



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 16, 2018 – 12:21 am GMT

PDB ID : 5TRE  
EMDB ID: : EMD-8458  
Title : Zinc and the Iron Donor Frataxin Regulate Oligomerization of the Scaffold Protein to Form New Fe-S Cluster Assembly Centers  
Authors : Ranatunga, W.; Gakh, O.; Galeano, B.K.; Smith IV, D.Y.; Thompson, J.R.; Isaya, G.  
Deposited on : 2016-10-26  
Resolution : 15.60 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

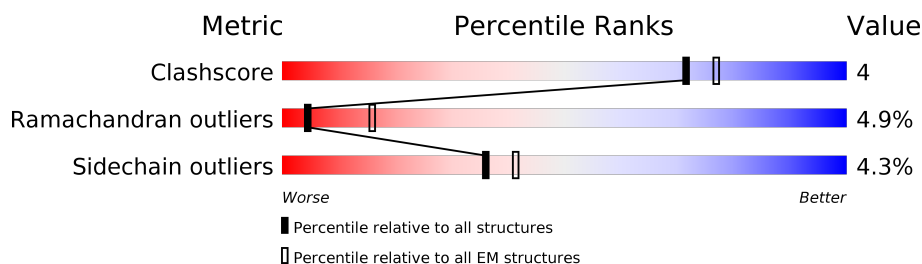
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 15.60 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.







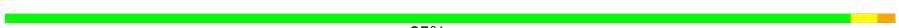











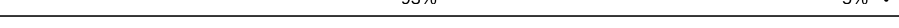








Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531

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  $\geq 3$ , 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% 8%
1	b	142	92% 8%
1	c	142	91% 9%
1	d	142	89% 9% .
1	e	142	90% 8% .
1	f	142	93% 6% .
1	g	142	92% 7% .
1	h	142	85% 13% .
1	i	142	89% 10% .

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Mol	Chain	Length	Quality of chain
1	j	142	 87% 12% .
1	k	142	 91% 8% .
1	l	142	 89% 11% .
1	m	142	 89% 11% .
1	n	142	 95% . .
1	o	142	 92% 8%
1	p	142	 87% 11% .
1	q	142	 90% 8% .
1	r	142	 89% 10% .
1	s	142	 87% 11% .
1	t	142	 92% 7% .
1	u	142	 92% 8% .
1	v	142	 88% 9% .
1	w	142	 92% 7% .
1	x	142	 90% 8% .
2	A	121	 93% 5% .
2	B	121	 83% 16% .
2	C	121	 80% 16% .
2	D	121	 91% 8% .
2	E	121	 90% 10%
2	F	121	 85% 13% .
2	G	121	 89% 10% .
2	H	121	 88% 11% .
2	I	121	 83% 12% .
2	J	121	 88% 12%

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Mol	Chain	Length	Quality of chain
2	K	121	 88% 11% .
2	L	121	 83% 16% .
2	M	121	 86% 13% .
2	N	121	 93% 7% .
2	O	121	 92% 8% .
2	P	121	 86% 12% .
2	Q	121	 89% 10% .
2	R	121	 88% 11% .
2	S	121	 83% 16% .
2	T	121	 84% 12% .
2	U	121	 93% 7% .
2	V	121	 84% 13% .
2	W	121	 85% 12% .
2	X	121	 86% 11% .

## 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 947	C 597	N 153	O 195	S 2	0	0
2	G	121	Total 947	C 597	N 153	O 195	S 2	0	0
2	H	121	Total 947	C 597	N 153	O 195	S 2	0	0
2	I	121	Total 947	C 597	N 153	O 195	S 2	0	0
2	J	121	Total 947	C 597	N 153	O 195	S 2	0	0
2	K	121	Total 947	C 597	N 153	O 195	S 2	0	0
2	L	121	Total 947	C 597	N 153	O 195	S 2	0	0
2	M	121	Total 947	C 597	N 153	O 195	S 2	0	0
2	N	121	Total 947	C 597	N 153	O 195	S 2	0	0
2	O	121	Total 947	C 597	N 153	O 195	S 2	0	0
2	P	121	Total 947	C 597	N 153	O 195	S 2	0	0
2	Q	121	Total 947	C 597	N 153	O 195	S 2	0	0
2	R	121	Total 947	C 597	N 153	O 195	S 2	0	0
2	S	121	Total 947	C 597	N 153	O 195	S 2	0	0
2	T	121	Total 947	C 597	N 153	O 195	S 2	0	0
2	U	121	Total 947	C 597	N 153	O 195	S 2	0	0
2	V	121	Total 947	C 597	N 153	O 195	S 2	0	0
2	W	121	Total 947	C 597	N 153	O 195	S 2	0	0
2	X	121	Total 947	C 597	N 153	O 195	S 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

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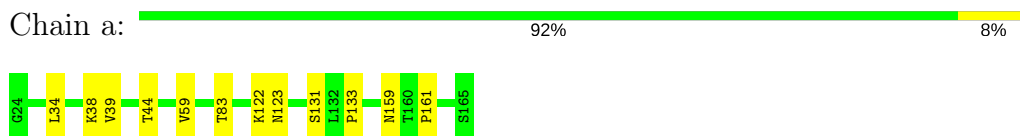
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Chain	Residue	Modelled	Actual	Comment	Reference
B	73	ALA	TYR	conflict	UNP Q07540
C	73	ALA	TYR	conflict	UNP Q07540
D	73	ALA	TYR	conflict	UNP Q07540
E	73	ALA	TYR	conflict	UNP Q07540
F	73	ALA	TYR	conflict	UNP Q07540
G	73	ALA	TYR	conflict	UNP Q07540
H	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

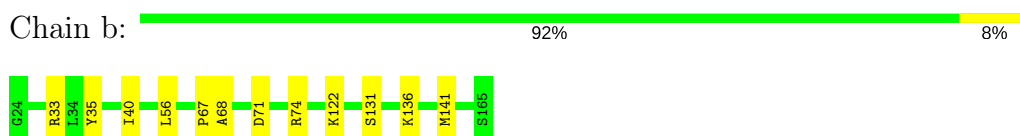
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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.

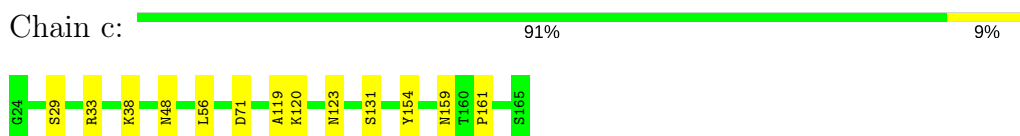
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



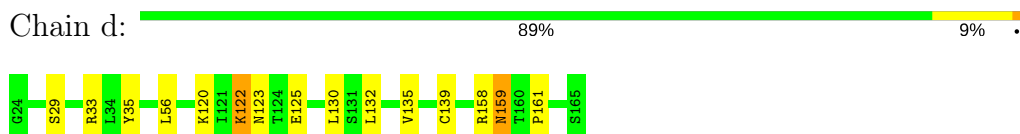
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



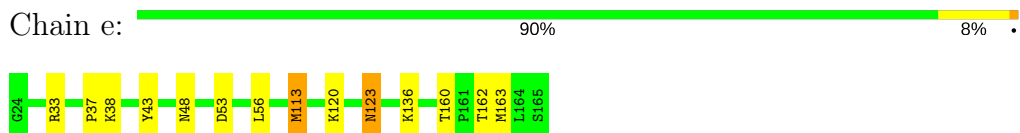
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



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

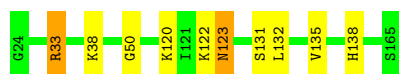


- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



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





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

Chain g: 92% 7%



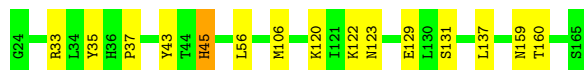
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain h: 85% 13%



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

Chain i: 89% 10%



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

Chain j: 87% 12%



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

Chain k: 91% 8%



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

Chain l: 89% 11%

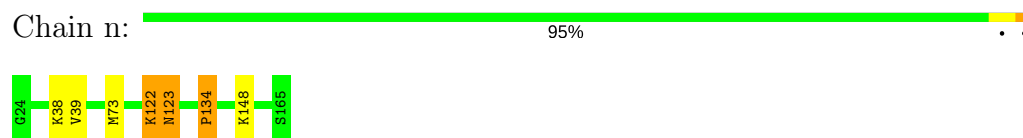


- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

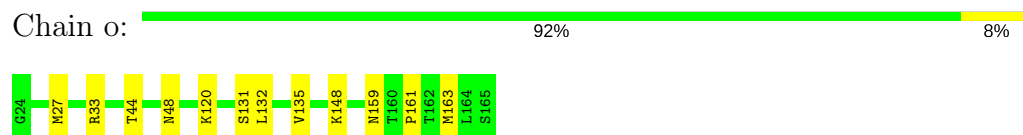
Chain m: 89% 11%



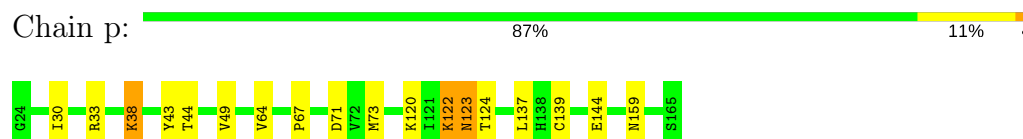
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



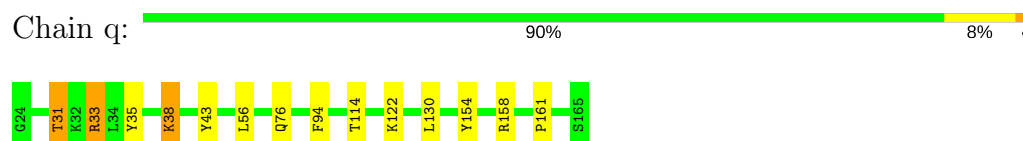
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



