



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:27 PM UTC

PDB ID : 5TRE / pdb\_00005tre  
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 EM Validation Report for a publicly released PDB 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

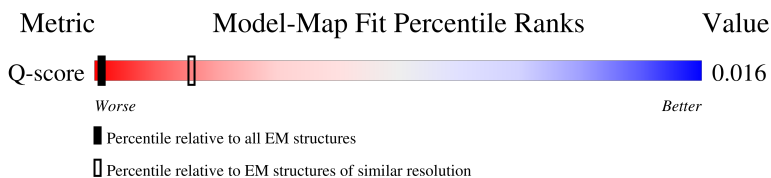
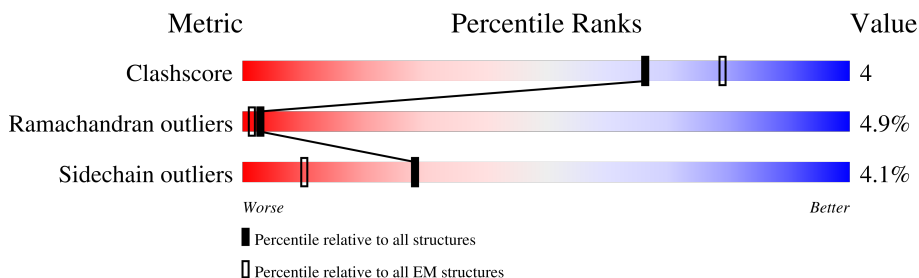
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	38 ( 15.30 - 16.10 )

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

Mol	Chain	Length	Quality of chain
1	a	142	<div> <div>39%</div> <div>78%</div> <div>18%</div> <div>.</div> </div>
1	b	142	<div> <div>44%</div> <div>77%</div> <div>23%</div> <div>.</div> </div>
1	c	142	<div> <div>39%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
1	d	142	<div> <div>44%</div> <div>81%</div> <div>16%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	e	142	42% 76% 20% ..
1	f	142	42% 82% 15% ..
1	g	142	39% 77% 20% .
1	h	142	46% 77% 19% .
1	i	142	41% 77% 20% .
1	j	142	46% 77% 18% 6%
1	k	142	42% 77% 20% .
1	l	142	44% 77% 20% .
1	m	142	44% 76% 20% .
1	n	142	40% 77% 19% ..
1	o	142	43% 84% 14% .
1	p	142	42% 75% 20% 5% .
1	q	142	39% 84% 13% .
1	r	142	46% 79% 18% ..
1	s	142	44% 81% 15% ..
1	t	142	43% 75% 19% 6%
1	u	142	44% 80% 17% .
1	v	142	46% 78% 18% .
1	w	142	43% 78% 20% .
1	x	142	43% 79% 19% ..
2	A	121	45% 81% 18% .
2	B	121	42% 77% 19% .
2	C	121	42% 77% 18% ..
2	D	121	45% 80% 20%
2	E	121	44% 86% 13% .

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Mol	Chain	Length	Quality of chain
2	F	121	<div> <div>46%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
2	G	121	<div> <div>45%</div> <div>83%</div> <div>17%</div> </div>
2	H	121	<div> <div>45%</div> <div>79%</div> <div>17%</div> <div>..</div> </div>
2	I	121	<div> <div>47%</div> <div>76%</div> <div>19%</div> <div>5%</div> </div>
2	J	121	<div> <div>50%</div> <div>78%</div> <div>22%</div> </div>
2	K	121	<div> <div>48%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
2	L	121	<div> <div>42%</div> <div>78%</div> <div>17%</div> <div>5%</div> </div>
2	M	121	<div> <div>45%</div> <div>79%</div> <div>17%</div> <div>.</div> </div>
2	N	121	<div> <div>45%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
2	O	121	<div> <div>46%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
2	P	121	<div> <div>45%</div> <div>79%</div> <div>16%</div> <div>5%</div> </div>
2	Q	121	<div> <div>48%</div> <div>78%</div> <div>22%</div> </div>
2	R	121	<div> <div>46%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
2	S	121	<div> <div>45%</div> <div>74%</div> <div>23%</div> <div>.</div> </div>
2	T	121	<div> <div>47%</div> <div>75%</div> <div>22%</div> <div>..</div> </div>
2	U	121	<div> <div>41%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
2	V	121	<div> <div>45%</div> <div>74%</div> <div>25%</div> <div>.</div> </div>
2	W	121	<div> <div>47%</div> <div>72%</div> <div>24%</div> <div>..</div> </div>
2	X	121	<div> <div>45%</div> <div>76%</div> <div>21%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 48456 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Iron sulfur cluster assembly protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
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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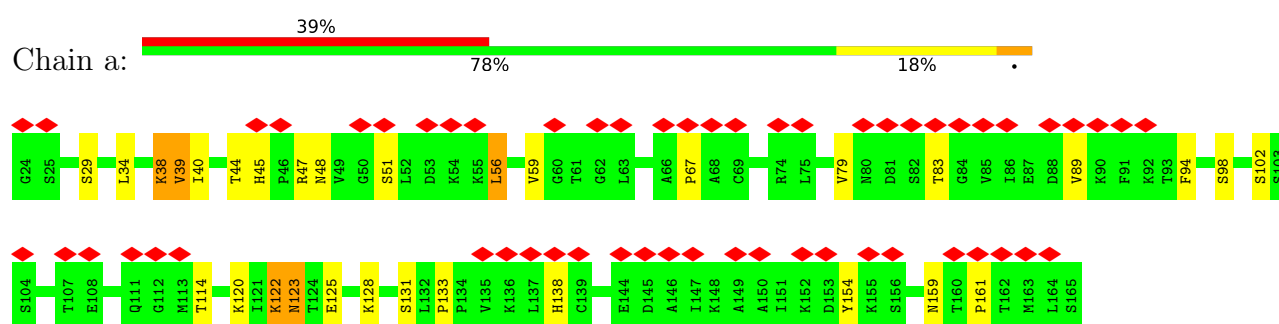
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Chain	Residue	Modelled	Actual	Comment	Reference
B	73	ALA	TYR	conflict	UNP Q07540
C	73	ALA	TYR	conflict	UNP Q07540
D	73	ALA	TYR	conflict	UNP Q07540
E	73	ALA	TYR	conflict	UNP Q07540
F	73	ALA	TYR	conflict	UNP Q07540
G	73	ALA	TYR	conflict	UNP Q07540
H	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

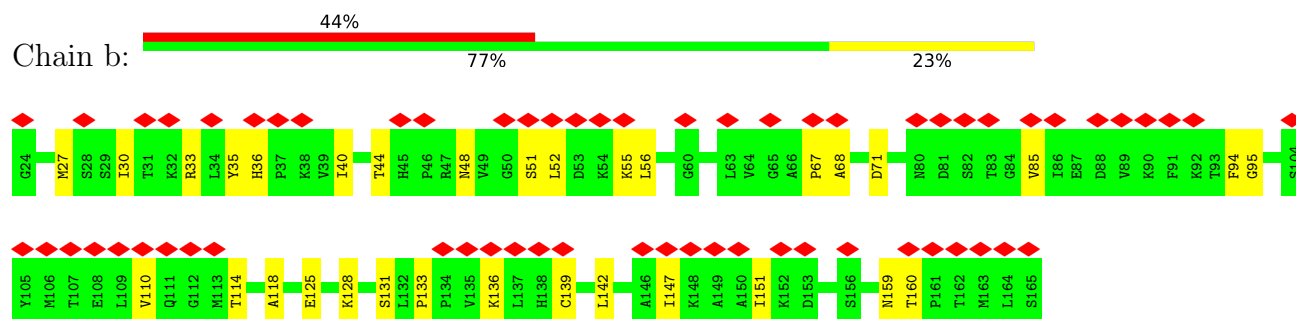
### 3 Residue-property plots [i](#)

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

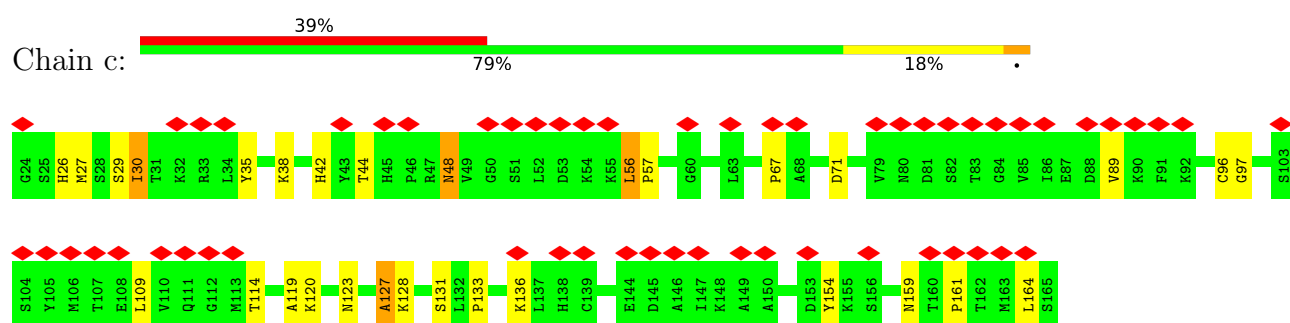
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



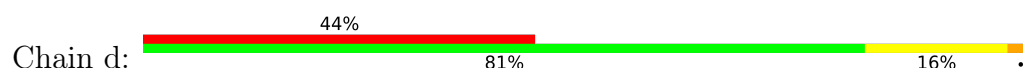
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

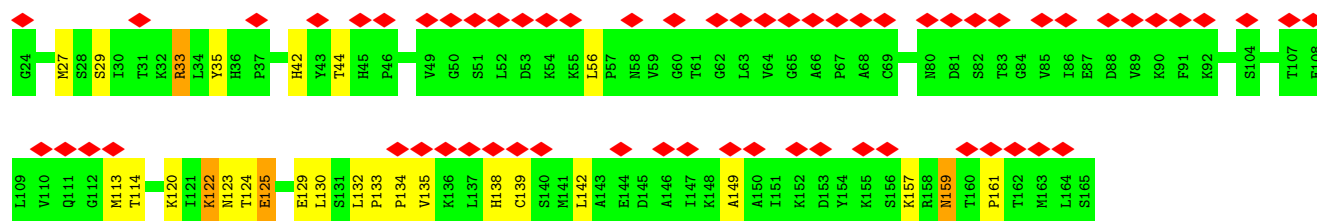


- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



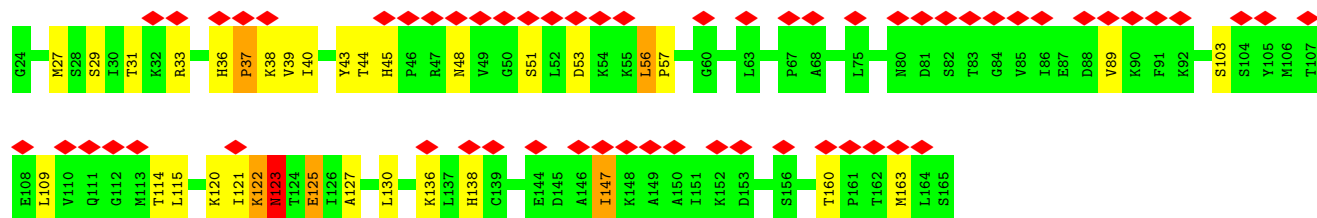
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial





