



wwPDB EM Map/Model Validation Report ⓘ

Aug 23, 2016 – 03:12 PM 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 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

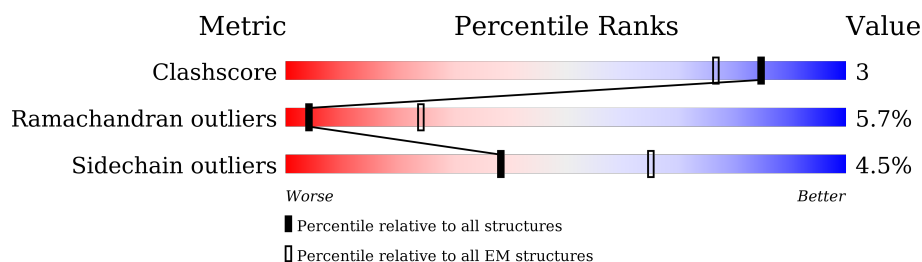
1 Overall quality at a glance

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.






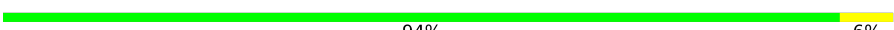






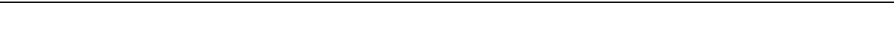

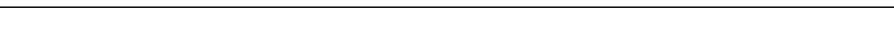
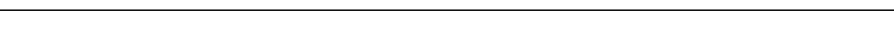
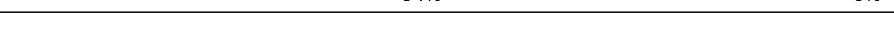
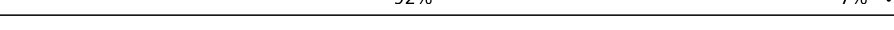









Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 $\leq 5\%$.

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

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Mol	Chain	Length	Quality of chain
1	j	142	 92% 8%
1	k	142	 90% 8% .
1	l	142	 89% 11%
1	m	142	 94% 6%
1	n	142	 93% 6% .
1	o	142	 94% 6%
1	p	142	 88% 12%
1	q	142	 91% 9%
1	r	142	 91% 8% .
1	s	142	 94% 6%
1	t	142	 91% 6% .
1	u	142	 94% 6%
1	v	142	 94% 6%
1	w	142	 94% 6%
1	x	142	 92% 7% .
2	A	121	 81% 15% .
2	B	121	 87% 12% .
2	C	121	 83% 14% .
2	D	121	 80% 18% .
2	E	121	 83% 13% .
2	F	121	 85% 14% .
2	G	121	 80% 17% .
2	H	121	 81% 16% .
2	I	121	 88% 12%
2	J	121	 81% 17% ..

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Mol	Chain	Length	Quality of chain
2	K	121	 79% 20% .
2	L	121	 84% 15% .
2	M	121	 87% 10% .
2	N	121	 76% 21% .
2	O	121	 88% 11% .
2	P	121	 83% 17%
2	Q	121	 85% 12% .
2	R	121	 88% 11% .
2	S	121	 85% 11% . .
2	T	121	 86% 12% .
2	U	121	 77% 19% .
2	V	121	 84% 13% .
2	W	121	 79% 19% .
2	X	121	 90% 8% .

2 Entry composition

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

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

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

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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

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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
2	A	121	Total	C	N	O	S	0	0
			947	597	153	195	2		
2	B	121	Total	C	N	O	S	0	0
			947	597	153	195	2		
2	C	121	Total	C	N	O	S	0	0
			947	597	153	195	2		
2	D	121	Total	C	N	O	S	0	0
			947	597	153	195	2		
2	E	121	Total	C	N	O	S	0	0
			947	597	153	195	2		

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

There are 24 discrepancies between the modelled and reference sequences:

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

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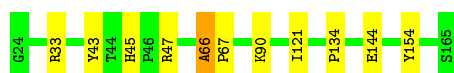
Chain	Residue	Modelled	Actual	Comment	Reference
B	73	ALA	TYR	conflict	UNP Q07540
C	73	ALA	TYR	conflict	UNP Q07540
D	73	ALA	TYR	conflict	UNP Q07540
E	73	ALA	TYR	conflict	UNP Q07540
F	73	ALA	TYR	conflict	UNP Q07540
G	73	ALA	TYR	conflict	UNP Q07540
H	73	ALA	TYR	conflict	UNP Q07540
I	73	ALA	TYR	conflict	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 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: Iron sulfur cluster assembly protein 1, mitochondrial

Chain a:  92% 7% .