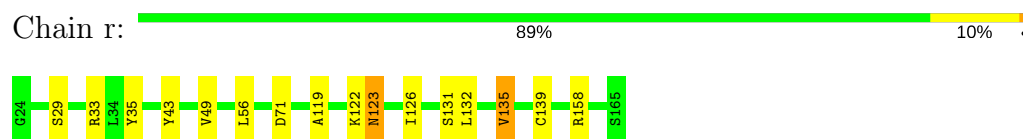
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



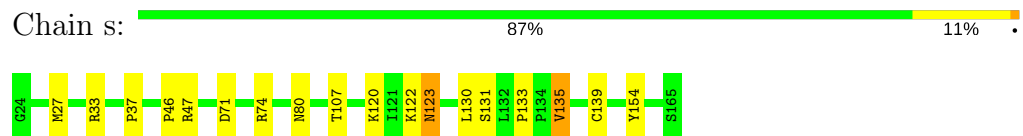
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



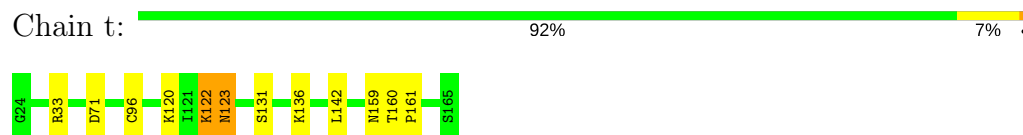
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial




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

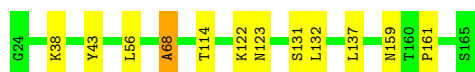


- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial




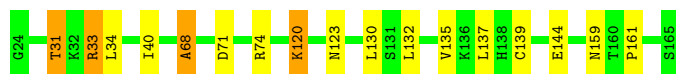
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain u:  92% 8%



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

Chain v:  88% 9%




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

Chain w:  92% 7%



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

Chain x:  90% 8%




- Molecule 2: Frataxin homolog, mitochondrial

Chain A:  93% 5%




- Molecule 2: Frataxin homolog, mitochondrial

Chain B:  83% 16%



- Molecule 2: Frataxin homolog, mitochondrial

Chain C:  80% 16%



- Molecule 2: Frataxin homolog, mitochondrial

Chain D:  91% 8%



- Molecule 2: Frataxin homolog, mitochondrial

Chain E: 90% 10%



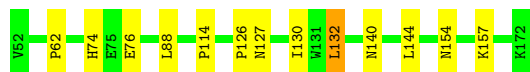
- Molecule 2: Frataxin homolog, mitochondrial

Chain F: 85% 13%



- Molecule 2: Frataxin homolog, mitochondrial

Chain G: 89% 10%



- Molecule 2: Frataxin homolog, mitochondrial

Chain H: 88% 11%



- Molecule 2: Frataxin homolog, mitochondrial

Chain I: 83% 12%



- Molecule 2: Frataxin homolog, mitochondrial

Chain J: 88% 12%




- Molecule 2: Frataxin homolog, mitochondrial

Chain K: 88% 11%




- Molecule 2: Frataxin homolog, mitochondrial

Chain L:  83% 16%



- Molecule 2: Frataxin homolog, mitochondrial

Chain M:  86% 13%



- Molecule 2: Frataxin homolog, mitochondrial

Chain N:  93% 7%




- Molecule 2: Frataxin homolog, mitochondrial

Chain O:  92% 8%




- Molecule 2: Frataxin homolog, mitochondrial

Chain P:  86% 12%




- Molecule 2: Frataxin homolog, mitochondrial

Chain Q:  89% 10%




- Molecule 2: Frataxin homolog, mitochondrial

Chain R:  88% 11%




- Molecule 2: Frataxin homolog, mitochondrial



Chain S:  83% 16%



- Molecule 2: Frataxin homolog, mitochondrial

Chain T:  84% 12%




- Molecule 2: Frataxin homolog, mitochondrial

Chain U:  93% 7%




- Molecule 2: Frataxin homolog, mitochondrial

Chain V:  84% 13%




- Molecule 2: Frataxin homolog, mitochondrial

Chain W:  85% 12%



- Molecule 2: Frataxin homolog, mitochondrial

Chain X:  86% 11%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, O	Depositor
Number of particles used	4218	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; The ctf.auto function from EMAN2 was applied.	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	210	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	115000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	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	1.06	0/1089	1.32	3/1466 (0.2%)
1	b	1.04	0/1089	1.26	4/1466 (0.3%)
1	c	1.06	0/1089	1.27	0/1466
1	d	1.04	0/1089	1.29	5/1466 (0.3%)
1	e	1.04	0/1089	1.30	5/1466 (0.3%)
1	f	1.04	0/1089	1.28	4/1466 (0.3%)
1	g	1.03	0/1089	1.30	3/1466 (0.2%)
1	h	1.04	0/1089	1.30	6/1466 (0.4%)
1	i	1.03	0/1089	1.30	3/1466 (0.2%)
1	j	1.00	1/1089 (0.1%)	1.27	1/1466 (0.1%)
1	k	1.05	0/1089	1.30	6/1466 (0.4%)
1	l	1.05	0/1089	1.26	2/1466 (0.1%)
1	m	1.03	0/1089	1.32	4/1466 (0.3%)
1	n	1.01	0/1089	1.32	3/1466 (0.2%)
1	o	1.05	0/1089	1.25	4/1466 (0.3%)
1	p	1.04	0/1089	1.30	5/1466 (0.3%)
1	q	1.02	0/1089	1.35	11/1466 (0.8%)
1	r	1.03	0/1089	1.33	7/1466 (0.5%)
1	s	1.05	0/1089	1.28	4/1466 (0.3%)
1	t	1.03	0/1089	1.26	2/1466 (0.1%)
1	u	1.00	0/1089	1.29	4/1466 (0.3%)
1	v	1.05	0/1089	1.34	3/1466 (0.2%)
1	w	1.04	0/1089	1.32	5/1466 (0.3%)
1	x	1.06	0/1089	1.32	8/1466 (0.5%)
2	A	0.99	0/967	1.28	5/1319 (0.4%)
2	B	1.01	0/967	1.26	2/1319 (0.2%)
2	C	1.01	1/967 (0.1%)	1.17	1/1319 (0.1%)
2	D	0.99	0/967	1.21	0/1319
2	E	1.01	0/967	1.21	0/1319
2	F	1.02	0/967	1.21	3/1319 (0.2%)
2	G	1.02	0/967	1.19	0/1319
2	H	1.00	0/967	1.22	1/1319 (0.1%)
2	I	1.04	1/967 (0.1%)	1.28	4/1319 (0.3%)
2	J	1.03	0/967	1.20	0/1319

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
2	K	1.03	0/967	1.19	3/1319 (0.2%)
2	L	1.00	0/967	1.21	3/1319 (0.2%)
2	M	1.04	0/967	1.19	1/1319 (0.1%)
2	N	1.03	0/967	1.20	3/1319 (0.2%)
2	O	1.03	0/967	1.19	0/1319
2	P	0.97	0/967	1.15	0/1319
2	Q	0.99	0/967	1.20	1/1319 (0.1%)
2	R	1.03	0/967	1.23	1/1319 (0.1%)
2	S	1.02	0/967	1.23	0/1319
2	T	1.02	0/967	1.17	2/1319 (0.2%)
2	U	1.01	0/967	1.19	1/1319 (0.1%)
2	V	1.03	0/967	1.22	3/1319 (0.2%)
2	W	0.99	0/967	1.20	1/1319 (0.1%)
2	X	1.03	0/967	1.27	6/1319 (0.5%)
All	All	1.03	3/49344 (0.0%)	1.26	143/66840 (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	h	0	1
1	i	0	1
1	l	0	1
1	s	0	1
1	t	0	1
1	v	0	1
1	x	0	1
2	A	0	1
2	B	0	1
2	C	0	1
2	F	0	1
2	K	0	1
All	All	0	12

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	96	PRO	N-CD	5.45	1.55	1.47
1	j	33	ARG	NE-CZ	5.17	1.39	1.33
2	C	153	ARG	NE-CZ	5.14	1.39	1.33