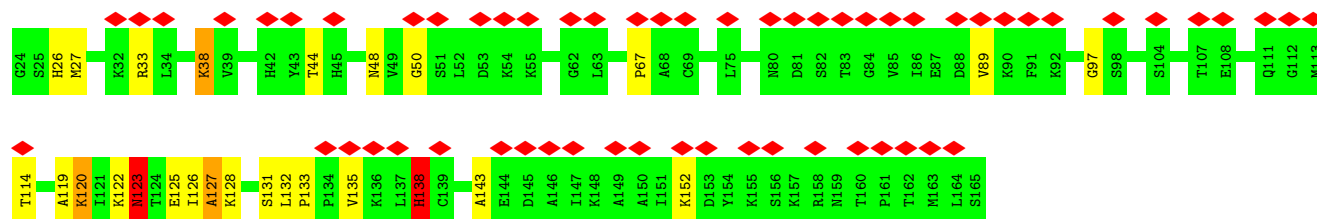
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain e: 42% 76% 20%



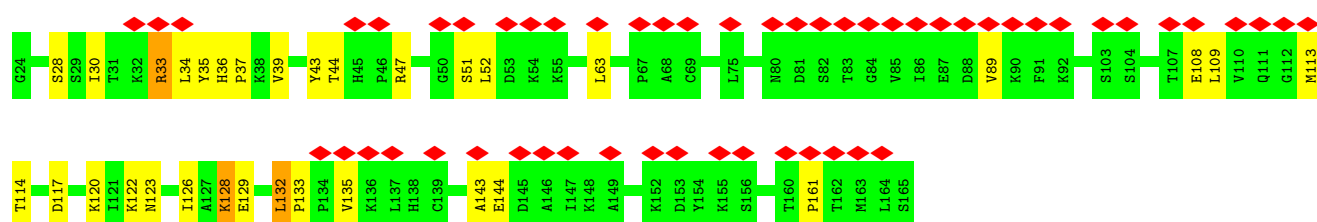
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain f: 42% 82% 15%



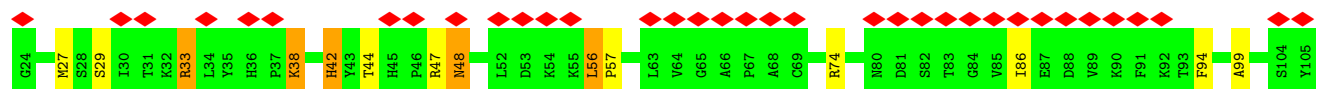
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

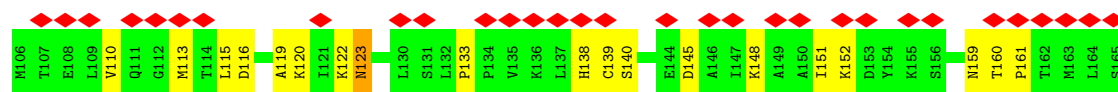
Chain g: 39% 77% 20%



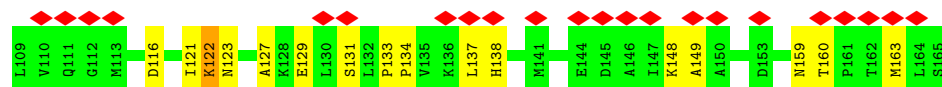
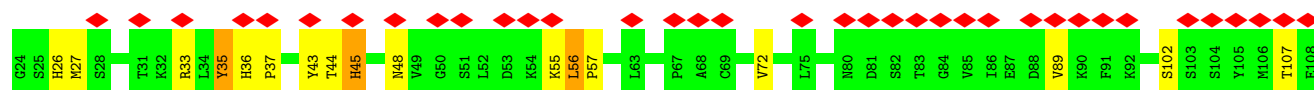
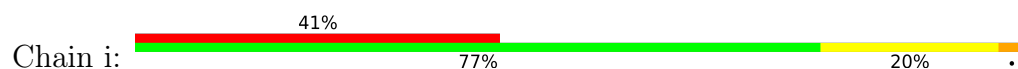
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain h: 46% 77% 19%

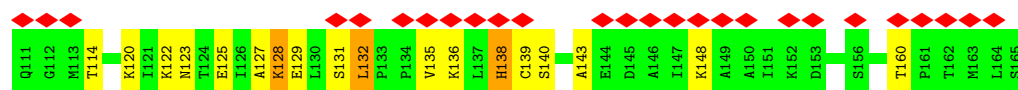
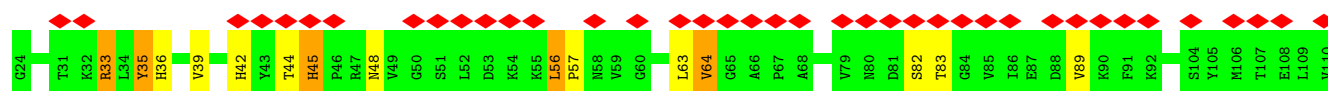
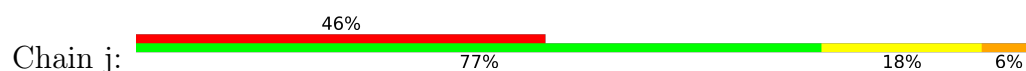




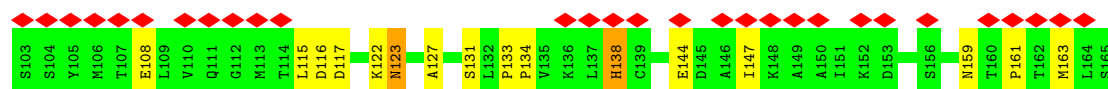
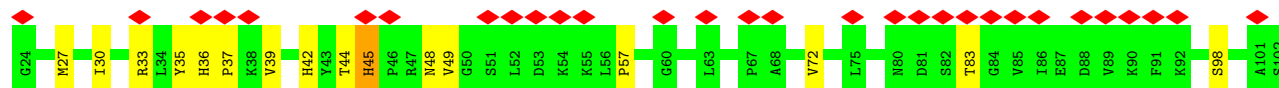
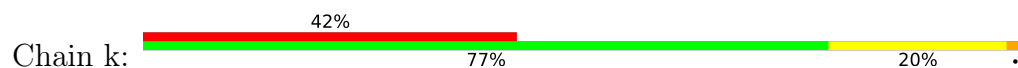
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



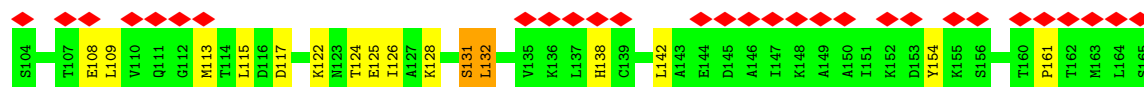
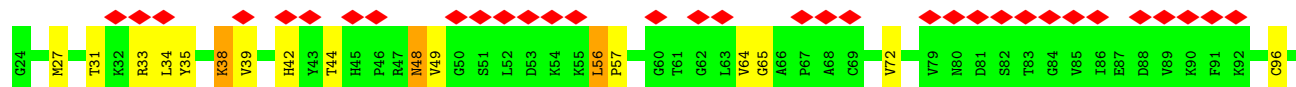
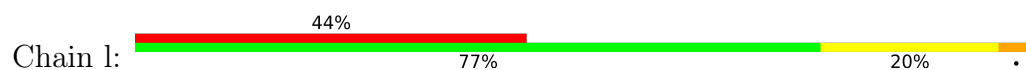
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



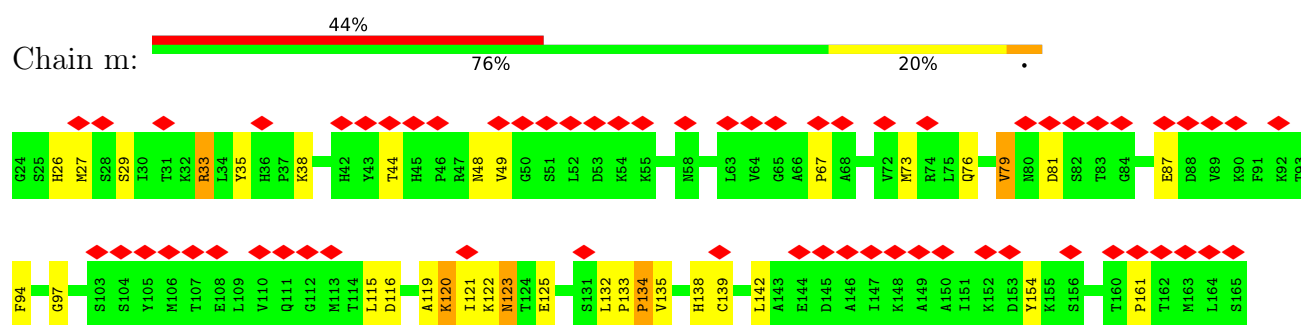
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



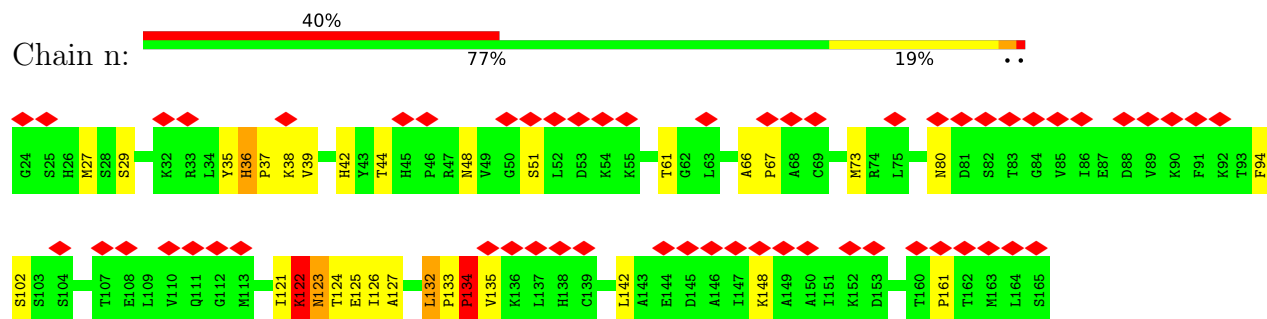
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



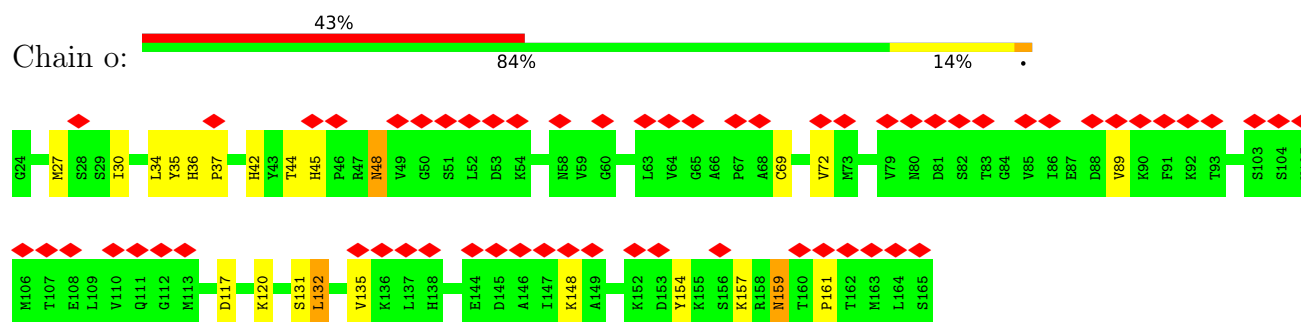
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