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

Chain b:  92% 7% .



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

Chain c:  90% 9% .



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

Chain d:  97% .



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

Chain e:  91% 8% .



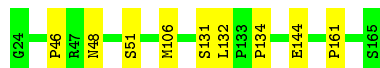
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain f:  93% 6% .



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

Chain g: 94% 6%



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

Chain h: 92% 8%



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

Chain i: 92% 8%



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

Chain j: 92% 8%



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

Chain k: 90% 8%



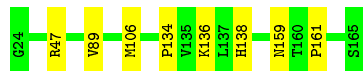
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain l: 89% 11%



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

Chain m: 94% 6%



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

Chain n:  93% 6%




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

Chain o:  94% 6%




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

Chain p:  88% 12%




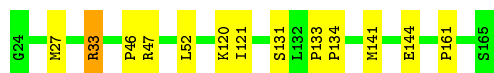
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain q:  91% 9%



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

Chain r:  91% 8%




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

Chain s:  94% 6%



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

Chain t:  91% 6%



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

Chain u:  94% 6%



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

Chain v:  94% 6%



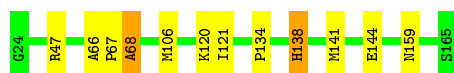
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain w:  94% 6%




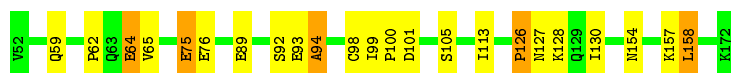
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain x:  92% 7% .



- Molecule 2: Frataxin homolog, mitochondrial

Chain A:  81% 15% .




- Molecule 2: Frataxin homolog, mitochondrial

Chain B:  87% 12% .




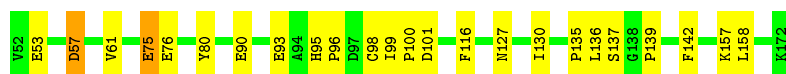
- Molecule 2: Frataxin homolog, mitochondrial

Chain C:  83% 14% .



- Molecule 2: Frataxin homolog, mitochondrial

Chain D:  80% 18% .



- Molecule 2: Frataxin homolog, mitochondrial

Chain E: 83% 13% .



- Molecule 2: Frataxin homolog, mitochondrial

Chain F: 85% 14% .



- Molecule 2: Frataxin homolog, mitochondrial

Chain G: 80% 17% .



- Molecule 2: Frataxin homolog, mitochondrial

Chain H: 81% 16% .



- Molecule 2: Frataxin homolog, mitochondrial

Chain I: 88% 12% .



- Molecule 2: Frataxin homolog, mitochondrial

Chain J: 81% 17% ..

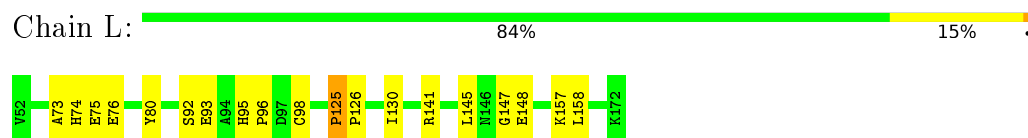


- Molecule 2: Frataxin homolog, mitochondrial

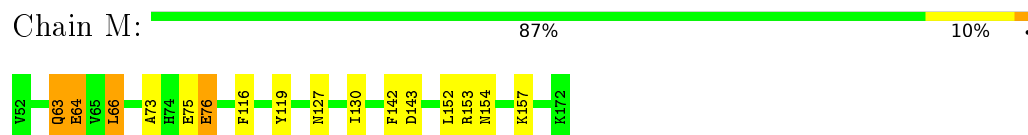
Chain K: 79% 20% .



