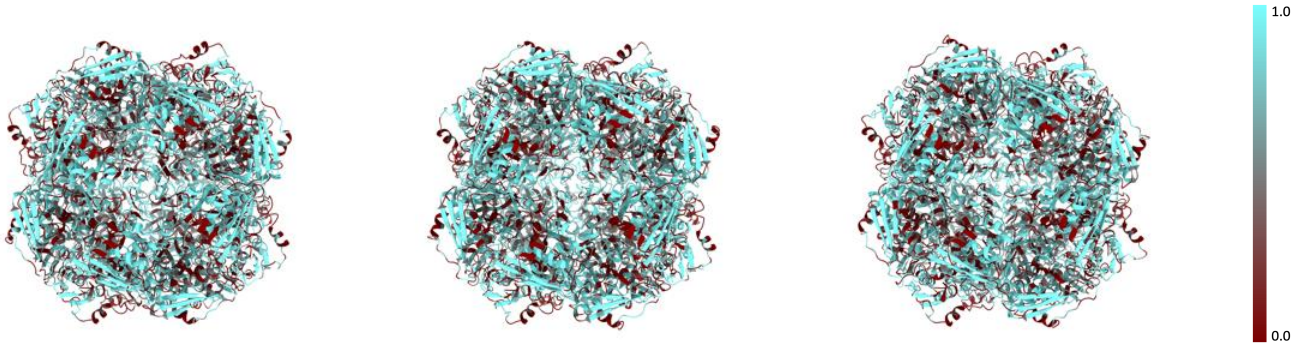
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

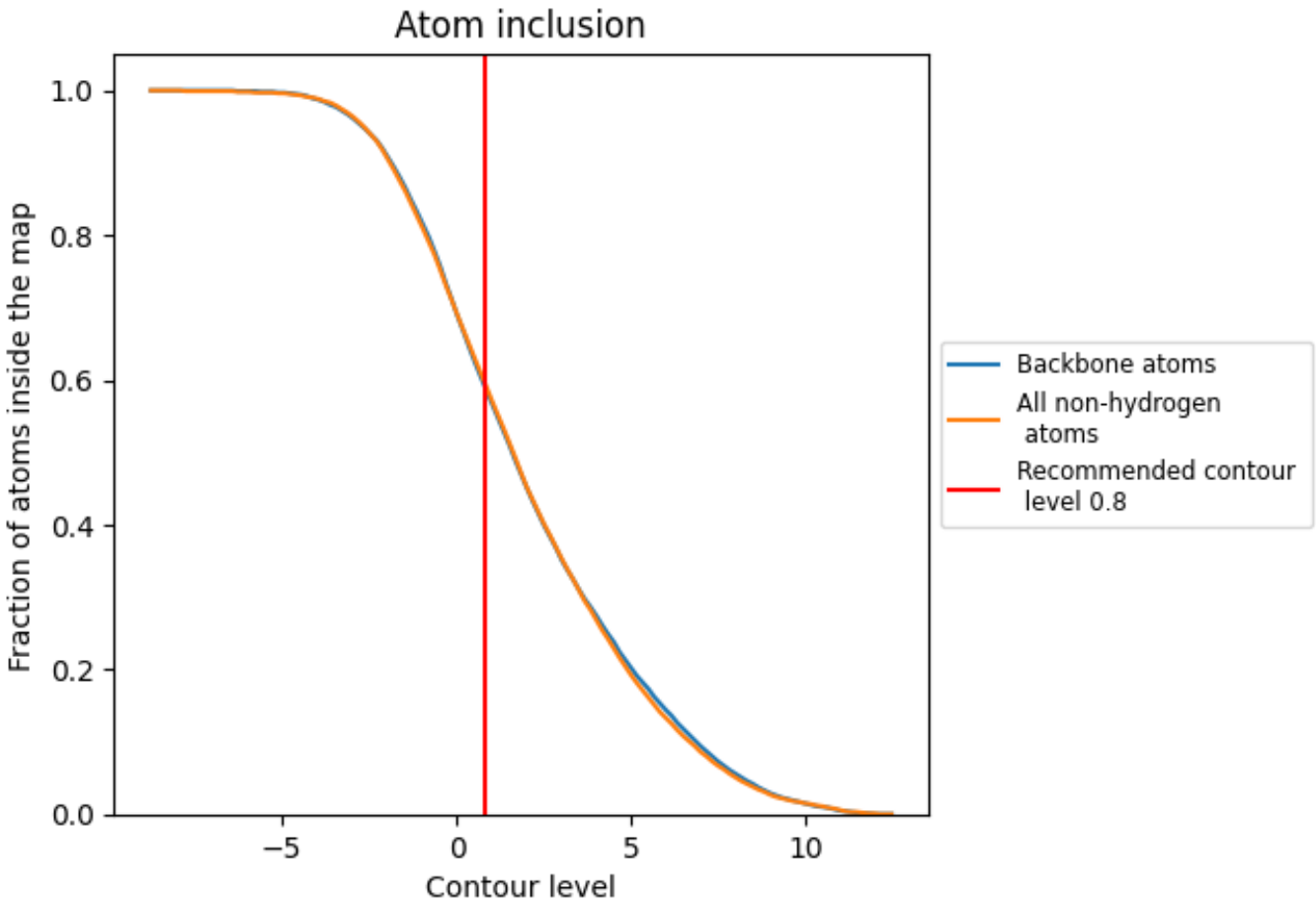
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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, 59% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.5980	0.0120
A	0.6230	0.0110
B	0.6420	0.0250
C	0.6450	0.0120
D	0.6090	0.0150
E	0.6460	0.0350
F	0.6220	0.0160
G	0.6290	0.0120
H	0.6410	0.0280
I	0.6390	0.0150
J	0.6180	0.0110
K	0.6580	0.0430
L	0.6400	0.0260
M	0.6120	0.0080
N	0.6450	0.0180
O	0.6230	0.0050
P	0.6150	0.0140
Q	0.6380	0.0280
R	0.6360	0.0140
S	0.6060	0.0030
T	0.6460	0.0260
U	0.6090	0.0080
V	0.6330	0.0190
W	0.6500	0.0260
X	0.6460	0.0160
a	0.5660	0.0070
b	0.5700	0.0090
c	0.5750	0.0060
d	0.5800	0.0150
e	0.5570	0.0010
f	0.5730	0.0010
g	0.5740	0.0120
h	0.5540	0.0110
i	0.5540	0.0070
j	0.5620	0.0110

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	0.5500	0.0110
l	0.5710	0.0030
m	0.5470	-0.0050
n	0.5680	0.0070
o	0.5760	-0.0020
p	0.5840	0.0110
q	0.5480	-0.0020
r	0.5860	0.0120
s	0.5630	0.0140
t	0.5660	0.0170
u	0.5730	0.0090
v	0.5780	0.0050
w	0.5540	0.0070
x	0.5760	0.0110