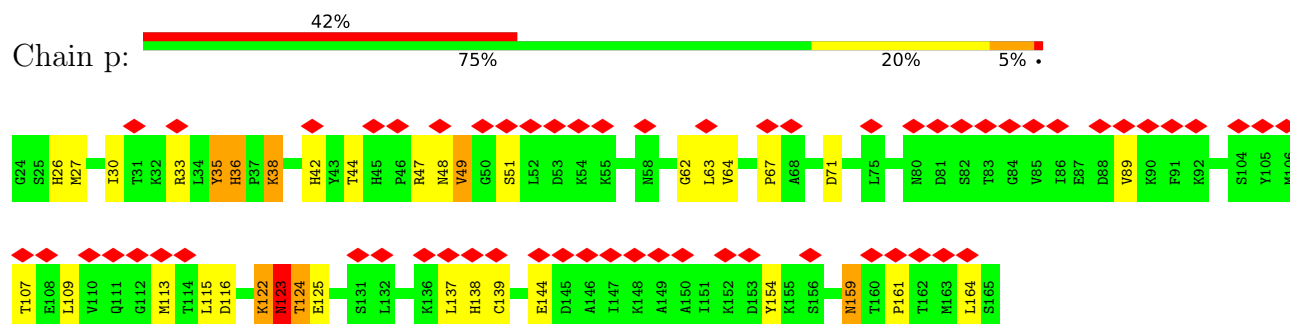
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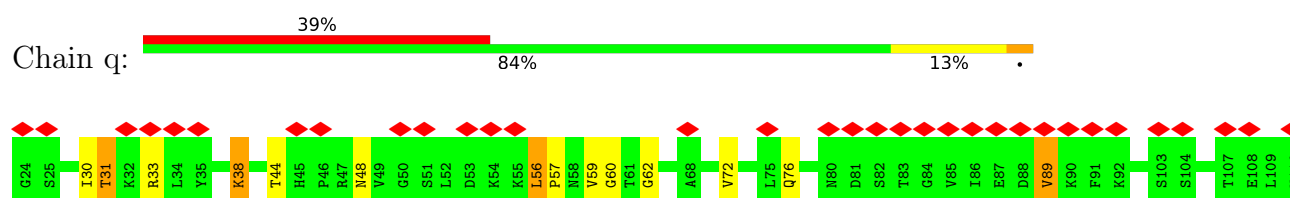
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

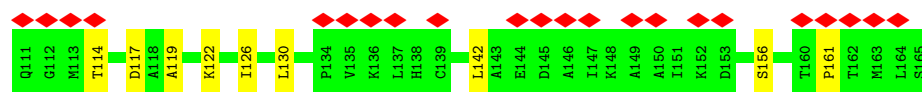


- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

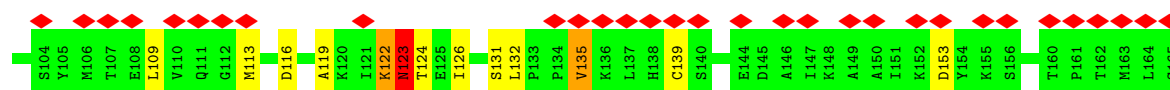
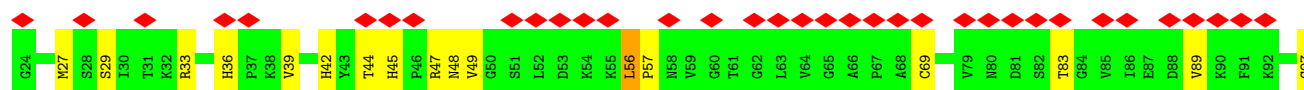
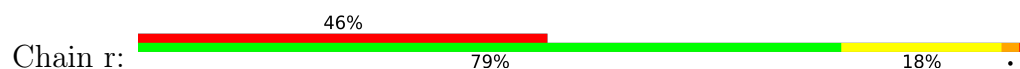


- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

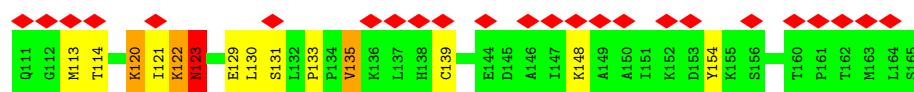
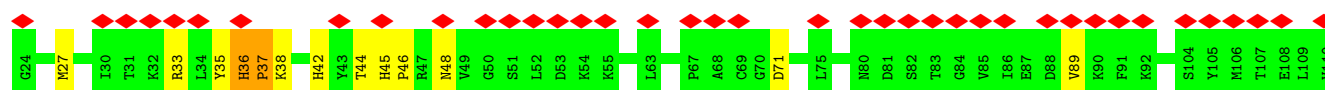
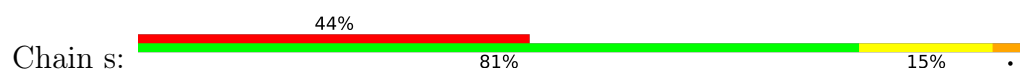




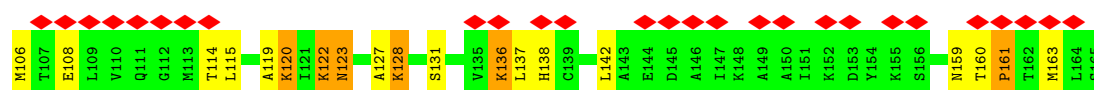
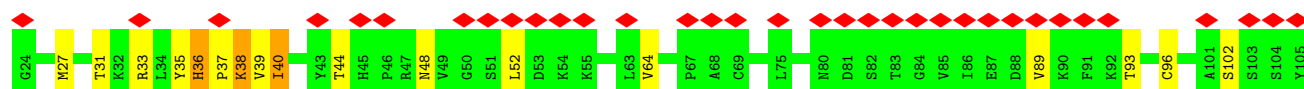
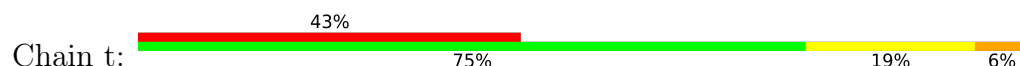
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



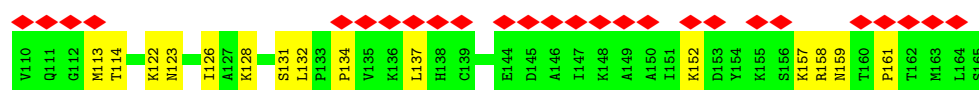
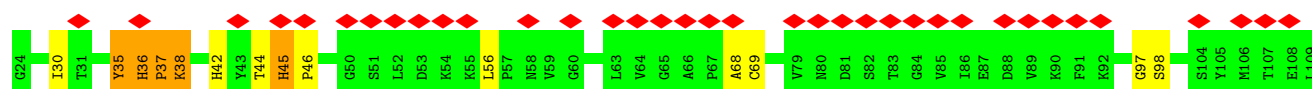
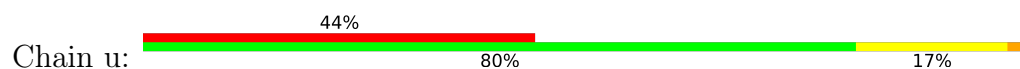
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



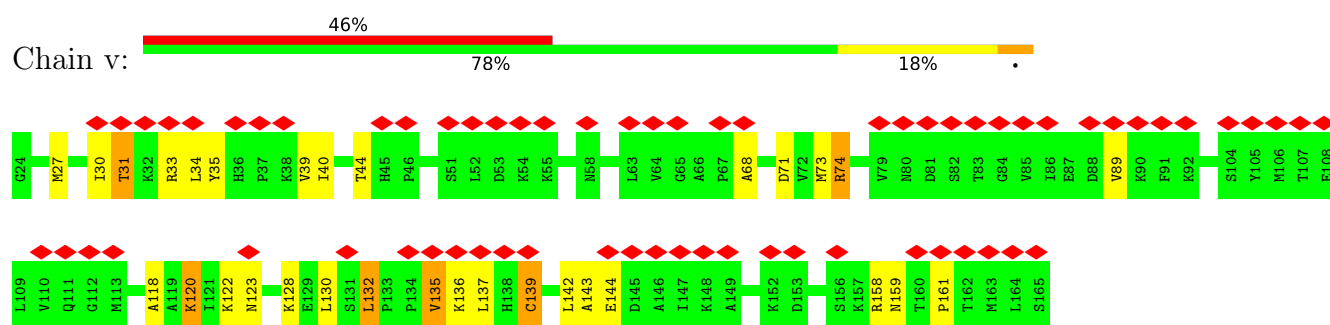
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



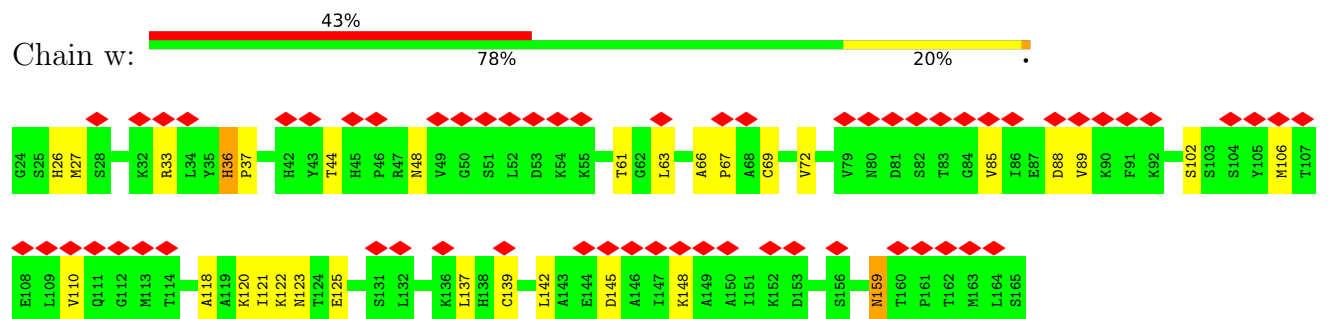
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



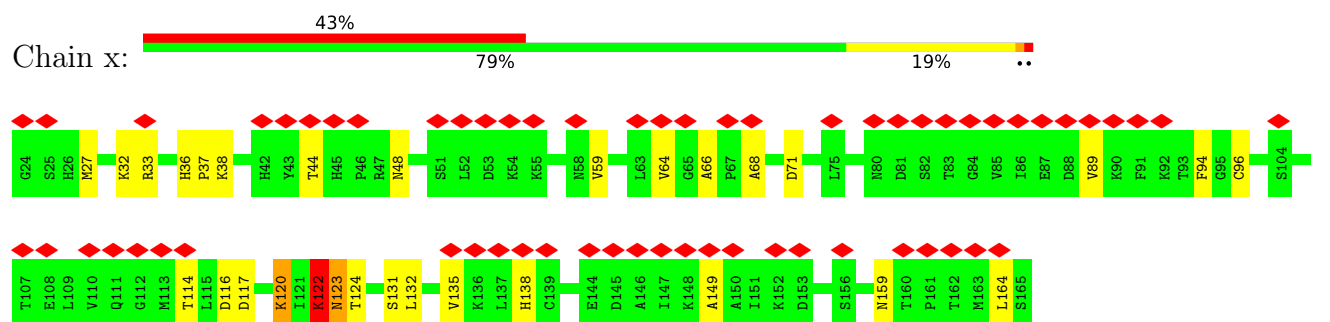
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