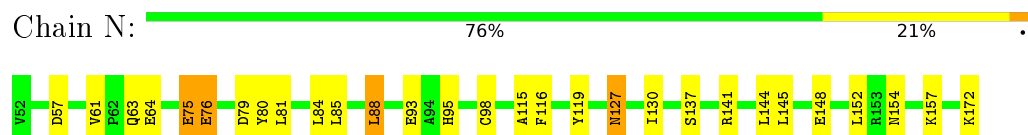
- Molecule 2: Frataxin homolog, mitochondrial



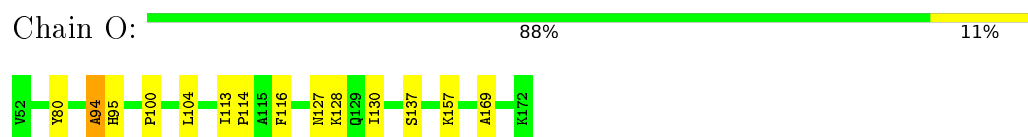
- Molecule 2: Frataxin homolog, mitochondrial



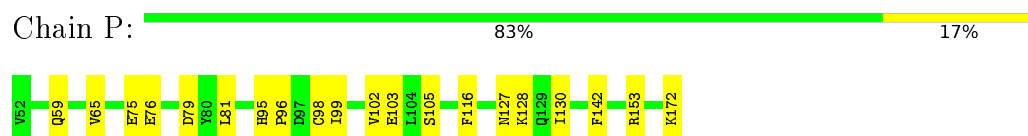
- Molecule 2: Frataxin homolog, mitochondrial



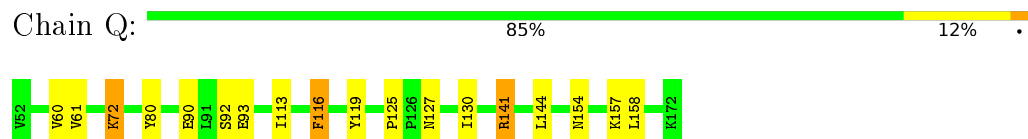
- Molecule 2: Frataxin homolog, mitochondrial



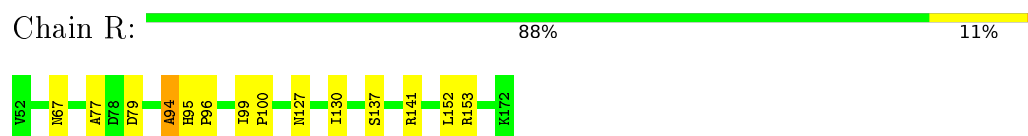
- Molecule 2: Frataxin homolog, mitochondrial




- Molecule 2: Frataxin homolog, mitochondrial

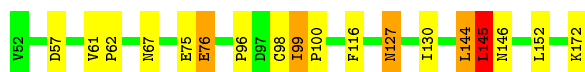


- Molecule 2: Frataxin homolog, mitochondrial




- Molecule 2: Frataxin homolog, mitochondrial

Chain S:  85% 11% . .




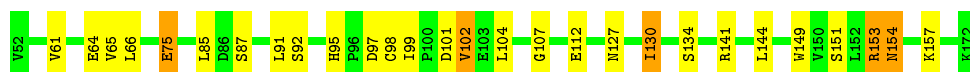
- Molecule 2: Frataxin homolog, mitochondrial

Chain T:  86% 12% .




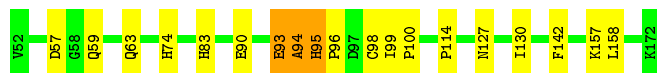
- Molecule 2: Frataxin homolog, mitochondrial

Chain U:  77% 19% .




- Molecule 2: Frataxin homolog, mitochondrial

Chain V:  84% 13% .




- Molecule 2: Frataxin homolog, mitochondrial

Chain W:  79% 19% .



- Molecule 2: Frataxin homolog, mitochondrial

Chain X:  90% 8% .