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	m	43	TYR	CB-CG-CD2	-10.44	114.73	121.00
2	V	142	PHE	CB-CG-CD1	9.62	127.53	120.80
1	g	35	TYR	CB-CG-CD1	9.20	126.52	121.00
1	m	43	TYR	CB-CG-CD1	8.99	126.39	121.00
1	q	35	TYR	CB-CG-CD1	8.93	126.36	121.00
2	A	80	TYR	CB-CG-CD1	8.77	126.26	121.00
2	A	80	TYR	CB-CG-CD2	-8.41	115.96	121.00
1	k	33	ARG	NE-CZ-NH1	-8.33	116.14	120.30
2	B	80	TYR	CB-CG-CD2	-7.98	116.21	121.00
1	e	43	TYR	CB-CG-CD1	7.49	125.50	121.00
1	r	122	LYS	C-N-CA	7.49	140.43	121.70
1	q	154	TYR	CB-CG-CD2	-7.42	116.55	121.00
1	d	35	TYR	CB-CG-CD2	-7.33	116.60	121.00
1	k	35	TYR	CB-CG-CD2	-7.24	116.65	121.00
1	i	123	ASN	N-CA-CB	7.22	123.60	110.60
1	q	35	TYR	CB-CG-CD2	-7.12	116.73	121.00
2	B	80	TYR	CB-CG-CD1	7.12	125.27	121.00
2	V	142	PHE	CB-CG-CD2	-7.11	115.82	120.80
1	q	33	ARG	NE-CZ-NH1	-6.99	116.81	120.30
1	d	122	LYS	C-N-CA	6.96	139.09	121.70
1	e	43	TYR	CB-CG-CD2	-6.94	116.83	121.00
1	a	122	LYS	C-N-CA	6.85	138.83	121.70
1	x	35	TYR	CB-CG-CD1	6.81	125.09	121.00
1	k	123	ASN	N-CA-CB	6.76	122.77	110.60
1	r	123	ASN	N-CA-CB	6.65	122.58	110.60
2	V	141	ARG	NE-CZ-NH1	-6.65	116.97	120.30
1	n	123	ASN	N-CA-CB	6.65	122.56	110.60
2	I	73	ALA	N-CA-CB	6.63	119.38	110.10
1	w	47	ARG	NE-CZ-NH1	-6.59	117.01	120.30
1	f	123	ASN	N-CA-CB	6.54	122.38	110.60
1	n	73	MET	CG-SD-CE	-6.51	89.78	100.20
1	l	122	LYS	C-N-CA	6.51	137.96	121.70
1	p	43	TYR	CB-CG-CD2	-6.46	117.12	121.00
1	k	122	LYS	C-N-CA	6.45	137.81	121.70
1	g	35	TYR	CB-CG-CD2	-6.43	117.14	121.00
1	v	31	THR	N-CA-CB	6.39	122.44	110.30
2	W	80	TYR	CB-CG-CD1	-6.39	117.17	121.00
1	b	131	SER	N-CA-CB	6.38	120.08	110.50
1	q	33	ARG	NE-CZ-NH2	6.35	123.47	120.30
1	q	158	ARG	NE-CZ-NH1	-6.35	117.12	120.30
2	A	73	ALA	N-CA-CB	6.29	118.91	110.10
1	q	43	TYR	CB-CG-CD2	-6.27	117.24	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	r	158	ARG	NE-CZ-NH1	-6.27	117.16	120.30
1	h	123	ASN	N-CA-CB	6.27	121.89	110.60
1	x	154	TYR	CB-CG-CD1	6.26	124.76	121.00
1	u	123	ASN	N-CA-CB	6.17	121.71	110.60
2	R	80	TYR	CB-CG-CD2	-6.15	117.31	121.00
1	m	123	ASN	N-CA-CB	6.14	121.65	110.60
2	X	119	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	e	123	ASN	N-CA-CB	6.03	121.46	110.60
1	u	43	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	u	122	LYS	C-N-CA	5.99	136.68	121.70
1	h	43	TYR	CB-CG-CD1	5.98	124.59	121.00
2	N	153	ARG	NE-CZ-NH2	-5.98	117.31	120.30
2	U	77	ALA	N-CA-CB	5.97	118.46	110.10
1	b	74	ARG	NE-CZ-NH2	5.94	123.27	120.30
2	C	141	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	x	35	TYR	CB-CG-CD2	-5.92	117.45	121.00
1	r	43	TYR	CB-CG-CD2	-5.90	117.46	121.00
2	H	118	THR	CA-CB-CG2	-5.87	104.18	112.40
1	p	123	ASN	N-CA-CB	5.86	121.14	110.60
1	i	45	HIS	N-CA-CB	5.84	121.11	110.60
2	F	78	ASP	C-N-CA	5.78	136.15	121.70
1	s	123	ASN	N-CA-CB	5.77	120.98	110.60
2	Q	116	PHE	CB-CG-CD2	-5.76	116.77	120.80
1	a	44	THR	C-N-CA	5.72	136.00	121.70
1	f	122	LYS	C-N-CA	5.69	135.93	121.70
1	x	123	ASN	N-CA-CB	5.68	120.83	110.60
1	n	122	LYS	C-N-CA	5.68	135.91	121.70
2	K	73	ALA	N-CA-CB	5.68	118.05	110.10
1	x	33	ARG	NE-CZ-NH2	5.66	123.13	120.30
2	X	75	GLU	C-N-CA	5.66	135.85	121.70
2	K	113	ILE	N-CA-C	-5.64	95.76	111.00
1	r	43	TYR	CB-CG-CD1	5.64	124.39	121.00
1	s	74	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	v	33	ARG	NE-CZ-NH2	5.63	123.11	120.30
1	b	35	TYR	CB-CG-CD2	-5.62	117.62	121.00
2	I	95	HIS	C-N-CD	5.61	140.18	128.40
1	o	44	THR	C-N-CA	5.55	135.59	121.70
1	h	43	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	q	38	LYS	N-CA-CB	5.55	120.59	110.60
1	r	35	TYR	CB-CG-CD2	-5.54	117.68	121.00
2	N	94	ALA	N-CA-CB	5.52	117.83	110.10
2	T	73	ALA	N-CA-CB	5.51	117.82	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	35	TYR	CB-CG-CD1	5.48	124.29	121.00
2	M	75	GLU	C-N-CA	5.47	135.38	121.70
2	I	80	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	x	154	TYR	CB-CG-CD2	-5.44	117.74	121.00
1	t	122	LYS	C-N-CA	5.43	135.27	121.70
2	L	141	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	w	44	THR	C-N-CA	5.41	135.23	121.70
1	m	122	LYS	C-N-CA	5.41	135.23	121.70
2	A	116	PHE	CB-CG-CD1	5.41	124.58	120.80
1	g	47	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	d	158	ARG	NE-CZ-NH2	5.39	123.00	120.30
1	o	33	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	x	43	TYR	CB-CG-CD2	-5.36	117.78	121.00
2	L	94	ALA	N-CA-CB	5.35	117.59	110.10
1	l	44	THR	C-N-CA	5.34	135.06	121.70
2	X	94	ALA	N-CA-CB	5.34	117.57	110.10
1	u	68	ALA	N-CA-CB	5.33	117.56	110.10
2	X	56	THR	CA-CB-CG2	-5.31	104.96	112.40
1	o	163	MET	CG-SD-CE	-5.31	91.71	100.20
2	F	133	ALA	N-CA-CB	5.30	117.52	110.10
2	X	127	ASN	N-CA-CB	5.29	120.12	110.60
1	i	35	TYR	CB-CG-CD2	-5.29	117.83	121.00
2	T	75	GLU	C-N-CA	5.29	134.91	121.70
2	K	116	PHE	CB-CG-CD2	-5.28	117.11	120.80
1	q	31	THR	N-CA-CB	5.27	120.31	110.30
1	e	113	MET	CG-SD-CE	-5.26	91.78	100.20
1	v	68	ALA	N-CA-CB	5.26	117.47	110.10
1	k	35	TYR	CB-CG-CD1	5.25	124.15	121.00
2	F	94	ALA	N-CA-CB	5.23	117.42	110.10
1	k	123	ASN	N-CA-C	-5.23	96.88	111.00
1	h	158	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	s	107	THR	CA-CB-CG2	-5.20	105.12	112.40
1	w	74	ARG	NE-CZ-NH2	5.19	122.90	120.30
1	f	33	ARG	NE-CZ-NH2	5.18	122.89	120.30
2	I	119	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	e	162	THR	CA-CB-CG2	-5.17	105.16	112.40
1	p	122	LYS	C-N-CA	5.16	134.59	121.70
1	j	44	THR	C-N-CA	5.16	134.59	121.70
1	q	94	PHE	CB-CG-CD2	-5.15	117.19	120.80
1	q	43	TYR	CB-CG-CD1	5.15	124.09	121.00
1	s	122	LYS	C-N-CA	5.14	134.56	121.70
1	w	74	ARG	NE-CZ-NH1	-5.14	117.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	r	158	ARG	NE-CZ-NH2	5.14	122.87	120.30
2	A	75	GLU	O-C-N	-5.13	114.49	122.70
1	h	44	THR	C-N-CA	5.13	134.53	121.70
1	t	123	ASN	N-CA-CB	5.13	119.84	110.60
2	X	99	ILE	N-CA-C	-5.13	97.15	111.00
1	p	73	MET	N-CA-CB	5.12	119.82	110.60
1	a	133	PRO	CA-C-N	5.11	131.42	117.10
1	o	27	MET	C-N-CA	5.11	134.48	121.70
1	h	71	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	f	123	ASN	N-CA-C	-5.09	97.25	111.00
1	p	44	THR	C-N-CA	5.09	134.43	121.70
1	w	33	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	x	44	THR	C-N-CA	5.05	134.32	121.70
2	L	67	ASN	N-CA-CB	5.04	119.67	110.60
2	N	131	TRP	CA-CB-CG	5.03	123.25	113.70
1	d	159	ASN	N-CA-CB	5.02	119.64	110.60
1	d	35	TYR	CB-CG-CD1	5.01	124.00	121.00

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	80	TYR	Sidechain
2	B	119	TYR	Sidechain
2	C	75	GLU	Peptide
2	F	128	LYS	Peptide
2	K	118	THR	Peptide
1	h	74	ARG	Sidechain
1	i	43	TYR	Sidechain
1	l	154	TYR	Sidechain
1	s	154	TYR	Sidechain
1	t	122	LYS	Peptide
1	v	74	ARG	Sidechain
1	x	122	LYS	Peptide

## 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	1106	0	0
1	c	1072	0	1106	0	0
1	d	1072	0	1106	0	0
1	e	1072	0	1108	0	0
1	f	1072	0	1106	0	0
1	g	1072	0	1108	0	0
1	h	1072	0	1106	0	0
1	i	1072	0	1108	0	0
1	j	1072	0	1106	0	0
1	k	1072	0	1108	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	1106	0	0
1	p	1072	0	1108	0	0
1	q	1072	0	1108	0	0
1	r	1072	0	1106	0	0
1	s	1072	0	1108	0	0
1	t	1072	0	1108	0	0
1	u	1072	0	1108	0	0
1	v	1072	0	1106	0	0
1	w	1072	0	1108	0	0
1	x	1072	0	1108	0	0
2	A	947	0	921	6	0
2	B	947	0	921	3	0
2	C	947	0	921	17	0
2	D	947	0	921	0	0
2	E	947	0	921	0	0
2	F	947	0	921	16	0
2	G	947	0	921	2	0
2	H	947	0	921	7	0
2	I	947	0	921	16	0
2	J	947	0	921	19	0
2	K	947	0	921	0	0
2	L	947	0	921	35	0
2	M	947	0	921	24	0
2	N	947	0	921	0	0
2	O	947	0	921	3	0
2	P	947	0	921	28	0
2	Q	947	0	921	3	0
2	R	947	0	921	6	0
2	S	947	0	921	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	947	0	921	1	0
2	U	947	0	921	0	0
2	V	947	0	921	45	0
2	W	947	0	921	37	0
2	X	947	0	921	0	0
All	All	48456	0	48674	284	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 4.