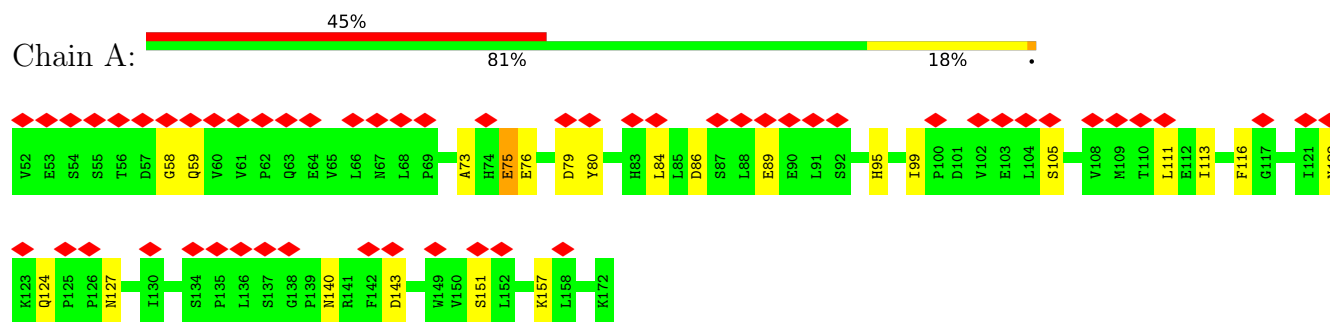
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



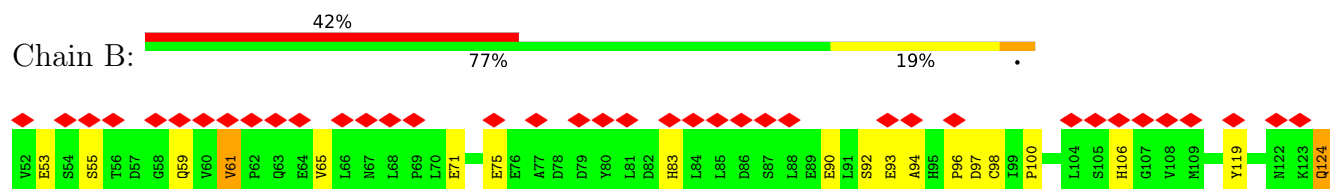
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



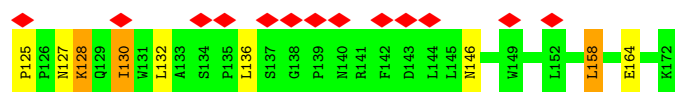
- Molecule 2: Frataxin homolog, mitochondrial



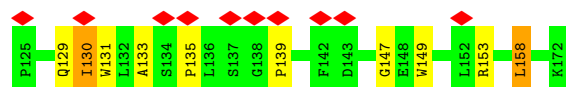
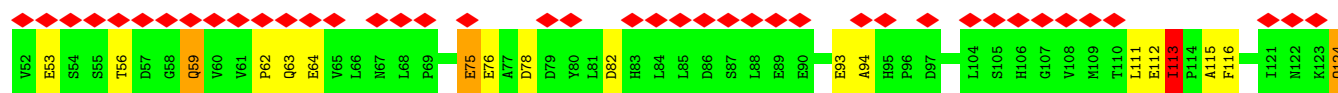
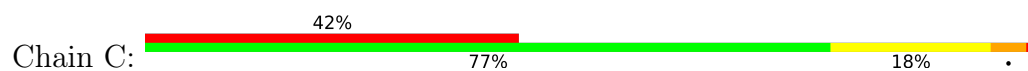
- Molecule 2: Frataxin homolog, mitochondrial



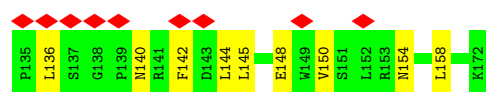
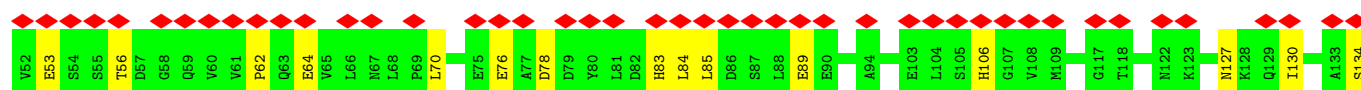
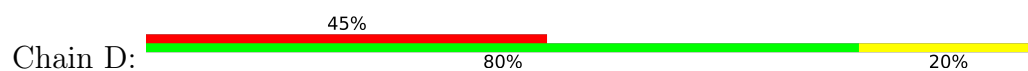




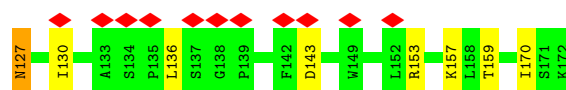
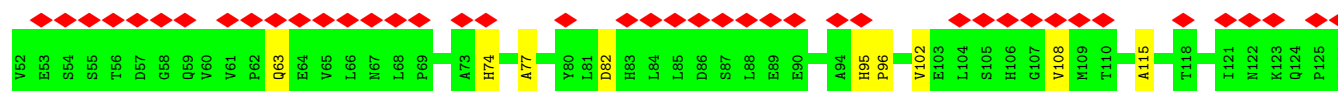
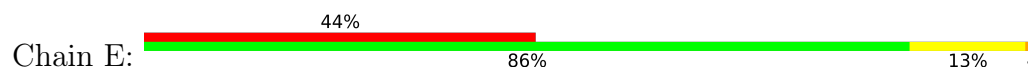
- Molecule 2: Frataxin homolog, mitochondrial



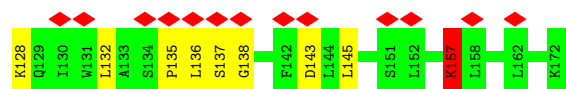
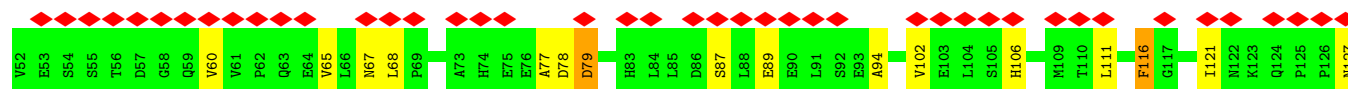
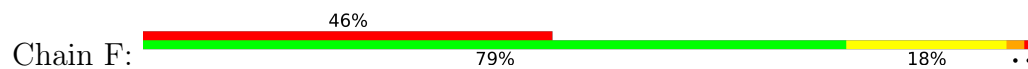
- Molecule 2: Frataxin homolog, mitochondrial



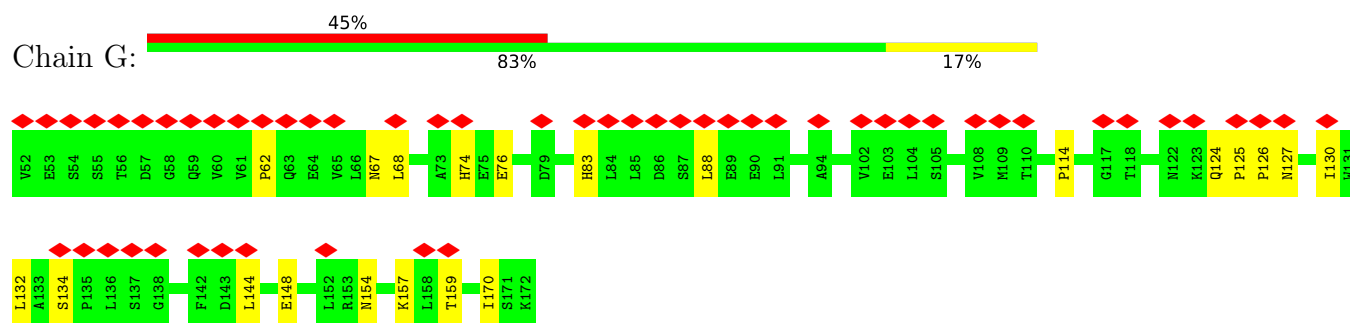
- Molecule 2: Frataxin homolog, mitochondrial



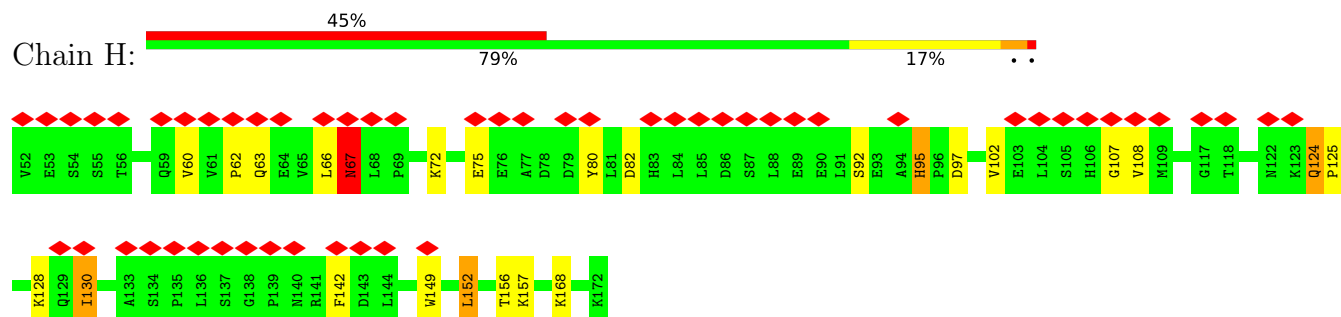
- Molecule 2: Frataxin homolog, mitochondrial



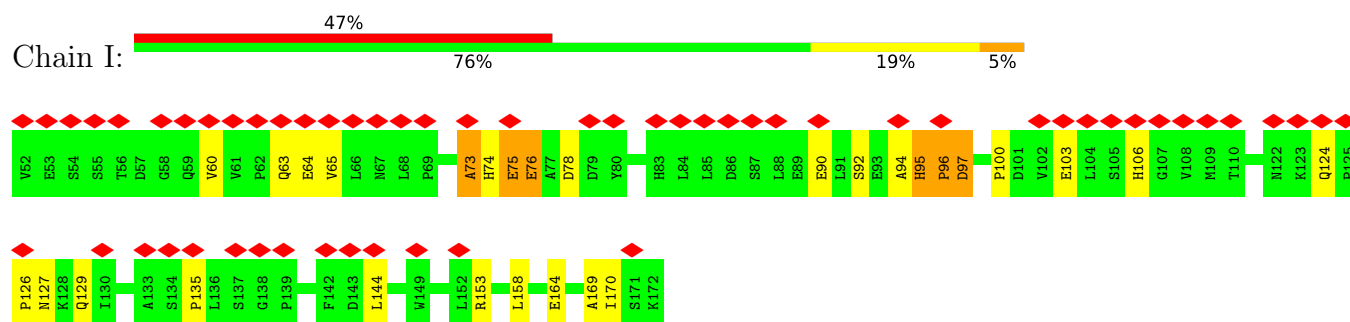
- Molecule 2: Frataxin homolog, mitochondrial