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	4153	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 ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	210	Depositor
Maximum defocus (nm)	2800	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	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 >2	RMSZ	# Z >2
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(°)	Ideal(°)
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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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

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	a	1072	0	1106	0	0
1	b	1072	0	1108	0	0
1	c	1072	0	1108	0	0
1	d	1072	0	1108	0	0
1	e	1072	0	1108	0	0
1	f	1072	0	1108	0	0
1	g	1072	0	1108	0	0
1	h	1072	0	1108	0	0
1	i	1072	0	1106	0	0
1	j	1072	0	1108	0	0
1	k	1072	0	1106	0	0
1	l	1072	0	1108	0	0
1	m	1072	0	1108	0	0
1	n	1072	0	1106	0	0
1	o	1072	0	1108	0	0
1	p	1072	0	1108	0	0
1	q	1072	0	1108	0	0
1	r	1072	0	1105	0	0
1	s	1072	0	1106	0	0
1	t	1072	0	1108	0	0
1	u	1072	0	1108	0	0
1	v	1072	0	1108	0	0
1	w	1072	0	1106	0	0
1	x	1072	0	1108	0	0
2	A	947	0	921	2	0
2	B	947	0	921	2	0
2	C	947	0	921	4	0
2	D	947	0	921	1	0
2	E	947	0	921	3	0
2	F	947	0	921	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	947	0	921	2	0
2	H	947	0	921	3	0
2	I	947	0	921	1	0
2	J	947	0	921	3	0
2	K	947	0	921	2	0
2	L	947	0	920	19	0
2	M	947	0	921	5	0
2	N	947	0	920	26	0
2	O	947	0	920	17	0
2	P	947	0	921	2	0
2	Q	947	0	921	1	0
2	R	947	0	921	2	0
2	S	947	0	921	6	0
2	T	947	0	921	2	0
2	U	947	0	921	6	0
2	V	947	0	921	3	0
2	W	947	0	920	13	0
2	X	947	0	921	1	0
All	All	48456	0	48677	118	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 3.