All (284) 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:S:131:TRP:CZ2	2:S:139:PRO:CB	1.75	1.62
2:S:131:TRP:CZ2	2:S:139:PRO:HB3	1.11	1.58
2:L:121:ILE:HG12	2:L:132:LEU:CD2	1.33	1.57
2:P:130:ILE:CD1	2:P:149:TRP:NE1	1.72	1.52
2:M:121:ILE:HG22	2:M:132:LEU:CD2	1.36	1.51
2:L:121:ILE:CG1	2:L:132:LEU:HD21	1.45	1.44
2:M:121:ILE:CG2	2:M:132:LEU:CD2	1.96	1.43
2:P:131:TRP:CH2	2:Q:76:GLU:OE2	1.73	1.41
2:S:131:TRP:CE2	2:S:139:PRO:HB3	1.56	1.41
2:L:121:ILE:CB	2:L:132:LEU:HD21	1.53	1.37
2:S:131:TRP:HZ2	2:S:139:PRO:CG	1.40	1.34
2:P:130:ILE:CD1	2:P:149:TRP:CD1	2.11	1.32
2:P:130:ILE:HD12	2:P:149:TRP:NE1	1.36	1.31
2:V:131:TRP:CH2	2:V:141:ARG:HB3	1.66	1.30
2:J:132:LEU:CD2	2:J:158:LEU:CD1	2.15	1.25
2:P:130:ILE:HD12	2:P:149:TRP:CE2	1.71	1.24
2:V:131:TRP:CZ3	2:V:141:ARG:HB3	1.73	1.23
2:S:132:LEU:HD12	2:S:142:PHE:CE1	1.74	1.23
2:L:121:ILE:HA	2:L:132:LEU:CD2	1.72	1.19
2:M:121:ILE:CG2	2:M:132:LEU:HD22	1.71	1.19
2:L:131:TRP:CZ2	2:L:139:PRO:HB3	1.78	1.19
2:J:132:LEU:CD2	2:J:158:LEU:HG	1.73	1.17
2:P:130:ILE:HD12	2:P:149:TRP:CD1	1.74	1.17
2:M:132:LEU:CD1	2:M:158:LEU:HB2	1.73	1.16
2:H:128:LYS:HE3	2:H:152:LEU:HD11	1.21	1.16
2:J:132:LEU:HD23	2:J:158:LEU:HD11	1.16	1.15
2:F:121:ILE:HG12	2:F:132:LEU:CD2	1.75	1.15
2:F:121:ILE:HD13	2:F:132:LEU:HD21	1.26	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:132:LEU:CD2	2:J:158:LEU:CG	2.25	1.13
2:J:132:LEU:HD23	2:J:158:LEU:CD1	1.77	1.12
2:L:121:ILE:HG12	2:L:132:LEU:HD22	1.26	1.12
2:M:121:ILE:HG22	2:M:132:LEU:HD22	1.26	1.12
2:V:131:TRP:CE2	2:V:142:PHE:N	2.17	1.12
2:V:131:TRP:NE1	2:V:142:PHE:O	1.81	1.12
2:I:95:HIS:HE1	2:I:170:ILE:HD11	1.12	1.11
2:W:132:LEU:HD11	2:W:158:LEU:HB2	1.25	1.10
2:L:121:ILE:HA	2:L:132:LEU:HD23	1.20	1.10
2:V:131:TRP:CZ3	2:V:141:ARG:CB	2.34	1.10
2:L:121:ILE:CG1	2:L:132:LEU:CD2	2.09	1.10
2:F:121:ILE:CD1	2:F:132:LEU:CD2	2.30	1.09
2:L:131:TRP:CZ2	2:L:139:PRO:CB	2.35	1.09
2:S:132:LEU:HD12	2:S:142:PHE:CZ	1.87	1.08
2:J:132:LEU:HD22	2:J:158:LEU:HG	1.31	1.08
2:F:121:ILE:CG1	2:F:132:LEU:CD2	2.31	1.08
2:P:130:ILE:HD11	2:P:149:TRP:NE1	1.53	1.07
2:P:131:TRP:HH2	2:Q:76:GLU:OE2	1.12	1.05
2:W:132:LEU:CD1	2:W:158:LEU:HB2	1.88	1.03
2:F:121:ILE:HG12	2:F:132:LEU:HD23	1.36	1.03
2:L:121:ILE:CG2	2:L:132:LEU:HD21	1.88	1.03
2:P:131:TRP:CZ3	2:Q:76:GLU:OE2	2.10	1.03
2:V:131:TRP:CD1	2:V:142:PHE:HB2	1.93	1.03
2:I:95:HIS:CE1	2:I:170:ILE:HD11	1.93	1.03
2:L:131:TRP:HE1	2:L:133:ALA:HB2	1.23	1.02
2:I:95:HIS:HD1	2:I:170:ILE:HG12	1.21	1.02
2:L:121:ILE:CB	2:L:132:LEU:CD2	2.36	1.02
2:P:73:ALA:HB1	2:P:80:TYR:CE1	1.94	1.01
2:V:130:ILE:O	2:V:131:TRP:HD1	1.41	1.00
2:L:121:ILE:CA	2:L:132:LEU:CD2	2.38	1.00
2:M:121:ILE:HG22	2:M:132:LEU:HD23	1.01	1.00
2:W:132:LEU:HD11	2:W:158:LEU:CB	1.91	0.99
2:M:121:ILE:HG21	2:M:132:LEU:CD2	1.91	0.98
2:J:132:LEU:HD11	2:J:142:PHE:CZ	1.98	0.98
2:P:130:ILE:HD13	2:P:149:TRP:CD1	1.98	0.97
2:H:128:LYS:HE3	2:H:152:LEU:CD1	1.93	0.97
2:W:132:LEU:HD12	2:W:161:ILE:HD12	1.45	0.97
2:C:131:TRP:HE1	2:C:133:ALA:HB2	1.26	0.96
2:S:131:TRP:CZ2	2:S:139:PRO:CG	2.30	0.95
2:V:131:TRP:CZ3	2:V:141:ARG:CG	2.48	0.95
2:S:131:TRP:HZ2	2:S:139:PRO:CB	1.37	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:132:LEU:CD1	2:W:161:ILE:HD12	1.95	0.95
2:J:132:LEU:HD22	2:J:158:LEU:CG	1.93	0.94
2:M:121:ILE:CG2	2:M:132:LEU:HD23	1.77	0.94
2:F:121:ILE:HD13	2:F:132:LEU:CD2	1.93	0.94
2:M:132:LEU:HD11	2:M:158:LEU:HD12	1.49	0.94
2:P:130:ILE:HD11	2:P:149:TRP:HE1	1.10	0.92
2:P:73:ALA:O	2:P:80:TYR:OH	1.86	0.92
2:J:132:LEU:HD21	2:J:158:LEU:CD1	1.99	0.92
2:S:131:TRP:CZ2	2:S:139:PRO:HB2	2.03	0.92
2:F:121:ILE:CD1	2:F:132:LEU:HD22	1.99	0.91
2:V:131:TRP:CE3	2:V:141:ARG:HA	2.06	0.90
2:A:76:GLU:CD	2:C:131:TRP:CZ3	2.46	0.89
2:I:95:HIS:ND1	2:I:170:ILE:HG12	1.87	0.89
2:I:95:HIS:CE1	2:I:170:ILE:CD1	2.56	0.88
2:V:130:ILE:O	2:V:131:TRP:CD1	2.26	0.88
2:A:76:GLU:CD	2:C:131:TRP:HZ3	1.77	0.88
2:J:132:LEU:HD21	2:J:158:LEU:CG	2.04	0.88
2:F:121:ILE:HG12	2:F:132:LEU:HD22	1.54	0.87
2:W:132:LEU:HD11	2:W:158:LEU:CA	2.05	0.87
2:V:131:TRP:NE1	2:V:142:PHE:N	2.19	0.86
2:M:132:LEU:HD11	2:M:158:LEU:HB2	1.55	0.86
2:J:132:LEU:CD2	2:J:158:LEU:HD11	1.89	0.85
2:V:131:TRP:HE1	2:V:142:PHE:C	1.79	0.85
2:J:132:LEU:HD21	2:J:158:LEU:HG	1.55	0.85
2:V:131:TRP:CD2	2:V:141:ARG:HA	2.12	0.84
2:I:92:SER:O	2:I:95:HIS:CD2	2.31	0.84
2:F:121:ILE:CG1	2:F:132:LEU:HD22	2.07	0.84
2:M:132:LEU:CD1	2:M:158:LEU:CB	2.55	0.84
2:S:131:TRP:CH2	2:S:139:PRO:CB	2.59	0.84
2:P:73:ALA:O	2:P:80:TYR:CZ	2.31	0.83
2:P:73:ALA:HB1	2:P:80:TYR:HE1	1.43	0.81
2:M:132:LEU:HD12	2:M:158:LEU:HB2	1.63	0.81
2:V:131:TRP:NE1	2:V:142:PHE:CA	2.44	0.80
2:W:132:LEU:CD1	2:W:158:LEU:CB	2.54	0.79
2:W:131:TRP:CZ2	2:W:140:ASN:HB2	2.18	0.79
2:L:121:ILE:HG23	2:L:132:LEU:HD21	1.64	0.79
2:L:131:TRP:CE2	2:L:139:PRO:HB3	2.17	0.79
2:S:132:LEU:CD1	2:S:142:PHE:CE1	2.62	0.79
2:F:121:ILE:CG1	2:F:132:LEU:HD23	2.04	0.78
2:V:131:TRP:CZ3	2:V:141:ARG:HG2	2.16	0.78
2:W:131:TRP:CH2	2:W:140:ASN:HB2	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:131:TRP:CE3	2:W:142:PHE:CD1	2.72	0.77
2:M:121:ILE:CG2	2:M:132:LEU:HD21	2.15	0.76
2:V:131:TRP:CE3	2:V:141:ARG:HG2	2.21	0.75
2:C:124:GLN:OE1	2:C:131:TRP:HE3	1.68	0.75
2:P:131:TRP:HE1	2:P:133:ALA:HB2	1.52	0.74
2:V:131:TRP:NE1	2:V:142:PHE:C	2.39	0.74
2:W:132:LEU:CD1	2:W:158:LEU:CA	2.65	0.74
2:W:131:TRP:CE3	2:W:142:PHE:HD1	2.05	0.74
2:P:130:ILE:HD12	2:P:149:TRP:CD2	2.22	0.74
2:J:132:LEU:HD21	2:J:158:LEU:HD12	1.68	0.74
2:J:132:LEU:CD2	2:J:158:LEU:HD12	2.16	0.73
2:W:132:LEU:CG	2:W:158:LEU:HB2	2.18	0.73
2:S:132:LEU:CD1	2:S:142:PHE:CZ	2.71	0.72
2:F:121:ILE:CD1	2:F:132:LEU:HD21	1.98	0.72
2:P:121:ILE:HG13	2:P:132:LEU:CD2	2.18	0.72
2:M:132:LEU:HD11	2:M:158:LEU:CD1	2.19	0.72
2:W:132:LEU:HD12	2:W:158:LEU:HA	1.72	0.72
2:M:132:LEU:HD12	2:M:158:LEU:CB	2.20	0.71
2:W:131:TRP:CZ3	2:W:142:PHE:HD1	2.07	0.71
2:P:130:ILE:HD12	2:P:149:TRP:CG	2.27	0.70
2:V:128:LYS:HB3	2:V:131:TRP:CE2	2.23	0.70
2:L:121:ILE:HG12	2:L:132:LEU:CG	2.19	0.70
2:L:121:ILE:HG23	2:L:132:LEU:CD2	2.20	0.70
2:I:92:SER:HA	2:I:95:HIS:NE2	2.07	0.70
2:M:121:ILE:HG21	2:M:132:LEU:HD22	1.58	0.69
2:W:131:TRP:CZ3	2:W:142:PHE:CD1	2.81	0.69
2:L:131:TRP:CZ2	2:L:139:PRO:HB2	2.26	0.69
2:W:132:LEU:CD1	2:W:158:LEU:HA	2.23	0.69
2:P:121:ILE:CG1	2:P:132:LEU:CD2	2.71	0.68
2:S:130:ILE:HD12	2:S:149:TRP:CE2	2.28	0.68
2:S:131:TRP:HZ2	2:S:139:PRO:HG3	1.50	0.68
2:W:132:LEU:HD11	2:W:158:LEU:O	1.95	0.67
2:L:121:ILE:CD1	2:L:132:LEU:HD11	2.25	0.67
2:V:131:TRP:CE2	2:V:142:PHE:O	2.48	0.66
2:P:130:ILE:CD1	2:P:149:TRP:CE2	2.50	0.66
2:W:132:LEU:HD13	2:W:161:ILE:HD12	1.78	0.66
2:V:131:TRP:HZ3	2:V:141:ARG:HD3	1.61	0.65
2:M:121:ILE:HG21	2:M:132:LEU:HD21	1.78	0.65
2:W:131:TRP:NE1	2:W:132:LEU:O	2.30	0.64
2:L:131:TRP:HZ2	2:L:139:PRO:CB	2.07	0.64
2:V:131:TRP:CE3	2:V:141:ARG:CA	2.81	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:132:LEU:HD11	2:W:158:LEU:C	2.18	0.64
2:M:75:GLU:H	2:M:76:GLU:HA	1.61	0.64
2:A:76:GLU:OE2	2:C:131:TRP:CZ3	2.52	0.63
2:F:121:ILE:HD11	2:F:132:LEU:HD22	1.79	0.62
2:L:121:ILE:HG12	2:L:132:LEU:CD1	2.29	0.62
2:J:132:LEU:HD11	2:J:142:PHE:CE2	2.34	0.62
2:S:131:TRP:CH2	2:S:139:PRO:HB2	2.32	0.62
2:V:131:TRP:CE3	2:V:141:ARG:CB	2.82	0.62
2:H:128:LYS:CE	2:H:152:LEU:CD1	2.75	0.61
2:W:132:LEU:HD12	2:W:161:ILE:CD1	2.27	0.61
2:C:130:ILE:HD12	2:C:149:TRP:CE2	2.35	0.61
2:L:121:ILE:HD13	2:L:132:LEU:HD11	1.83	0.61
2:L:121:ILE:CG1	2:L:132:LEU:HD22	2.04	0.61
2:V:132:LEU:HD12	2:V:132:LEU:O	2.02	0.60
2:V:131:TRP:NE1	2:V:142:PHE:HB2	2.17	0.59
2:J:132:LEU:HD11	2:J:142:PHE:CE1	2.36	0.59
2:A:76:GLU:OE2	2:C:131:TRP:HZ3	1.84	0.58
2:M:132:LEU:HD11	2:M:158:LEU:CB	2.25	0.58