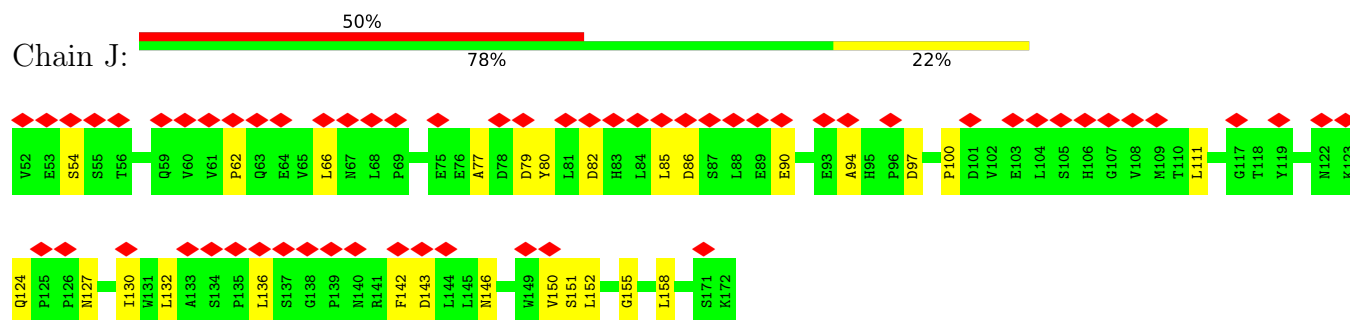
- Molecule 2: Frataxin homolog, mitochondrial



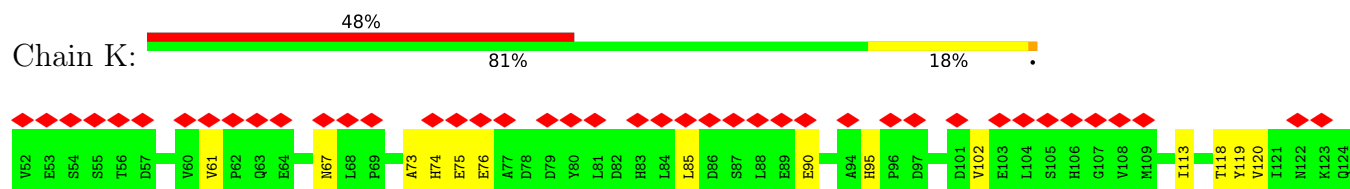
- Molecule 2: Frataxin homolog, mitochondrial

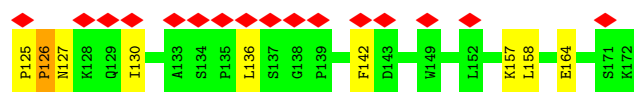


- Molecule 2: Frataxin homolog, mitochondrial

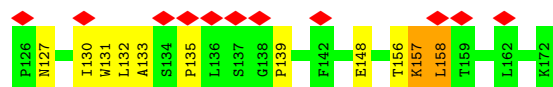
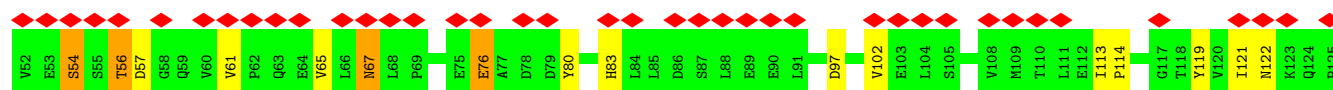
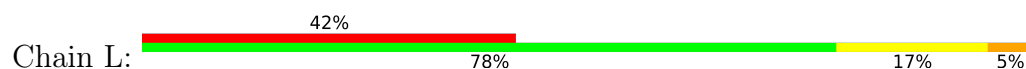


- Molecule 2: Frataxin homolog, mitochondrial

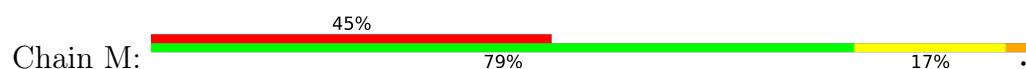




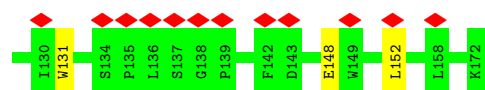
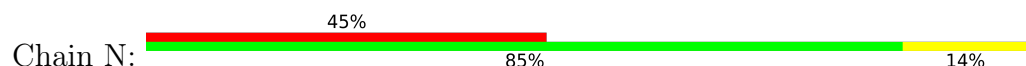
- Molecule 2: Frataxin homolog, mitochondrial



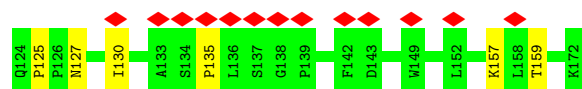
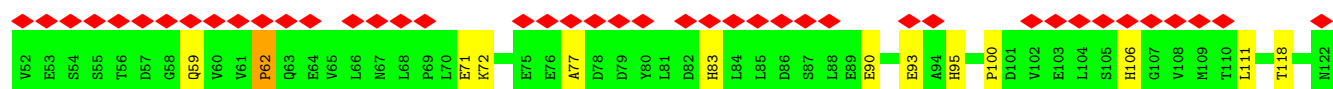
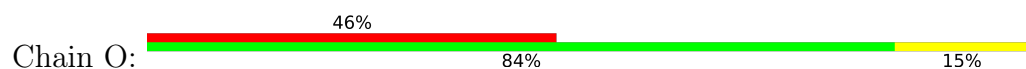
- Molecule 2: Frataxin homolog, mitochondrial



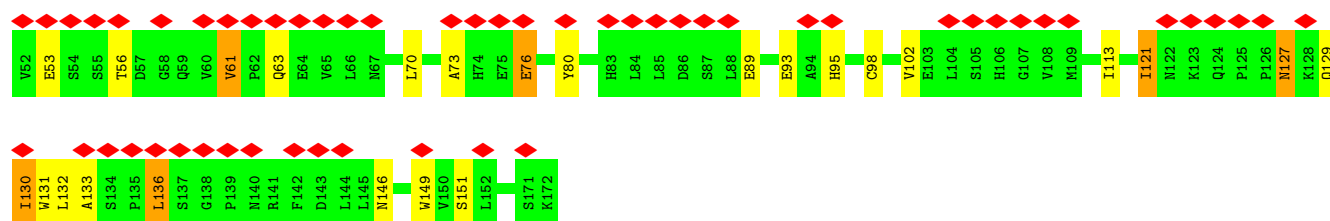
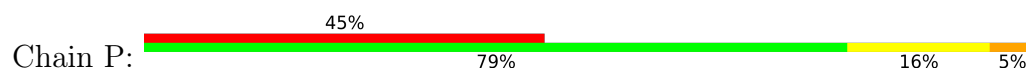
- Molecule 2: Frataxin homolog, mitochondrial



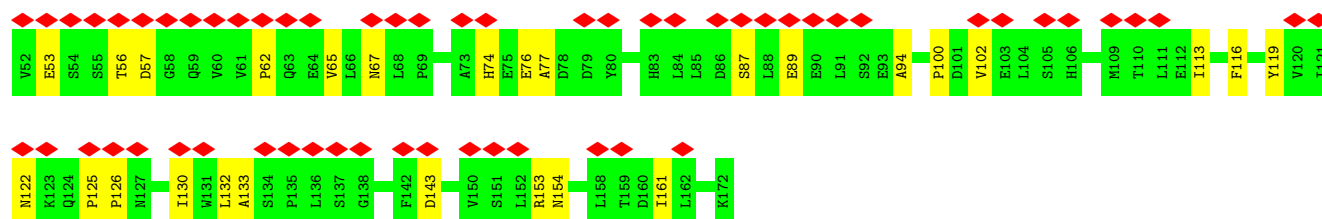
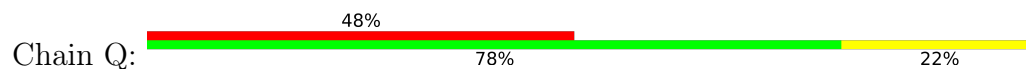
- Molecule 2: Frataxin homolog, mitochondrial



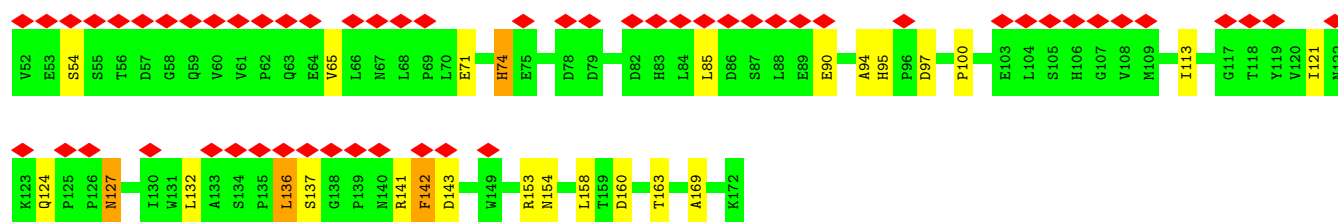
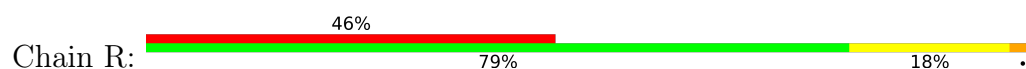
- Molecule 2: Frataxin homolog, mitochondrial



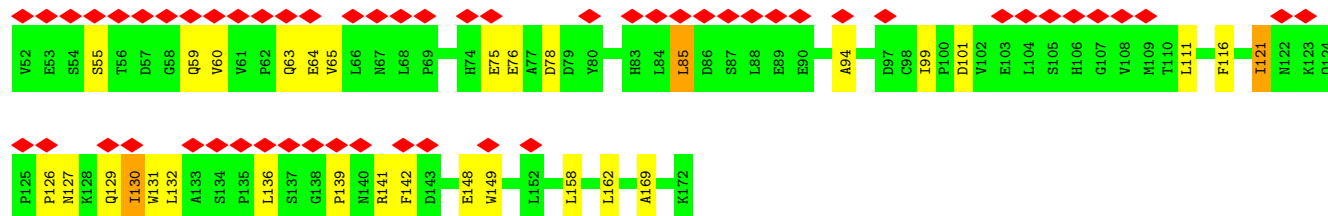
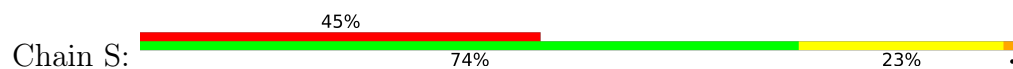
- Molecule 2: Frataxin homolog, mitochondrial



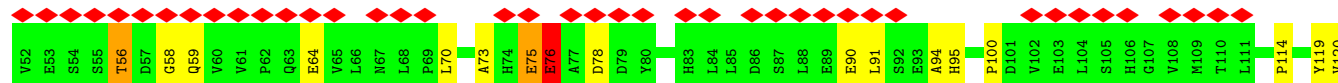
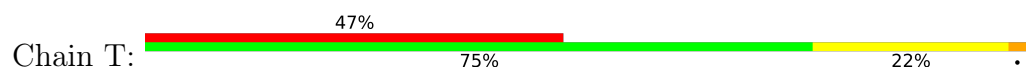
- Molecule 2: Frataxin homolog, mitochondrial