All (118) 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:O:113:ILE:CG2	2:O:116:PHE:CD2	2.12	1.31
2:L:76:GLU:O	2:L:80:TYR:CD1	1.86	1.29
2:O:113:ILE:HG22	2:O:116:PHE:CD2	1.68	1.27
2:N:75:GLU:CD	2:N:80:TYR:CD2	2.17	1.18
2:O:113:ILE:HG21	2:O:116:PHE:CD2	1.82	1.15
2:N:80:TYR:HE1	2:N:148:GLU:CG	1.61	1.11
2:N:75:GLU:CD	2:N:80:TYR:HD2	1.48	1.10
2:O:116:PHE:HB3	2:O:128:LYS:NZ	24.18	1.10
2:W:80:TYR:CE1	2:W:148:GLU:HA	1.81	1.09
2:N:75:GLU:OE1	2:N:80:TYR:CD2	2.06	1.08
2:L:76:GLU:O	2:L:80:TYR:CE1	2.10	1.05
2:N:80:TYR:HE1	2:N:148:GLU:HG3	1.21	1.04
2:O:116:PHE:HB3	2:O:128:LYS:HZ3	23.66	1.02
2:O:113:ILE:HG22	2:O:116:PHE:HD2	0.99	1.02
2:W:80:TYR:HE1	2:W:148:GLU:HA	1.18	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:80:TYR:CE1	2:N:148:GLU:HG3	1.99	0.97
2:N:80:TYR:CE1	2:N:148:GLU:HA	1.99	0.97
2:W:76:GLU:HA	2:W:80:TYR:HE2	1.26	0.96
2:W:76:GLU:HA	2:W:80:TYR:CE2	2.01	0.95
2:L:76:GLU:O	2:L:80:TYR:HD1	1.30	0.95
2:O:116:PHE:O	2:O:128:LYS:HD2	25.94	0.93
2:L:80:TYR:HE2	2:L:148:GLU:HG3	1.35	0.90
2:N:75:GLU:OE1	2:N:80:TYR:CE2	2.27	0.87
2:N:80:TYR:CE1	2:N:148:GLU:CG	2.54	0.86
2:N:75:GLU:CD	2:N:80:TYR:CE2	2.55	0.80
2:N:75:GLU:OE2	2:N:80:TYR:HD2	1.65	0.80
2:L:80:TYR:CE2	2:L:148:GLU:HG3	2.18	0.76
2:L:75:GLU:H	2:L:76:GLU:HA	1.54	0.73
2:C:75:GLU:H	2:C:76:GLU:HA	1.53	0.72
2:L:80:TYR:OH	2:L:147:GLY:HA3	1.90	0.72
2:N:75:GLU:OE1	2:N:80:TYR:HD2	1.53	0.71
2:L:80:TYR:OH	2:L:147:GLY:CA	2.16	0.71
2:O:116:PHE:HB3	2:O:128:LYS:HZ2	24.64	0.69
2:N:80:TYR:CE1	2:N:148:GLU:CA	2.75	0.69
2:O:116:PHE:CZ	2:O:169:ALA:HA	2.30	0.67
2:N:80:TYR:CZ	2:N:148:GLU:HA	2.29	0.67
2:O:113:ILE:CG2	2:O:116:PHE:CE2	2.76	0.67
2:L:80:TYR:CE2	2:L:148:GLU:HA	2.30	0.67
2:L:80:TYR:HE2	2:L:148:GLU:CG	2.07	0.67
2:O:113:ILE:CG2	2:O:116:PHE:HD2	1.71	0.66
2:W:80:TYR:O	2:W:84:LEU:HB3	1.99	0.62
2:N:80:TYR:HE1	2:N:148:GLU:CB	2.12	0.61
2:O:113:ILE:HG21	2:O:116:PHE:CG	2.36	0.60
2:M:75:GLU:H	2:M:76:GLU:HA	1.66	0.60
2:C:144:LEU:HD12	2:C:144:LEU:H	1.67	0.59
2:N:80:TYR:CE1	2:N:148:GLU:CB	2.85	0.59
2:O:116:PHE:HZ	2:O:169:ALA:HA	1.69	0.58
2:L:74:HIS:HD2	2:L:80:TYR:OH	1.89	0.56
2:O:113:ILE:HB	2:O:116:PHE:HB2	1.87	0.56
2:N:75:GLU:CG	2:N:80:TYR:CE2	2.90	0.55
2:N:75:GLU:OE2	2:N:80:TYR:CD2	2.49	0.55
2:U:92:SER:HB3	2:U:102:VAL:HG12	1.90	0.54
2:W:76:GLU:CA	2:W:80:TYR:CE2	2.84	0.53
2:N:75:GLU:HB3	2:N:79:ASP:H	1.74	0.53
2:M:153:ARG:HD2	2:N:80:TYR:CE2	2.43	0.53
2:L:76:GLU:H	2:L:76:GLU:CD	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:80:TYR:CE1	2:W:148:GLU:CA	2.75	0.52
2:J:158:LEU:HD23	2:J:158:LEU:H	1.75	0.51