2:W:132:LEU:CD1	2:W:158:LEU:O	2.52	0.58
2:V:131:TRP:CD1	2:V:142:PHE:CB	2.78	0.58
2:M:121:ILE:CB	2:M:132:LEU:HD23	2.33	0.58
2:R:121:ILE:HG22	2:R:132:LEU:HD22	1.86	0.58
2:I:95:HIS:CE1	2:I:170:ILE:CG1	2.87	0.57
2:I:95:HIS:CE1	2:I:170:ILE:HG12	2.40	0.57
2:M:121:ILE:H	2:M:121:ILE:HD12	5.03	0.57
2:P:131:TRP:CD1	2:P:132:LEU:N	2.73	0.57
2:W:131:TRP:CH2	2:W:140:ASN:CB	2.88	0.56
2:I:75:GLU:H	2:I:76:GLU:HA	1.70	0.56
2:S:131:TRP:CZ2	2:S:139:PRO:HG2	2.38	0.56
2:V:131:TRP:CH2	2:V:141:ARG:CB	2.61	0.56
2:V:131:TRP:HZ3	2:V:141:ARG:CD	2.19	0.55
2:R:136:LEU:HD13	2:R:136:LEU:H	1.72	0.55
2:V:131:TRP:CZ3	2:V:141:ARG:HD3	2.42	0.55
2:C:131:TRP:CZ2	2:C:139:PRO:HB3	2.42	0.55
2:F:121:ILE:HG23	2:F:132:LEU:HD23	1.88	0.55
2:R:132:LEU:HD12	2:R:142:PHE:CE1	2.41	0.55
2:V:132:LEU:HD12	2:V:132:LEU:C	2.27	0.55
2:V:131:TRP:NE1	2:V:142:PHE:CB	2.70	0.55
2:S:55:SER:H	2:S:59:GLN:HB2	1.72	0.54
2:C:113:ILE:HG22	2:C:115:ALA:H	1.73	0.54
2:V:131:TRP:CE3	2:V:141:ARG:CG	2.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:131:TRP:CZ3	2:V:141:ARG:CD	2.90	0.54
2:S:132:LEU:HD11	2:S:158:LEU:CB	2.38	0.54
2:L:131:TRP:CH2	2:L:139:PRO:HB2	2.43	0.53
2:V:131:TRP:CD2	2:V:141:ARG:CA	2.90	0.53
2:B:55:SER:H	2:B:59:GLN:HB3	1.72	0.53
2:I:95:HIS:HE1	2:I:170:ILE:CD1	1.94	0.53
2:S:130:ILE:CD1	2:S:149:TRP:CE2	2.91	0.53
2:C:124:GLN:OE1	2:C:131:TRP:CE3	2.57	0.53
2:W:131:TRP:CE2	2:W:140:ASN:HB2	2.44	0.53
2:P:129:GLN:O	2:P:130:ILE:HB	2.09	0.53
2:V:130:ILE:C	2:V:131:TRP:CD1	2.81	0.53
2:V:131:TRP:HD1	2:V:142:PHE:HB2	1.66	0.52
2:P:121:ILE:HG13	2:P:132:LEU:HD23	1.90	0.52
2:V:131:TRP:CD1	2:V:142:PHE:N	2.72	0.52
2:S:132:LEU:HD11	2:S:158:LEU:HB2	1.92	0.52
2:L:158:LEU:HD23	2:L:158:LEU:H	1.75	0.51
2:L:119:TYR:HE1	2:L:132:LEU:HD13	1.75	0.51
2:J:150:VAL:HG22	2:J:151:SER:H	1.75	0.51
2:R:158:LEU:HD23	2:R:158:LEU:H	1.75	0.51
2:P:121:ILE:HG12	2:P:132:LEU:CD2	2.41	0.51
2:L:131:TRP:NE1	2:L:133:ALA:HB2	2.07	0.51
2:P:121:ILE:HG12	2:P:132:LEU:HD21	1.93	0.50
2:C:131:TRP:C	2:C:131:TRP:CD1	2.86	0.50
2:I:92:SER:O	2:I:95:HIS:NE2	2.45	0.50
2:V:131:TRP:HZ3	2:V:141:ARG:CG	2.18	0.49
2:S:131:TRP:CD1	2:S:131:TRP:C	2.86	0.49
2:V:66:LEU:HD12	2:V:66:LEU:H	1.77	0.49
2:B:124:GLN:HB3	2:B:130:ILE:H	1.78	0.49
2:W:131:TRP:CD1	2:W:132:LEU:C	2.86	0.49
2:I:144:LEU:H	2:I:144:LEU:HD12	1.77	0.48
2:I:96:PRO:O	2:I:97:ASP:CB	2.61	0.48
2:W:132:LEU:HG	2:W:158:LEU:HB2	1.94	0.48
2:W:131:TRP:CZ3	2:W:140:ASN:HB2	2.50	0.47
2:P:131:TRP:C	2:P:131:TRP:CD1	2.88	0.46
2:R:71:GLU:HB3	2:R:74:HIS:CE1	2.50	0.46
2:W:131:TRP:HE1	2:W:133:ALA:HA	1.80	0.46
2:H:80:TYR:HB3	2:H:149:TRP:HE1	1.79	0.46
2:M:121:ILE:CB	2:M:132:LEU:CD2	2.85	0.46
2:W:131:TRP:HE3	2:W:142:PHE:CD1	2.32	0.46
2:I:75:GLU:H	2:I:76:GLU:CA	2.29	0.46
2:R:136:LEU:HD22	2:R:137:SER:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:157:LYS:HD2	2:W:157:LYS:H	1.81	0.46
2:L:121:ILE:CG2	2:L:132:LEU:CD2	2.70	0.45
2:F:121:ILE:CG2	2:F:132:LEU:HD23	2.46	0.45
2:C:129:GLN:O	2:C:130:ILE:HB	2.16	0.45
2:L:131:TRP:C	2:L:131:TRP:CD1	2.90	0.45
2:J:132:LEU:HD21	2:J:142:PHE:CE2	2.52	0.45
2:M:132:LEU:HD12	2:M:158:LEU:HB3	1.98	0.45
2:S:121:ILE:CG2	2:S:132:LEU:HD23	2.47	0.45
2:W:131:TRP:CG	2:W:132:LEU:N	2.85	0.44
2:L:56:THR:HB	2:L:57:ASP:HA	1.99	0.44
2:V:91:LEU:HB3	2:V:166:VAL:HG11	1.99	0.44
2:H:95:HIS:CE1	2:H:97:ASP:HB3	2.53	0.44
2:L:119:TYR:CE1	2:L:132:LEU:HD13	2.52	0.44
2:P:121:ILE:HG13	2:P:132:LEU:HD22	1.97	0.44
2:W:131:TRP:CE2	2:W:132:LEU:O	2.70	0.44
2:G:74:HIS:CE1	2:G:144:LEU:HD22	2.52	0.43
2:V:131:TRP:CD2	2:V:142:PHE:N	2.70	0.43
2:O:93:GLU:HG2	2:V:132:LEU:H	23.36	0.43
2:S:129:GLN:O	2:S:130:ILE:HB	2.19	0.43
2:W:131:TRP:NE1	2:W:133:ALA:HA	2.33	0.43
2:V:131:TRP:CZ2	2:V:142:PHE:N	2.79	0.43
2:L:131:TRP:HE1	2:L:133:ALA:CB	2.12	0.43
2:S:131:TRP:CD1	2:S:132:LEU:N	2.87	0.42
2:H:72:LYS:H	2:H:72:LYS:HD2	1.84	0.42
2:A:75:GLU:HB3	2:A:76:GLU:HA	2.00	0.42
2:S:121:ILE:HG22	2:S:132:LEU:HD23	2.02	0.42
2:L:131:TRP:HZ2	2:L:139:PRO:CG	2.32	0.42
2:F:157:LYS:HD2	2:F:157:LYS:H	1.84	0.42
2:A:76:GLU:OE1	2:C:131:TRP:HZ3	2.01	0.42
2:C:131:TRP:CZ2	2:C:139:PRO:CB	3.02	0.42
2:I:96:PRO:O	2:I:97:ASP:HB2	2.20	0.42
2:V:131:TRP:CZ2	2:V:142:PHE:O	2.73	0.42
2:O:72:LYS:HD2	2:O:72:LYS:H	1.84	0.41
2:W:113:ILE:H	2:W:118:THR:HG22	1.85	0.41
2:B:93:GLU:HB2	2:O:132:LEU:HD23	20.75	0.41
2:C:59:GLN:HE22	2:J:66:LEU:HG	1.85	0.41
2:W:131:TRP:HA	2:W:142:PHE:HB2	2.02	0.41
2:L:131:TRP:CZ2	2:L:139:PRO:CG	3.03	0.41
2:V:131:TRP:NE1	2:V:142:PHE:H	1.56	0.41
2:M:158:LEU:H	2:M:158:LEU:HD23	1.86	0.41
2:C:94:ALA:H	2:L:132:LEU:HB2	22.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:124:GLN:H	2:H:130:ILE:H	1.68	0.41
2:V:95:HIS:CE1	2:V:170:ILE:HG13	2.55	0.41
2:T:75:GLU:N	2:T:76:GLU:HA	2.36	0.41
2:W:130:ILE:HG22	2:W:131:TRP:N	2.36	0.41
2:S:130:ILE:HG21	2:S:158:LEU:HD22	2.02	0.41
2:S:130:ILE:HD12	2:S:149:TRP:CD2	2.56	0.41
2:S:132:LEU:HD11	2:S:158:LEU:HB3	2.02	0.40
2:C:75:GLU:N	2:C:76:GLU:HA	2.36	0.40
2:F:121:ILE:CG2	2:F:132:LEU:CD2	2.99	0.40
2:G:132:LEU:C	2:G:132:LEU:HD22	4.07	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	121 (86%)	12 (9%)	7 (5%)	2	26
1	b	140/142 (99%)	124 (89%)	11 (8%)	5 (4%)	4	32
1	c	140/142 (99%)	122 (87%)	10 (7%)	8 (6%)	2	23
1	d	140/142 (99%)	123 (88%)	9 (6%)	8 (6%)	2	23
1	e	140/142 (99%)	123 (88%)	11 (8%)	6 (4%)	3	28
1	f	140/142 (99%)	120 (86%)	14 (10%)	6 (4%)	3	28
1	g	140/142 (99%)	118 (84%)	20 (14%)	2 (1%)	12	52
1	h	140/142 (99%)	118 (84%)	15 (11%)	7 (5%)	2	26
1	i	140/142 (99%)	124 (89%)	10 (7%)	6 (4%)	3	28
1	j	140/142 (99%)	118 (84%)	12 (9%)	10 (7%)	1	19
1	k	140/142 (99%)	120 (86%)	13 (9%)	7 (5%)	2	26
1	l	140/142 (99%)	122 (87%)	12 (9%)	6 (4%)	3	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	m	140/142 (99%)	118 (84%)	17 (12%)	5 (4%)	4	32
1	n	140/142 (99%)	118 (84%)	19 (14%)	3 (2%)	8	43
1	o	140/142 (99%)	121 (86%)	14 (10%)	5 (4%)	4	32
1	p	140/142 (99%)	123 (88%)	11 (8%)	6 (4%)	3	28
1	q	140/142 (99%)	122 (87%)	12 (9%)	6 (4%)	3	28
1	r	140/142 (99%)	118 (84%)	14 (10%)	8 (6%)	2	23
1	s	140/142 (99%)	125 (89%)	7 (5%)	8 (6%)	2	23
1	t	140/142 (99%)	120 (86%)	13 (9%)	7 (5%)	2	26
1	u	140/142 (99%)	122 (87%)	11 (8%)	7 (5%)	2	26
1	v	140/142 (99%)	119 (85%)	12 (9%)	9 (6%)	1	21
1	w	140/142 (99%)	118 (84%)	18 (13%)	4 (3%)	5	36
1	x	140/142 (99%)	124 (89%)	11 (8%)	5 (4%)	4	32
2	A	119/121 (98%)	93 (78%)	24 (20%)	2 (2%)	10	49
2	B	119/121 (98%)	95 (80%)	14 (12%)	10 (8%)	1	15
2	C	119/121 (98%)	96 (81%)	18 (15%)	5 (4%)	3	29
2	D	119/121 (98%)	102 (86%)	11 (9%)	6 (5%)	2	26
2	E	119/121 (98%)	92 (77%)	20 (17%)	7 (6%)	2	22
2	F	119/121 (98%)	92 (77%)	20 (17%)	7 (6%)	2	22
2	G	119/121 (98%)	99 (83%)	14 (12%)	6 (5%)	2	26
2	H	119/121 (98%)	98 (82%)	18 (15%)	3 (2%)	6	39
2	I	119/121 (98%)	101 (85%)	11 (9%)	7 (6%)	2	22
2	J	119/121 (98%)	94 (79%)	20 (17%)	5 (4%)	3	29
2	K	119/121 (98%)	97 (82%)	15 (13%)	7 (6%)	2	22
2	L	119/121 (98%)	95 (80%)	15 (13%)	9 (8%)	1	17
2	M	119/121 (98%)	97 (82%)	14 (12%)	8 (7%)	1	20
2	N	119/121 (98%)	98 (82%)	16 (13%)	5 (4%)	3	29
2	O	119/121 (98%)	94 (79%)	21 (18%)	4 (3%)	4	33
2	P	119/121 (98%)	99 (83%)	13 (11%)	7 (6%)	2	22
2	Q	119/121 (98%)	90 (76%)	22 (18%)	7 (6%)	2	22
2	R	119/121 (98%)	97 (82%)	18 (15%)	4 (3%)	4	33
2	S	119/121 (98%)	95 (80%)	19 (16%)	5 (4%)	3	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T	119/121 (98%)	100 (84%)	8 (7%)	11 (9%)	1	14
2	U	119/121 (98%)	97 (82%)	16 (13%)	6 (5%)	2	26
2	V	119/121 (98%)	100 (84%)	13 (11%)	6 (5%)	2	26
2	W	119/121 (98%)	93 (78%)	21 (18%)	5 (4%)	3	29
2	X	119/121 (98%)	98 (82%)	12 (10%)	9 (8%)	1	17
All	All	6216/6312 (98%)	5213 (84%)	701 (11%)	302 (5%)	4	26