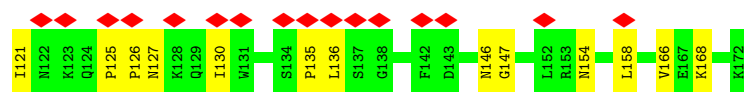


- Molecule 2: Frataxin homolog, mitochondrial

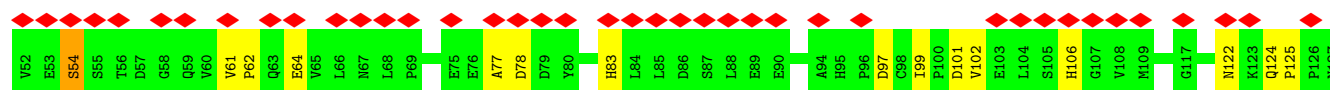
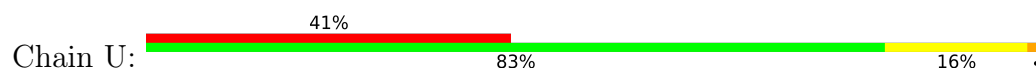


- Molecule 2: Frataxin homolog, mitochondrial

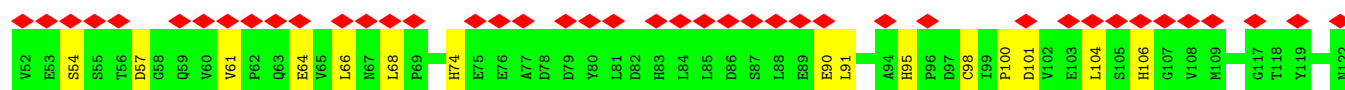
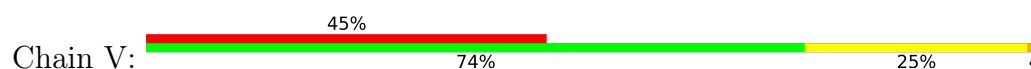




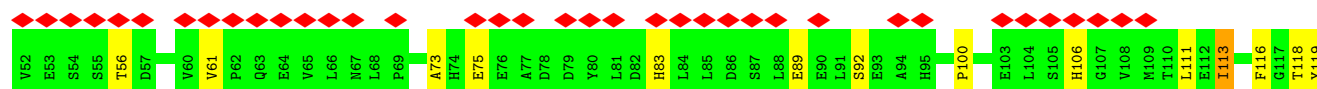
- Molecule 2: Frataxin homolog, mitochondrial



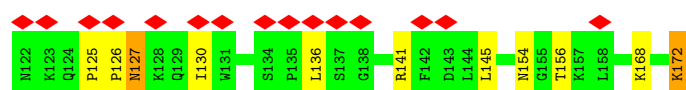
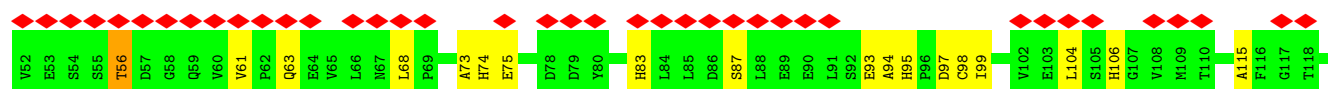
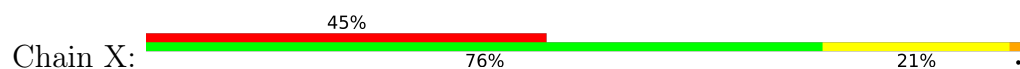
- Molecule 2: Frataxin homolog, mitochondrial



- Molecule 2: Frataxin homolog, mitochondrial



- Molecule 2: Frataxin homolog, mitochondrial



## 4 Experimental information

Property	Value	Source
EM 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
Maximum map value	8.189	Depositor
Minimum map value	-5.767	Depositor
Average map value	0.023	Depositor
Map value standard deviation	0.570	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	297.79202, 297.79202, 297.79202	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.034, 1.034, 1.034	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	a	1.48	2/1089 (0.2%)	1.98	28/1466 (1.9%)
1	b	1.44	4/1089 (0.4%)	1.89	28/1466 (1.9%)
1	c	1.41	1/1089 (0.1%)	1.91	25/1466 (1.7%)
1	d	1.42	1/1089 (0.1%)	1.92	29/1466 (2.0%)
1	e	1.45	0/1089	1.95	38/1466 (2.6%)
1	f	1.41	0/1089	1.95	34/1466 (2.3%)
1	g	1.40	1/1089 (0.1%)	1.93	33/1466 (2.3%)
1	h	1.44	0/1089	1.90	31/1466 (2.1%)
1	i	1.40	2/1089 (0.2%)	1.95	29/1466 (2.0%)
1	j	1.37	2/1089 (0.2%)	1.90	25/1466 (1.7%)
1	k	1.45	2/1089 (0.2%)	1.91	37/1466 (2.5%)
1	l	1.43	1/1089 (0.1%)	1.93	33/1466 (2.3%)
1	m	1.38	0/1089	1.93	39/1466 (2.7%)
1	n	1.40	1/1089 (0.1%)	1.96	36/1466 (2.5%)
1	o	1.42	1/1089 (0.1%)	1.84	21/1466 (1.4%)
1	p	1.47	2/1089 (0.2%)	1.91	33/1466 (2.3%)
1	q	1.41	1/1089 (0.1%)	1.90	22/1466 (1.5%)
1	r	1.40	1/1089 (0.1%)	1.95	32/1466 (2.2%)
1	s	1.45	0/1089	1.92	25/1466 (1.7%)
1	t	1.40	1/1089 (0.1%)	1.93	36/1466 (2.5%)
1	u	1.40	0/1089	1.89	27/1466 (1.8%)
1	v	1.41	2/1089 (0.2%)	1.93	21/1466 (1.4%)
1	w	1.42	2/1089 (0.2%)	1.92	23/1466 (1.6%)
1	x	1.44	1/1089 (0.1%)	1.94	31/1466 (2.1%)
2	A	1.35	2/967 (0.2%)	1.84	20/1319 (1.5%)
2	B	1.37	2/967 (0.2%)	1.83	17/1319 (1.3%)
2	C	1.37	1/967 (0.1%)	1.74	10/1319 (0.8%)
2	D	1.36	1/967 (0.1%)	1.80	19/1319 (1.4%)
2	E	1.40	0/967	1.71	13/1319 (1.0%)
2	F	1.41	0/967	1.84	21/1319 (1.6%)
2	G	1.38	0/967	1.71	11/1319 (0.8%)
2	H	1.35	0/967	1.82	21/1319 (1.6%)
2	I	1.45	3/967 (0.3%)	1.80	19/1319 (1.4%)
2	J	1.37	0/967	1.73	20/1319 (1.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	K	1.40	1/967 (0.1%)	1.79	16/1319 (1.2%)
2	L	1.36	1/967 (0.1%)	1.81	21/1319 (1.6%)
2	M	1.43	2/967 (0.2%)	1.76	19/1319 (1.4%)
2	N	1.41	0/967	1.81	16/1319 (1.2%)
2	O	1.39	1/967 (0.1%)	1.78	17/1319 (1.3%)
2	P	1.39	3/967 (0.3%)	1.72	10/1319 (0.8%)
2	Q	1.39	0/967	1.86	20/1319 (1.5%)
2	R	1.39	2/967 (0.2%)	1.73	21/1319 (1.6%)
2	S	1.38	2/967 (0.2%)	1.83	15/1319 (1.1%)
2	T	1.37	1/967 (0.1%)	1.74	20/1319 (1.5%)
2	U	1.39	2/967 (0.2%)	1.78	19/1319 (1.4%)
2	V	1.39	0/967	1.78	16/1319 (1.2%)
2	W	1.37	2/967 (0.2%)	1.90	28/1319 (2.1%)
2	X	1.43	3/967 (0.3%)	1.86	21/1319 (1.6%)
All	All	1.41	57/49344 (0.1%)	1.86	1146/66840 (1.7%)

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 (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	95	HIS	C-N	8.14	1.41	1.33
1	p	62	GLY	CA-C	-6.83	1.47	1.52
2	O	106	HIS	ND1-CE1	6.80	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	k	45	HIS	ND1-CE1	6.67	1.39	1.32
2	X	104	LEU	CA-C	-6.57	1.44	1.52
1	j	132	LEU	CA-CB	6.47	1.57	1.52
1	a	138	HIS	ND1-CE1	6.38	1.39	1.32
1	j	33	ARG	NE-CZ	6.11	1.39	1.33
2	C	153	ARG	NE-CZ	6.08	1.39	1.33
1	i	138	HIS	ND1-CE1	6.02	1.38	1.32
1	l	65	GLY	CA-C	-6.01	1.48	1.52
2	P	95	HIS	ND1-CE1	5.93	1.38	1.32
2	U	83	HIS	ND1-CE1	5.87	1.38	1.32
1	t	137	LEU	CA-C	-5.72	1.45	1.53
1	g	47	ARG	NE-CZ	5.66	1.39	1.33
1	a	47	ARG	NE-CZ	5.54	1.39	1.33
2	T	95	HIS	ND1-CE1	5.54	1.38	1.32
2	M	99	ILE	CA-C	-5.54	1.48	1.53
2	I	96	PRO	N-CD	5.52	1.55	1.47
2	A	122	ASN	CA-C	-5.51	1.45	1.52
1	b	85	VAL	C-N	5.49	1.39	1.33
1	d	33	ARG	NE-CZ	5.45	1.39	1.33
2	U	141	ARG	CD-NE	5.45	1.53	1.46
2	D	134	SER	CA-C	-5.43	1.48	1.52
1	w	61	THR	C-N	5.38	1.38	1.33
2	M	111	LEU	N-CA	-5.37	1.40	1.46
1	b	36	HIS	ND1-CE1	5.28	1.37	1.32
2	B	83	HIS	ND1-CE1	5.28	1.37	1.32
1	c	26	HIS	ND1-CE1	5.28	1.37	1.32
2	X	141	ARG	NE-CZ	5.27	1.38	1.33
1	q	62	GLY	CA-C	-5.26	1.48	1.52
2	S	141	ARG	NE-CZ	5.26	1.38	1.33
1	n	61	THR	C-N	5.23	1.38	1.33
2	X	145	LEU	CA-C	-5.23	1.48	1.52
2	W	153	ARG	CD-NE	5.22	1.53	1.46
2	L	113	ILE	N-CA	-5.17	1.41	1.46
2	P	70	LEU	CA-C	-5.16	1.45	1.52
2	P	98	CYS	N-CA	-5.16	1.40	1.46
1	b	125	GLU	CA-C	-5.14	1.46	1.52
1	i	45	HIS	ND1-CE1	5.12	1.37	1.32
1	k	138	HIS	ND1-CE1	5.12	1.37	1.32
2	R	153	ARG	CD-NE	5.12	1.53	1.46
2	K	95	HIS	ND1-CE1	5.12	1.37	1.32
1	x	138	HIS	ND1-CE1	5.12	1.37	1.32
1	v	158	ARG	NE-CZ	5.11	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	100	PRO	N-CA	-5.10	1.43	1.47
2	I	74	HIS	ND1-CE1	5.10	1.37	1.32
2	S	162	LEU	CA-C	-5.09	1.46	1.52
1	w	88	ASP	CA-C	-5.09	1.46	1.52
2	A	95	HIS	ND1-CE1	5.07	1.37	1.32
2	B	53	GLU	CA-C	-5.07	1.46	1.52
1	b	160	THR	N-CA	-5.06	1.41	1.46
2	W	146	ASN	CA-CB	5.06	1.57	1.53
1	v	74	ARG	NE-CZ	5.05	1.38	1.33
1	p	47	ARG	NE-CZ	5.04	1.38	1.33
1	r	36	HIS	ND1-CE1	5.04	1.37	1.32
1	o	45	HIS	ND1-CE1	5.00	1.37	1.32