2:L:76:GLU:O	2:L:80:TYR:HE1	1.82	0.51
2:S:144:LEU:H	2:S:144:LEU:HD12	1.75	0.51
2:C:70:LEU:HG	2:C:71:GLU:H	1.75	0.50
2:N:141:ARG:HB2	2:N:152:LEU:HD12	1.93	0.50
2:W:104:LEU:H	2:W:104:LEU:HD23	1.77	0.50
2:W:61:VAL:H	2:W:62:PRO:HD3	1.76	0.49
2:M:63:GLN:HE22	2:M:66:LEU:HD22	1.78	0.49
2:M:143:ASP:HB3	2:M:152:LEU:HD11	1.95	0.48
2:W:80:TYR:CE2	2:W:147:GLY:O	2.38	0.48
2:L:74:HIS:CD2	2:L:80:TYR:OH	2.67	0.48
2:J:93:GLU:HB3	2:V:94:ALA:HB3	1.96	0.47
2:A:105:SER:HA	2:E:105:SER:HB3	1.97	0.47
2:B:95:HIS:CD2	2:B:98:CYS:HB2	2.49	0.47
2:L:80:TYR:CE2	2:L:148:GLU:CA	2.96	0.46
2:S:145:LEU:HD22	2:U:151:SER:HB3	1.95	0.46
2:O:116:PHE:CB	2:O:128:LYS:NZ	24.89	0.46
2:O:116:PHE:CB	2:O:128:LYS:HZ2	25.36	0.46
2:R:141:ARG:HE	2:R:152:LEU:HD12	1.81	0.45
2:T:110:THR:HG22	2:T:121:ILE:H	1.80	0.45
2:W:76:GLU:O	2:W:80:TYR:CD2	2.70	0.45
2:G:113:ILE:H	2:G:114:PRO:HD3	1.82	0.45
2:R:96:PRO:HG2	2:R:99:ILE:H	1.82	0.45
2:U:102:VAL:HG23	2:U:112:GLU:H	1.82	0.45
2:W:80:TYR:O	2:W:84:LEU:CB	2.63	0.45
2:F:75:GLU:HB3	2:F:80:TYR:H	1.81	0.45
2:S:99:ILE:H	2:X:89:GLU:HG2	1.82	0.44
2:V:74:HIS:CE1	2:V:83:HIS:CD2	3.06	0.44
2:K:88:LEU:HB2	2:K:166:VAL:HB	2.00	0.44
2:S:152:LEU:HD21	2:U:153:ARG:HH21	1.83	0.44
2:W:61:VAL:H	2:W:62:PRO:CD	2.30	0.43
2:H:92:SER:HA	2:H:102:VAL:H	1.83	0.43
2:D:158:LEU:HD23	2:D:158:LEU:H	1.84	0.43
2:J:92:SER:O	2:J:99:ILE:HD13	2.19	0.43
2:S:75:GLU:N	2:S:76:GLU:HA	2.34	0.43
2:P:103:GLU:HG3	2:P:105:SER:H	1.85	0.42
2:K:113:ILE:HD12	2:K:116:PHE:HB2	2.01	0.42
2:L:80:TYR:CE2	2:L:148:GLU:CG	2.92	0.42
2:L:80:TYR:OH	2:L:148:GLU:OE1	2.37	0.42
2:E:75:GLU:N	2:E:76:GLU:HA	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:77:ALA:HA	2:I:80:TYR:CD2	2.54	0.42
2:G:99:ILE:HD12	2:G:99:ILE:HA	2.01	0.42
2:T:75:GLU:N	2:T:76:GLU:HA	2.35	0.42
2:L:158:LEU:HD23	2:L:158:LEU:H	1.85	0.42
2:N:80:TYR:HE1	2:N:148:GLU:HG2	1.70	0.42
2:H:75:GLU:H	2:H:79:ASP:HB2	1.85	0.41
2:M:153:ARG:HD2	2:N:80:TYR:CZ	2.55	0.41
2:Q:113:ILE:HB	2:Q:116:PHE:CD1	2.55	0.41
2:V:93:GLU:O	2:V:95:HIS:CE1	2.73	0.41
2:E:113:ILE:HD12	2:E:116:PHE:HB3	2.03	0.41
2:N:81:LEU:O	2:N:84:LEU:HB3	2.21	0.41
2:S:145:LEU:HD23	2:U:153:ARG:H	1.86	0.41
2:L:75:GLU:H	2:L:76:GLU:CA	2.27	0.41
2:N:76:GLU:CD	2:N:76:GLU:H	2.24	0.41
2:N:95:HIS:CE1	2:P:98:CYS:HB3	2.56	0.41
2:H:109:MET:HB3	2:H:121:ILE:H	1.86	0.41
2:U:130:ILE:HD12	2:U:149:TRP:CE3	2.56	0.41
2:O:113:ILE:HG22	2:O:116:PHE:CE2	2.38	0.40
2:B:144:LEU:H	2:B:144:LEU:HD12	1.86	0.40
2:C:145:LEU:HD12	2:C:145:LEU:HA	1.99	0.40
2:A:75:GLU:H	2:A:76:GLU:HA	1.87	0.40