All (302) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	39	VAL
1	b	68	ALA
2	B	127	ASN
2	B	136	LEU
1	c	123	ASN
1	c	131	SER
1	d	135	VAL
1	d	139	CYS
1	d	159	ASN
2	E	127	ASN
1	f	123	ASN
1	f	131	SER
2	F	77	ALA
2	F	79	ASP
2	F	94	ALA
2	F	116	PHE
2	F	127	ASN
1	g	135	VAL
2	H	67	ASN
1	i	131	SER
2	I	97	ASP
2	J	127	ASN
1	k	123	ASN
2	L	67	ASN
2	L	127	ASN
1	m	139	CYS
2	M	65	VAL
2	M	127	ASN
1	n	123	ASN
1	n	134	PRO

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Mol	Chain	Res	Type
2	N	77	ALA
2	N	94	ALA
2	N	116	PHE
1	o	131	SER
1	o	161	PRO
2	O	127	ASN
2	P	127	ASN
2	P	130	ILE
2	P	136	LEU
1	r	123	ASN
1	r	135	VAL
1	r	139	CYS
2	R	127	ASN
1	s	120	LYS
1	s	123	ASN
1	s	135	VAL
1	s	139	CYS
2	S	101	ASP
2	S	127	ASN
1	t	131	SER
1	t	136	LYS
2	T	127	ASN
1	u	38	LYS
2	U	77	ALA
2	U	141	ARG
1	v	31	THR
1	v	135	VAL
1	v	139	CYS
2	V	127	ASN
2	W	130	ILE
1	x	135	VAL
2	X	94	ALA
2	X	115	ALA
1	a	34	LEU
1	a	131	SER
2	A	73	ALA
1	b	136	LYS
2	B	97	ASP
2	B	98	CYS
2	B	100	PRO
1	c	38	LYS
2	C	130	ILE