All (1146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	113	ILE	N-CA-C	-10.71	97.55	108.15
1	r	122	LYS	CA-C-N	10.40	140.43	121.70
1	r	122	LYS	C-N-CA	10.40	140.43	121.70
1	d	122	LYS	CA-C-N	9.66	139.09	121.70
1	d	122	LYS	C-N-CA	9.66	139.09	121.70
1	a	122	LYS	CA-C-N	9.52	138.83	121.70
1	a	122	LYS	C-N-CA	9.52	138.83	121.70
2	H	67	ASN	CA-CB-CG	9.33	121.93	112.60
1	l	122	LYS	CA-C-N	9.04	137.96	121.70
1	l	122	LYS	C-N-CA	9.04	137.96	121.70
1	k	122	LYS	CA-C-N	8.95	137.81	121.70
1	k	122	LYS	C-N-CA	8.95	137.81	121.70
1	b	128	LYS	N-CA-C	8.80	120.95	111.36
2	J	62	PRO	N-CA-C	-8.68	103.57	114.68
1	q	60	GLY	N-CA-C	-8.65	103.71	111.67
2	A	113	ILE	N-CA-C	-8.40	99.52	109.01
2	Q	125	PRO	CA-C-O	-8.35	114.89	120.90
1	u	122	LYS	CA-C-N	8.32	136.68	121.70
1	u	122	LYS	C-N-CA	8.32	136.68	121.70
1	o	69	CYS	N-CA-C	-8.31	104.01	114.56
1	d	133	PRO	N-CA-C	-8.12	100.80	110.70
1	r	69	CYS	N-CA-C	-8.07	104.31	114.56
1	n	125	GLU	N-CA-C	7.97	120.05	111.36
1	a	44	THR	CA-C-N	7.95	136.00	121.70
1	a	44	THR	C-N-CA	7.95	136.00	121.70
1	f	122	LYS	CA-C-N	7.91	135.93	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	122	LYS	C-N-CA	7.91	135.93	121.70
1	n	122	LYS	CA-C-N	7.89	135.91	121.70
1	n	122	LYS	C-N-CA	7.89	135.91	121.70
2	O	135	PRO	N-CA-C	-7.89	104.58	114.68
2	Q	65	VAL	N-CA-C	-7.88	105.33	112.90
2	X	75	GLU	CA-C-N	7.86	135.85	121.70
2	X	75	GLU	C-N-CA	7.86	135.85	121.70
2	T	64	GLU	N-CA-C	-7.84	102.55	114.16
2	A	157	LYS	CA-C-N	7.77	130.69	120.28
2	A	157	LYS	C-N-CA	7.77	130.69	120.28
1	o	44	THR	CA-C-N	7.71	135.59	121.70
1	o	44	THR	C-N-CA	7.71	135.59	121.70
1	i	123	ASN	N-CA-CB	7.71	123.60	110.50
2	U	99	ILE	CA-C-O	-7.69	115.94	119.94
1	m	133	PRO	CA-C-O	-7.66	109.46	120.56
2	F	78	ASP	CA-C-N	7.65	136.15	121.54
2	F	78	ASP	C-N-CA	7.65	136.15	121.54
2	Q	125	PRO	CA-C-N	7.61	129.36	119.84
2	Q	125	PRO	C-N-CA	7.61	129.36	119.84
2	M	75	GLU	CA-C-N	7.60	135.38	121.70
2	M	75	GLU	C-N-CA	7.60	135.38	121.70
2	F	136	LEU	N-CA-C	-7.54	106.02	114.62
1	m	133	PRO	N-CA-C	7.54	119.90	110.70
1	t	122	LYS	CA-C-N	7.54	135.27	121.70
1	t	122	LYS	C-N-CA	7.54	135.27	121.70
1	a	133	PRO	N-CA-C	7.54	119.90	110.70
1	w	44	THR	CA-C-N	7.52	135.23	121.70
1	w	44	THR	C-N-CA	7.52	135.23	121.70
1	m	122	LYS	CA-C-N	7.51	135.23	121.70
1	m	122	LYS	C-N-CA	7.51	135.23	121.70
1	g	39	VAL	CA-C-N	7.49	130.58	120.77
1	g	39	VAL	C-N-CA	7.49	130.58	120.77
2	N	60	VAL	N-CA-C	-7.49	105.47	112.96
2	G	67	ASN	N-CA-C	-7.47	104.29	113.41
2	O	90	GLU	CA-C-N	7.43	130.24	120.28
2	O	90	GLU	C-N-CA	7.43	130.24	120.28
1	l	44	THR	CA-C-N	7.42	135.06	121.70
1	l	44	THR	C-N-CA	7.42	135.06	121.70
1	e	163	MET	N-CA-C	-7.42	104.26	113.38
1	n	132	LEU	O-C-N	-7.40	114.97	121.71
2	T	75	GLU	CA-C-N	7.34	134.91	121.70
2	T	75	GLU	C-N-CA	7.34	134.91	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	125	GLU	N-CA-C	-7.32	102.31	112.12
1	s	129	GLU	N-CA-C	7.29	119.23	111.28
1	l	48	ASN	CA-CB-CG	7.26	119.86	112.60
1	k	123	ASN	N-CA-CB	7.21	122.77	110.50
1	a	67	PRO	N-CA-C	-7.21	106.34	114.92
2	X	156	THR	CA-C-N	7.20	131.62	120.75
2	X	156	THR	C-N-CA	7.20	131.62	120.75
2	V	74	HIS	N-CA-C	-7.18	105.71	114.75
1	h	113	MET	CA-C-N	7.17	130.90	120.71
1	h	113	MET	C-N-CA	7.17	130.90	120.71
2	I	135	PRO	CA-C-N	7.17	129.89	120.28
2	I	135	PRO	C-N-CA	7.17	129.89	120.28
2	B	65	VAL	N-CA-C	-7.16	105.36	112.17
1	p	122	LYS	CA-C-N	7.16	134.59	121.70
1	p	122	LYS	C-N-CA	7.16	134.59	121.70
1	j	44	THR	CA-C-N	7.16	134.59	121.70
1	j	44	THR	C-N-CA	7.16	134.59	121.70
2	H	102	VAL	N-CA-C	-7.16	97.86	108.45
1	s	122	LYS	CA-C-N	7.15	134.56	121.70
1	s	122	LYS	C-N-CA	7.15	134.56	121.70
1	h	44	THR	CA-C-N	7.13	134.53	121.70
1	h	44	THR	C-N-CA	7.13	134.53	121.70
1	o	30	ILE	N-CA-C	-7.13	105.08	113.42
1	r	123	ASN	N-CA-CB	7.10	122.58	110.50
1	n	123	ASN	N-CA-CB	7.10	122.56	110.50
1	o	27	MET	CA-C-N	7.10	134.48	121.70
1	o	27	MET	C-N-CA	7.10	134.48	121.70
1	p	44	THR	CA-C-N	7.07	134.43	121.70
1	p	44	THR	C-N-CA	7.07	134.43	121.70
1	v	31	THR	N-CA-CB	7.07	122.44	110.49
1	q	59	VAL	N-CA-C	-7.04	106.28	113.10
1	u	69	CYS	N-CA-C	-7.02	106.62	114.62
1	x	44	THR	CA-C-N	7.01	134.32	121.70
1	x	44	THR	C-N-CA	7.01	134.32	121.70
1	f	123	ASN	N-CA-CB	6.99	122.38	110.50
2	B	124	GLN	CA-C-N	6.96	124.74	119.66
2	B	124	GLN	C-N-CA	6.96	124.74	119.66
1	s	44	THR	CA-C-N	6.94	134.19	121.70
1	s	44	THR	C-N-CA	6.94	134.19	121.70
1	x	120	LYS	N-CA-C	6.93	121.31	112.86
1	u	157	LYS	CA-C-N	6.90	129.53	120.28
1	u	157	LYS	C-N-CA	6.90	129.53	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	u	134	PRO	N-CA-C	-6.88	105.87	114.68
1	h	116	ASP	CA-C-N	6.85	129.77	120.38
1	h	116	ASP	C-N-CA	6.85	129.77	120.38
1	g	35	TYR	CA-C-N	6.84	134.01	121.70
1	g	35	TYR	C-N-CA	6.84	134.01	121.70
1	e	138	HIS	CA-C-N	6.84	131.85	122.07
1	e	138	HIS	C-N-CA	6.84	131.85	122.07
2	X	125	PRO	CA-C-N	6.83	128.38	119.84
2	X	125	PRO	C-N-CA	6.83	128.38	119.84
1	j	138	HIS	N-CA-C	-6.83	100.35	110.46
1	i	48	ASN	CA-C-N	6.82	133.97	121.70
1	i	48	ASN	C-N-CA	6.82	133.97	121.70
1	q	48	ASN	CA-C-N	6.81	133.96	121.70
1	q	48	ASN	C-N-CA	6.81	133.96	121.70
1	v	128	LYS	N-CA-C	6.81	118.79	111.36
2	A	58	GLY	CA-C-N	6.80	130.07	120.28
2	A	58	GLY	C-N-CA	6.80	130.07	120.28
2	F	65	VAL	N-CA-C	-6.79	105.72	112.17
1	n	133	PRO	N-CA-C	6.78	118.97	110.70
1	m	116	ASP	CA-C-N	6.76	129.34	120.28
1	m	116	ASP	C-N-CA	6.76	129.34	120.28
2	H	152	LEU	N-CA-C	-6.75	104.79	113.16
2	W	138	GLY	CA-C-N	6.74	126.78	119.90
2	W	138	GLY	C-N-CA	6.74	126.78	119.90
1	a	94	PHE	CA-CB-CG	-6.74	107.06	113.80
2	O	62	PRO	N-CA-C	-6.72	106.92	114.92
2	F	60	VAL	N-CA-C	6.72	117.48	110.62
1	q	122	LYS	CA-C-N	6.71	129.27	120.28
1	q	122	LYS	C-N-CA	6.71	129.27	120.28
2	K	125	PRO	CA-C-N	6.71	128.22	119.84
2	K	125	PRO	C-N-CA	6.71	128.22	119.84
1	h	123	ASN	N-CA-CB	6.70	121.89	110.50
1	n	133	PRO	CA-C-O	-6.69	110.85	120.56
1	a	38	LYS	CA-C-N	6.69	134.01	121.97
1	a	38	LYS	C-N-CA	6.69	134.01	121.97
1	a	133	PRO	CA-C-O	-6.67	110.89	120.56
1	i	44	THR	CA-C-N	6.67	133.70	121.70
1	i	44	THR	C-N-CA	6.67	133.70	121.70
1	r	44	THR	CA-C-N	6.66	133.68	121.70
1	r	44	THR	C-N-CA	6.66	133.68	121.70
1	o	157	LYS	CA-C-N	6.64	129.18	120.28
1	o	157	LYS	C-N-CA	6.64	129.18	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	124	GLN	CA-C-O	-6.64	114.02	120.19
2	F	138	GLY	CA-C-N	6.63	126.66	119.89
2	F	138	GLY	C-N-CA	6.63	126.66	119.89
1	i	122	LYS	CA-C-N	6.63	133.63	121.70
1	i	122	LYS	C-N-CA	6.63	133.63	121.70