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	a	140/142 (99%)	124 (89%)	11 (8%)	5 (4%)	4	38
1	b	140/142 (99%)	120 (86%)	17 (12%)	3 (2%)	9	50
1	c	140/142 (99%)	119 (85%)	15 (11%)	6 (4%)	3	34
1	d	140/142 (99%)	123 (88%)	16 (11%)	1 (1%)	26	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	e	140/142 (99%)	117 (84%)	18 (13%)	5 (4%)	4	38
1	f	140/142 (99%)	118 (84%)	18 (13%)	4 (3%)	6	43
1	g	140/142 (99%)	121 (86%)	13 (9%)	6 (4%)	3	34
1	h	140/142 (99%)	116 (83%)	19 (14%)	5 (4%)	4	38
1	i	140/142 (99%)	122 (87%)	12 (9%)	6 (4%)	3	34
1	j	140/142 (99%)	123 (88%)	12 (9%)	5 (4%)	4	38
1	k	140/142 (99%)	119 (85%)	14 (10%)	7 (5%)	3	31
1	l	140/142 (99%)	119 (85%)	13 (9%)	8 (6%)	2	28
1	m	140/142 (99%)	126 (90%)	10 (7%)	4 (3%)	6	43
1	n	140/142 (99%)	127 (91%)	9 (6%)	4 (3%)	6	43
1	o	140/142 (99%)	121 (86%)	16 (11%)	3 (2%)	9	50
1	p	140/142 (99%)	123 (88%)	10 (7%)	7 (5%)	3	31
1	q	140/142 (99%)	121 (86%)	12 (9%)	7 (5%)	3	31
1	r	140/142 (99%)	120 (86%)	15 (11%)	5 (4%)	4	38
1	s	140/142 (99%)	124 (89%)	13 (9%)	3 (2%)	9	50
1	t	140/142 (99%)	118 (84%)	16 (11%)	6 (4%)	3	34
1	u	140/142 (99%)	127 (91%)	10 (7%)	3 (2%)	9	50
1	v	140/142 (99%)	127 (91%)	8 (6%)	5 (4%)	4	38
1	w	140/142 (99%)	127 (91%)	11 (8%)	2 (1%)	14	58
1	x	140/142 (99%)	116 (83%)	19 (14%)	5 (4%)	4	38
2	A	119/121 (98%)	89 (75%)	15 (13%)	15 (13%)	0	8
2	B	119/121 (98%)	89 (75%)	21 (18%)	9 (8%)	1	20
2	C	119/121 (98%)	96 (81%)	12 (10%)	11 (9%)	1	17
2	D	119/121 (98%)	83 (70%)	21 (18%)	15 (13%)	0	8
2	E	119/121 (98%)	95 (80%)	14 (12%)	10 (8%)	1	18
2	F	119/121 (98%)	88 (74%)	23 (19%)	8 (7%)	1	24
2	G	119/121 (98%)	87 (73%)	15 (13%)	17 (14%)	0	6
2	H	119/121 (98%)	94 (79%)	13 (11%)	12 (10%)	1	14
2	I	119/121 (98%)	87 (73%)	24 (20%)	8 (7%)	1	24
2	J	119/121 (98%)	88 (74%)	18 (15%)	13 (11%)	0	11
2	K	119/121 (98%)	93 (78%)	13 (11%)	13 (11%)	0	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	119/121 (98%)	94 (79%)	16 (13%)	9 (8%)	1	20
2	M	119/121 (98%)	99 (83%)	14 (12%)	6 (5%)	3	31
2	N	119/121 (98%)	98 (82%)	14 (12%)	7 (6%)	2	27
2	O	119/121 (98%)	97 (82%)	17 (14%)	5 (4%)	3	34
2	P	119/121 (98%)	90 (76%)	20 (17%)	9 (8%)	1	20
2	Q	119/121 (98%)	98 (82%)	15 (13%)	6 (5%)	3	31
2	R	119/121 (98%)	93 (78%)	21 (18%)	5 (4%)	3	34
2	S	119/121 (98%)	98 (82%)	9 (8%)	12 (10%)	1	14
2	T	119/121 (98%)	98 (82%)	16 (13%)	5 (4%)	3	34
2	U	119/121 (98%)	85 (71%)	18 (15%)	16 (13%)	0	7
2	V	119/121 (98%)	90 (76%)	19 (16%)	10 (8%)	1	18
2	W	119/121 (98%)	89 (75%)	18 (15%)	12 (10%)	1	14
2	X	119/121 (98%)	95 (80%)	16 (13%)	8 (7%)	1	24
All	All	6216/6312 (98%)	5131 (82%)	729 (12%)	356 (6%)	4	28