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Mol	Chain	Res	Type
1	d	123	ASN
1	e	53	ASP
1	e	123	ASN
2	G	130	ILE
1	h	123	ASN
1	h	159	ASN
2	I	65	VAL
2	I	127	ASN
1	j	39	VAL
1	j	131	SER
1	j	136	LYS
1	k	131	SER
1	k	138	HIS
2	K	76	GLU
2	L	130	ILE
1	m	123	ASN
1	m	135	VAL
2	M	63	GLN
2	M	115	ALA
2	M	130	ILE
1	n	39	VAL
1	o	159	ASN
2	O	100	PRO
2	O	111	LEU
1	p	123	ASN
1	p	159	ASN
1	q	38	LYS
1	q	114	THR
1	q	161	PRO
2	Q	116	PHE
2	R	94	ALA
2	S	130	ILE
1	t	96	CYS
2	T	73	ALA
1	u	114	THR
1	u	159	ASN
2	U	97	ASP
1	v	40	ILE
1	v	159	ASN
1	x	38	LYS
2	X	56	THR
2	X	130	ILE

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Mol	Chain	Res	Type
1	a	159	ASN
2	B	94	ALA
1	c	29	SER
1	c	119	ALA
1	c	159	ASN
1	d	130	LEU
2	D	127	ASN
1	e	37	PRO
1	e	136	LYS
2	E	63	GLN
1	f	50	GLY
1	g	161	PRO
1	h	140	SER
2	H	130	ILE
1	i	45	HIS
1	i	159	ASN
1	j	135	VAL
2	J	97	ASP
2	K	73	ALA
2	K	126	PRO
1	l	38	LYS
2	L	54	SER
2	L	156	THR
1	m	29	SER
2	M	114	PRO
2	N	126	PRO
1	p	64	VAL
1	p	139	CYS
2	Q	94	ALA
2	Q	119	TYR
2	Q	126	PRO
2	Q	130	ILE
1	s	131	SER
1	t	161	PRO
2	T	119	TYR
2	T	147	GLY
2	U	130	ILE
2	U	137	SER
1	v	68	ALA
1	v	120	LYS
1	v	123	ASN
2	V	98	CYS

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Mol	Chain	Res	Type
2	V	135	PRO
2	W	75	GLU
1	x	123	ASN
1	x	131	SER
1	x	159	ASN
2	X	127	ASN
1	a	161	PRO
1	b	40	ILE
1	b	67	PRO
2	B	146	ASN
2	C	62	PRO
2	D	62	PRO
2	D	64	GLU
2	D	154	ASN
1	f	38	LYS
1	f	132	LEU
2	F	135	PRO
2	F	137	SER
2	G	62	PRO
2	G	127	ASN
2	G	154	ASN
1	h	161	PRO
2	I	73	ALA
1	j	45	HIS
2	J	94	ALA
1	k	45	HIS
1	k	161	PRO
2	K	120	VAL
2	K	130	ILE
1	l	31	THR
2	L	61	VAL
2	L	76	GLU
2	L	97	ASP
1	p	38	LYS
2	P	53	GLU
2	P	76	GLU
1	q	130	LEU
1	r	56	LEU
1	r	119	ALA
1	r	131	SER
2	R	97	ASP
2	S	126	PRO

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Mol	Chain	Res	Type
1	t	123	ASN
2	T	56	THR
2	T	94	ALA
2	T	130	ILE
1	u	131	SER
2	U	64	GLU
2	V	101	ASP
1	w	36	HIS
1	w	137	LEU
2	W	56	THR
2	X	97	ASP
2	X	154	ASN
1	a	123	ASN
1	b	56	LEU
2	B	75	GLU
2	B	130	ILE
1	c	56	LEU
2	C	53	GLU
2	C	63	GLN
2	C	116	PHE
1	d	29	SER
2	D	130	ILE
1	e	56	LEU
2	E	77	ALA
2	E	115	ALA
2	E	130	ILE
2	E	153	ARG
2	G	114	PRO
1	h	38	LYS
1	h	42	HIS
2	H	63	GLN
1	i	56	LEU
2	I	63	GLN
2	I	94	ALA
2	I	100	PRO
1	j	56	LEU
1	j	82	SER
1	j	140	SER
2	J	130	ILE
1	k	159	ASN
2	K	61	VAL
2	K	127	ASN

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Mol	Chain	Res	Type
1	l	131	SER
1	l	161	PRO
1	m	134	PRO
2	M	53	GLU
1	o	135	VAL
2	O	130	ILE
2	P	146	ASN
1	q	31	THR
1	q	56	LEU
2	Q	100	PRO
1	s	37	PRO
2	S	94	ALA
1	t	160	THR
2	T	100	PRO
2	T	121	ILE
2	T	146	ASN
2	T	154	ASN
2	V	130	ILE
1	w	159	ASN
2	W	100	PRO
2	W	153	ARG
2	X	73	ALA
2	X	98	CYS
1	a	59	VAL
2	A	127	ASN
1	d	56	LEU
1	d	161	PRO
2	D	56	THR
1	e	160	THR
1	i	37	PRO
1	j	63	LEU
1	j	160	THR
1	l	56	LEU
2	M	74	HIS
2	N	127	ASN
1	o	120	LYS
2	P	63	GLN
2	Q	133	ALA
1	r	29	SER
1	r	132	LEU
2	R	154	ASN
1	t	159	ASN