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
2	L	96	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	121/121 (100%)	118 (98%)	3 (2%)	55	81
1	b	121/121 (100%)	117 (97%)	4 (3%)	45	76
1	c	121/121 (100%)	114 (94%)	7 (6%)	25	61
1	d	121/121 (100%)	118 (98%)	3 (2%)	55	81
1	e	121/121 (100%)	117 (97%)	4 (3%)	45	76
1	f	121/121 (100%)	115 (95%)	6 (5%)	30	66
1	g	121/121 (100%)	119 (98%)	2 (2%)	68	87
1	h	121/121 (100%)	117 (97%)	4 (3%)	45	76
1	i	121/121 (100%)	115 (95%)	6 (5%)	30	66
1	j	121/121 (100%)	115 (95%)	6 (5%)	30	66
1	k	121/121 (100%)	118 (98%)	3 (2%)	55	81
1	l	121/121 (100%)	117 (97%)	4 (3%)	45	76
1	m	121/121 (100%)	117 (97%)	4 (3%)	45	76
1	n	121/121 (100%)	118 (98%)	3 (2%)	55	81
1	o	121/121 (100%)	117 (97%)	4 (3%)	45	76
1	p	121/121 (100%)	115 (95%)	6 (5%)	30	66
1	q	121/121 (100%)	117 (97%)	4 (3%)	45	76
1	r	121/121 (100%)	115 (95%)	6 (5%)	30	66
1	s	121/121 (100%)	117 (97%)	4 (3%)	45	76
1	t	121/121 (100%)	113 (93%)	8 (7%)	21	57
1	u	121/121 (100%)	116 (96%)	5 (4%)	37	71
1	v	121/121 (100%)	120 (99%)	1 (1%)	86	94
1	w	121/121 (100%)	114 (94%)	7 (6%)	25	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	x	121/121 (100%)	115 (95%)	6 (5%)	30	66
2	A	109/109 (100%)	101 (93%)	8 (7%)	17	54
2	B	109/109 (100%)	104 (95%)	5 (5%)	33	68
2	C	109/109 (100%)	104 (95%)	5 (5%)	33	68
2	D	109/109 (100%)	103 (94%)	6 (6%)	27	63
2	E	109/109 (100%)	104 (95%)	5 (5%)	33	68
2	F	109/109 (100%)	102 (94%)	7 (6%)	22	58
2	G	109/109 (100%)	103 (94%)	6 (6%)	27	63
2	H	109/109 (100%)	104 (95%)	5 (5%)	33	68
2	I	109/109 (100%)	106 (97%)	3 (3%)	51	78
2	J	109/109 (100%)	102 (94%)	7 (6%)	22	58
2	K	109/109 (100%)	100 (92%)	9 (8%)	14	49
2	L	109/109 (100%)	106 (97%)	3 (3%)	51	78
2	M	109/109 (100%)	105 (96%)	4 (4%)	41	73
2	N	109/109 (100%)	98 (90%)	11 (10%)	9	38
2	O	109/109 (100%)	104 (95%)	5 (5%)	33	68
2	P	109/109 (100%)	104 (95%)	5 (5%)	33	68
2	Q	109/109 (100%)	99 (91%)	10 (9%)	11	43
2	R	109/109 (100%)	106 (97%)	3 (3%)	51	78
2	S	109/109 (100%)	106 (97%)	3 (3%)	51	78
2	T	109/109 (100%)	102 (94%)	7 (6%)	22	58
2	U	109/109 (100%)	101 (93%)	8 (7%)	17	54
2	V	109/109 (100%)	104 (95%)	5 (5%)	33	68
2	W	109/109 (100%)	104 (95%)	5 (5%)	33	68
2	X	109/109 (100%)	106 (97%)	3 (3%)	51	78
All	All	5520/5520 (100%)	5272 (96%)	248 (4%)	38	69

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

Some 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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 carbohydrates 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.