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Mol	Chain	Res	Type
1	u	68	ALA
1	u	161	PRO
2	B	61	VAL
2	E	96	PRO
2	J	100	PRO
1	v	161	PRO
2	V	100	PRO
2	G	126	PRO
1	u	56	LEU
1	c	161	PRO
1	h	56	LEU
1	k	57	PRO
1	l	39	VAL
1	w	67	PRO
1	f	135	VAL
1	i	160	THR
2	L	114	PRO
1	p	67	PRO
1	s	133	PRO
1	s	46	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%)	119 (98%)	2 (2%)	63	83
1	b	121/121 (100%)	117 (97%)	4 (3%)	41	67
1	c	121/121 (100%)	116 (96%)	5 (4%)	33	62
1	d	121/121 (100%)	116 (96%)	5 (4%)	33	62
1	e	121/121 (100%)	115 (95%)	6 (5%)	27	57
1	f	121/121 (100%)	118 (98%)	3 (2%)	50	74
1	g	121/121 (100%)	113 (93%)	8 (7%)	18	49
1	h	121/121 (100%)	111 (92%)	10 (8%)	12	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	i	121/121 (100%)	115 (95%)	6 (5%)	27	57
1	j	121/121 (100%)	114 (94%)	7 (6%)	22	53
1	k	121/121 (100%)	118 (98%)	3 (2%)	50	74
1	l	121/121 (100%)	113 (93%)	8 (7%)	18	49
1	m	121/121 (100%)	112 (93%)	9 (7%)	15	45
1	n	121/121 (100%)	117 (97%)	4 (3%)	41	67
1	o	121/121 (100%)	118 (98%)	3 (2%)	50	74
1	p	121/121 (100%)	111 (92%)	10 (8%)	12	41
1	q	121/121 (100%)	118 (98%)	3 (2%)	50	74
1	r	121/121 (100%)	116 (96%)	5 (4%)	33	62
1	s	121/121 (100%)	114 (94%)	7 (6%)	22	53
1	t	121/121 (100%)	117 (97%)	4 (3%)	41	67
1	u	121/121 (100%)	119 (98%)	2 (2%)	63	83
1	v	121/121 (100%)	113 (93%)	8 (7%)	18	49
1	w	121/121 (100%)	115 (95%)	6 (5%)	27	57
1	x	121/121 (100%)	117 (97%)	4 (3%)	41	67
2	A	109/109 (100%)	106 (97%)	3 (3%)	47	71
2	B	109/109 (100%)	105 (96%)	4 (4%)	37	65
2	C	109/109 (100%)	101 (93%)	8 (7%)	15	46
2	D	109/109 (100%)	103 (94%)	6 (6%)	24	55
2	E	109/109 (100%)	104 (95%)	5 (5%)	29	59
2	F	109/109 (100%)	103 (94%)	6 (6%)	24	55
2	G	109/109 (100%)	104 (95%)	5 (5%)	29	59
2	H	109/109 (100%)	105 (96%)	4 (4%)	37	65
2	I	109/109 (100%)	104 (95%)	5 (5%)	29	59
2	J	109/109 (100%)	105 (96%)	4 (4%)	37	65
2	K	109/109 (100%)	103 (94%)	6 (6%)	24	55
2	L	109/109 (100%)	107 (98%)	2 (2%)	62	82
2	M	109/109 (100%)	105 (96%)	4 (4%)	37	65
2	N	109/109 (100%)	107 (98%)	2 (2%)	62	82
2	O	109/109 (100%)	106 (97%)	3 (3%)	47	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	109/109 (100%)	105 (96%)	4 (4%)	37	65
2	Q	109/109 (100%)	104 (95%)	5 (5%)	29	59
2	R	109/109 (100%)	107 (98%)	2 (2%)	62	82
2	S	109/109 (100%)	104 (95%)	5 (5%)	29	59
2	T	109/109 (100%)	101 (93%)	8 (7%)	15	46
2	U	109/109 (100%)	106 (97%)	3 (3%)	47	71
2	V	109/109 (100%)	106 (97%)	3 (3%)	47	71
2	W	109/109 (100%)	105 (96%)	4 (4%)	37	65
2	X	109/109 (100%)	103 (94%)	6 (6%)	24	55
All	All	5520/5520 (100%)	5281 (96%)	239 (4%)	36	61

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	38	LYS
1	a	83	THR
2	A	89	GLU
2	A	131	TRP
2	A	140	ASN
1	b	33	ARG
1	b	71	ASP
1	b	122	LYS
1	b	141	MET
2	B	128	LYS
2	B	132	LEU
2	B	158	LEU
2	B	164	GLU
1	c	33	ARG
1	c	48	ASN
1	c	71	ASP
1	c	120	LYS
1	c	154	TYR
2	C	56	THR
2	C	59	GLN
2	C	74	HIS
2	C	76	GLU
2	C	93	GLU
2	C	111	LEU
2	C	113	ILE

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Mol	Chain	Res	Type
2	C	158	LEU
1	d	33	ARG
1	d	120	LYS
1	d	122	LYS
1	d	125	GLU
1	d	132	LEU
2	D	59	GLN
2	D	64	GLU
2	D	72	LYS
2	D	76	GLU
2	D	140	ASN
2	D	144	LEU
1	e	33	ARG
1	e	38	LYS
1	e	48	ASN
1	e	113	MET
1	e	120	LYS
1	e	163	MET
2	E	64	GLU
2	E	76	GLU
2	E	108	VAL
2	E	111	LEU
2	E	131	TRP
1	f	33	ARG
1	f	120	LYS
1	f	138	HIS
2	F	67	ASN
2	F	89	GLU
2	F	111	LEU
2	F	145	LEU
2	F	157	LYS
2	F	168	LYS
1	g	33	ARG
1	g	34	LEU
1	g	47	ARG
1	g	63	LEU
1	g	120	LYS
1	g	126	ILE
1	g	128	LYS
1	g	132	LEU
2	G	76	GLU
2	G	88	LEU

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Mol	Chain	Res	Type
2	G	132	LEU
2	G	140	ASN
2	G	157	LYS
1	h	33	ARG
1	h	38	LYS
1	h	47	ARG
1	h	48	ASN
1	h	87	GLU
1	h	92	LYS
1	h	115	LEU
1	h	120	LYS
1	h	148	LYS
1	h	160	THR
2	H	60	VAL
2	H	67	ASN
2	H	109	MET
2	H	168	LYS
1	i	33	ARG
1	i	106	MET
1	i	120	LYS
1	i	122	LYS
1	i	129	GLU
1	i	137	LEU
2	I	76	GLU
2	I	103	GLU
2	I	126	PRO
2	I	158	LEU
2	I	164	GLU
1	j	33	ARG
1	j	48	ASN
1	j	120	LYS
1	j	129	GLU
1	j	132	LEU
1	j	141	MET
1	j	148	LYS
2	J	59	GLN
2	J	145	LEU
2	J	152	LEU
2	J	168	LYS
1	k	49	VAL
1	k	71	ASP
1	k	158	ARG

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Mol	Chain	Res	Type
2	K	64	GLU
2	K	75	GLU
2	K	119	TYR
2	K	126	PRO
2	K	128	LYS
2	K	136	LEU
1	l	33	ARG
1	l	34	LEU
1	l	38	LYS
1	l	48	ASN
1	l	49	VAL
1	l	64	VAL
1	l	109	LEU
1	l	120	LYS
2	L	157	LYS
2	L	158	LEU
1	m	33	ARG
1	m	49	VAL
1	m	71	ASP
1	m	76	GLN
1	m	87	GLU
1	m	113	MET
1	m	120	LYS
1	m	125	GLU
1	m	132	LEU
2	M	72	LYS
2	M	111	LEU
2	M	157	LYS
2	M	168	LYS
1	n	38	LYS
1	n	122	LYS
1	n	134	PRO
1	n	148	LYS
2	N	67	ASN
2	N	84	LEU
1	o	48	ASN
1	o	132	LEU
1	o	148	LYS
2	O	118	THR
2	O	157	LYS
2	O	158	LEU
1	p	30	ILE

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Mol	Chain	Res	Type
1	p	33	ARG
1	p	38	LYS
1	p	49	VAL
1	p	71	ASP
1	p	120	LYS
1	p	122	LYS
1	p	124	THR
1	p	137	LEU
1	p	144	GLU
2	P	61	VAL
2	P	76	GLU
2	P	93	GLU
2	P	136	LEU
1	q	33	ARG
1	q	76	GLN
1	q	122	LYS
2	Q	53	GLU
2	Q	102	VAL
2	Q	113	ILE
2	Q	132	LEU
2	Q	153	ARG
1	r	33	ARG
1	r	49	VAL
1	r	71	ASP
1	r	126	ILE
1	r	135	VAL
2	R	136	LEU
2	R	141	ARG
1	s	27	MET
1	s	33	ARG
1	s	47	ARG
1	s	71	ASP
1	s	80	ASN
1	s	130	LEU
1	s	135	VAL
2	S	63	GLN
2	S	76	GLU
2	S	111	LEU
2	S	136	LEU
2	S	157	LYS
1	t	33	ARG
1	t	71	ASP

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Mol	Chain	Res	Type
1	t	120	LYS
1	t	142	LEU
2	T	56	THR
2	T	70	LEU
2	T	76	GLU
2	T	103	GLU
2	T	131	TRP
2	T	136	LEU
2	T	158	LEU
2	T	168	LYS
1	u	132	LEU
1	u	137	LEU
2	U	57	ASP
2	U	61	VAL
2	U	102	VAL
1	v	33	ARG
1	v	34	LEU
1	v	71	ASP
1	v	120	LYS
1	v	130	LEU
1	v	132	LEU
1	v	137	LEU
1	v	144	GLU
2	V	57	ASP
2	V	61	VAL
2	V	129	GLN
1	w	33	ARG
1	w	106	MET
1	w	122	LYS
1	w	125	GLU
1	w	137	LEU
1	w	148	LYS
2	W	111	LEU
2	W	119	TYR
2	W	142	PHE
2	W	157	LYS
1	x	35	TYR
1	x	48	ASN
1	x	71	ASP
1	x	120	LYS
2	X	61	VAL
2	X	119	TYR

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Mol	Chain	Res	Type
2	X	126	PRO
2	X	136	LEU
2	X	149	TRP
2	X	172	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	b	138	HIS
1	c	138	HIS
2	C	59	GLN
2	C	74	HIS
2	C	106	HIS
2	C	124	GLN
2	D	95	HIS
2	D	124	GLN
2	E	74	HIS
1	f	138	HIS
2	F	67	ASN
2	F	122	ASN
2	G	74	HIS
2	G	129	GLN
2	H	67	ASN
2	H	74	HIS
2	H	95	HIS
2	H	127	ASN
2	I	67	ASN
2	I	127	ASN
2	J	106	HIS
1	k	123	ASN
2	K	95	HIS
1	l	48	ASN
2	L	122	ASN
2	N	67	ASN
2	N	95	HIS
2	N	124	GLN
2	O	63	GLN
2	P	74	HIS
1	r	76	GLN
2	R	74	HIS
2	R	124	GLN
2	R	140	ASN

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Mol	Chain	Res	Type
1	s	26	HIS
1	s	80	ASN
2	S	74	HIS
2	S	154	ASN
1	t	138	HIS
2	U	83	HIS
2	V	124	GLN
2	V	129	GLN
1	x	48	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.