2	H	62	PRO	N-CA-C	-6.63	105.39	114.80
2	H	142	PHE	CA-CB-CG	-6.62	107.18	113.80
2	U	62	PRO	N-CA-C	-6.61	105.33	114.98
1	u	123	ASN	N-CA-CB	6.60	121.71	110.50
2	L	158	LEU	N-CA-C	6.59	118.46	111.28
1	i	127	ALA	N-CA-C	6.59	118.12	111.07
1	m	123	ASN	N-CA-CB	6.56	121.65	110.50
2	W	169	ALA	CA-C-N	6.55	129.76	120.53
2	W	169	ALA	C-N-CA	6.55	129.76	120.53
1	i	116	ASP	CA-C-N	6.54	128.94	120.44
1	i	116	ASP	C-N-CA	6.54	128.94	120.44
1	t	40	ILE	CB-CA-C	-6.54	103.31	112.14
1	o	48	ASN	CA-C-N	6.54	133.47	121.70
1	o	48	ASN	C-N-CA	6.54	133.47	121.70
1	d	122	LYS	N-CA-C	-6.54	100.53	110.14
1	n	48	ASN	CA-C-N	6.54	133.46	121.70
1	n	48	ASN	C-N-CA	6.54	133.46	121.70
1	e	122	LYS	CA-C-N	6.53	133.45	121.70
1	e	122	LYS	C-N-CA	6.53	133.45	121.70
2	N	124	GLN	CA-C-N	6.53	127.11	120.38
2	N	124	GLN	C-N-CA	6.53	127.11	120.38
1	x	122	LYS	CA-C-N	6.53	133.46	121.70
1	x	122	LYS	C-N-CA	6.53	133.46	121.70
1	w	121	ILE	N-CA-C	-6.52	99.05	108.17
1	n	102	SER	CA-C-N	6.51	128.91	120.44
1	n	102	SER	C-N-CA	6.51	128.91	120.44
2	C	135	PRO	CA-C-N	6.51	128.90	120.44
2	C	135	PRO	C-N-CA	6.51	128.90	120.44
1	k	117	ASP	CA-C-N	6.51	129.00	120.28
1	k	117	ASP	C-N-CA	6.51	129.00	120.28
1	u	35	TYR	CA-C-N	6.50	133.40	121.70
1	u	35	TYR	C-N-CA	6.50	133.40	121.70
1	u	44	THR	CA-C-N	6.49	133.38	121.70
1	u	44	THR	C-N-CA	6.49	133.38	121.70
1	s	38	LYS	CA-C-N	6.49	129.63	120.42
1	s	38	LYS	C-N-CA	6.49	129.63	120.42
2	W	125	PRO	CA-C-N	6.47	126.50	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	125	PRO	C-N-CA	6.47	126.50	119.90
1	k	163	MET	N-CA-C	-6.46	106.03	114.04
2	W	61	VAL	N-CA-C	-6.46	100.70	108.45
1	h	29	SER	N-CA-C	-6.46	104.17	113.21
1	f	128	LYS	CA-C-N	6.46	128.93	120.28
1	f	128	LYS	C-N-CA	6.46	128.93	120.28
1	e	123	ASN	N-CA-CB	6.45	121.46	110.50
1	d	44	THR	CA-C-N	6.45	133.30	121.70
1	d	44	THR	C-N-CA	6.45	133.30	121.70
2	M	138	GLY	CA-C-N	6.45	126.97	120.14
2	M	138	GLY	C-N-CA	6.45	126.97	120.14
2	N	152	LEU	N-CA-C	-6.44	105.38	112.72
1	b	48	ASN	CA-C-N	6.44	133.29	121.70
1	b	48	ASN	C-N-CA	6.44	133.29	121.70
1	i	133	PRO	N-CA-C	6.44	118.56	110.70
2	S	148	GLU	N-CA-C	-6.44	99.28	109.07
1	v	122	LYS	CA-C-N	6.44	133.29	121.70
1	v	122	LYS	C-N-CA	6.44	133.29	121.70
2	H	124	GLN	N-CA-C	-6.44	101.43	110.31
1	v	35	TYR	CA-C-N	6.42	133.26	121.70
1	v	35	TYR	C-N-CA	6.42	133.26	121.70
2	I	95	HIS	CA-C-N	-6.42	113.13	120.89
2	I	95	HIS	C-N-CA	-6.42	113.13	120.89
1	b	114	THR	CA-C-N	6.40	128.76	120.44
1	b	114	THR	C-N-CA	6.40	128.76	120.44
1	r	124	THR	CA-C-N	6.39	130.41	120.82
1	r	124	THR	C-N-CA	6.39	130.41	120.82
1	b	142	LEU	CA-C-N	6.38	129.69	120.38
1	b	142	LEU	C-N-CA	6.38	129.69	120.38
1	n	44	THR	CA-C-N	6.38	133.18	121.70
1	n	44	THR	C-N-CA	6.38	133.18	121.70
1	p	48	ASN	CA-C-N	6.37	133.17	121.70
1	p	48	ASN	C-N-CA	6.37	133.17	121.70
2	W	156	THR	CA-C-N	6.37	130.18	120.82
2	W	156	THR	C-N-CA	6.37	130.18	120.82
2	T	90	GLU	CA-C-N	6.35	128.79	120.28
2	T	90	GLU	C-N-CA	6.35	128.79	120.28
2	M	77	ALA	N-CA-C	6.35	118.28	111.36
1	b	95	GLY	CA-C-N	6.34	130.76	121.31
1	b	95	GLY	C-N-CA	6.34	130.76	121.31
1	h	152	LYS	CA-C-N	6.33	128.67	120.44
1	h	152	LYS	C-N-CA	6.33	128.67	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	x	114	THR	CA-C-N	6.33	128.77	120.28
1	x	114	THR	C-N-CA	6.33	128.77	120.28
1	e	44	THR	CA-C-N	6.32	133.08	121.70
1	e	44	THR	C-N-CA	6.32	133.08	121.70
1	l	122	LYS	O-C-N	-6.32	114.73	122.19
1	h	48	ASN	CA-C-N	6.30	133.04	121.70
1	h	48	ASN	C-N-CA	6.30	133.04	121.70
1	j	122	LYS	CA-C-N	6.29	133.03	121.70
1	j	122	LYS	C-N-CA	6.29	133.03	121.70
1	e	48	ASN	CA-C-N	6.29	133.03	121.70
1	e	48	ASN	C-N-CA	6.29	133.03	121.70
1	p	27	MET	CA-C-N	6.29	133.02	121.70
1	p	27	MET	C-N-CA	6.29	133.02	121.70
1	f	120	LYS	N-CA-C	6.27	120.24	112.47
1	j	35	TYR	CA-C-N	6.26	132.98	121.70
1	j	35	TYR	C-N-CA	6.26	132.98	121.70
1	p	123	ASN	N-CA-CB	6.26	121.14	110.50
1	q	142	LEU	CA-C-N	6.25	128.56	120.44
1	q	142	LEU	C-N-CA	6.25	128.56	120.44
1	b	133	PRO	N-CA-C	6.25	118.32	110.70
1	i	45	HIS	N-CA-CB	6.24	121.11	110.50
2	R	143	ASP	CA-C-N	6.22	129.54	120.71
2	R	143	ASP	C-N-CA	6.22	129.54	120.71
2	V	150	VAL	N-CA-C	-6.22	98.74	108.81
1	f	26	HIS	CA-C-N	6.22	128.90	120.44
1	f	26	HIS	C-N-CA	6.22	128.90	120.44
1	a	98	SER	CA-C-N	6.20	128.59	120.28
1	a	98	SER	C-N-CA	6.20	128.59	120.28
1	s	42	HIS	CA-C-N	6.19	128.57	120.28
1	s	42	HIS	C-N-CA	6.19	128.57	120.28
2	D	84	LEU	CA-C-N	6.18	128.56	120.28
2	D	84	LEU	C-N-CA	6.18	128.56	120.28
2	T	76	GLU	CA-C-N	6.17	128.47	120.44
2	T	76	GLU	C-N-CA	6.17	128.47	120.44
2	S	65	VAL	N-CA-C	-6.17	106.72	112.83
1	k	39	VAL	N-CA-C	-6.17	106.98	112.90
2	F	87	SER	CA-C-N	6.17	128.54	120.28
2	F	87	SER	C-N-CA	6.17	128.54	120.28
2	H	108	VAL	N-CA-C	-6.17	99.54	108.17
1	s	123	ASN	N-CA-CB	6.16	120.98	110.50
1	d	27	MET	CA-C-N	6.15	132.78	121.70
1	d	27	MET	C-N-CA	6.15	132.78	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	r	122	LYS	N-CA-C	-6.15	101.67	110.59
1	u	152	LYS	CA-C-N	6.15	128.43	120.44
1	u	152	LYS	C-N-CA	6.15	128.43	120.44
1	d	134	PRO	CA-C-N	6.14	133.03	121.97
1	d	134	PRO	C-N-CA	6.14	133.03	121.97
1	k	44	THR	CA-C-N	6.14	132.76	121.70
1	k	44	THR	C-N-CA	6.14	132.76	121.70
2	C	78	ASP	CA-C-N	6.14	128.79	120.38
2	C	78	ASP	C-N-CA	6.14	128.79	120.38
1	m	115	LEU	CA-C-N	6.14	129.33	120.79
1	m	115	LEU	C-N-CA	6.14	129.33	120.79
1	k	108	GLU	CA-C-N	6.14	128.42	120.44
1	k	108	GLU	C-N-CA	6.14	128.42	120.44
1	k	42	HIS	CE1-NE2-CD2	-6.14	102.86	109.00
1	w	72	VAL	N-CA-C	-6.13	100.25	108.35
1	i	72	VAL	N-CA-C	-6.13	100.26	108.35
1	a	48	ASN	CA-C-N	6.13	132.73	121.70
1	a	48	ASN	C-N-CA	6.13	132.73	121.70
1	n	126	ILE	CA-C-N	6.12	128.48	120.28
1	n	126	ILE	C-N-CA	6.12	128.48	120.28
2	P	113	ILE	CA-C-N	6.12	125.82	119.64
2	P	113	ILE	C-N-CA	6.12	125.82	119.64
1	v	136	LYS	CA-C-N	6.12	129.39	120.71
1	v	136	LYS	C-N-CA	6.12	129.39	120.71
1	c	114	THR	CA-C-N	6.11	128.46	120.28
1	c	114	THR	C-N-CA	6.11	128.46	120.28
2	L	157	LYS	CA-C-N	6.11	128.46	120.28
2	L	157	LYS	C-N-CA	6.11	128.46	120.28
1	a	45	HIS	CE1-NE2-CD2	-6.10	102.90	109.00
1	l	72	VAL	N-CA-C	-6.10	100.30	108.35
2	H	107	GLY	N-CA-C	-6.10	106.55	115.63
1	h	94	PHE	N-CA-C	-6.10	100.97	110.42
1	m	26	HIS	CE1-NE2-CD2	-6.09	102.91	109.00
2	A	75	GLU	O-C-N	-6.09	114.49	122.59
1	x	68	ALA	CA-C-N	6.09	128.94	120.29
1	x	68	ALA	C-N-CA	6.09	128.94	120.29
1	r	122	LYS	O-C-N	-6.09	115.56	122.68
1	q	72	VAL	N-CA-C	-6.09	100.31	108.35
1	g	143	ALA	CA-C-N	6.08	128.75	120.54
1	g	143	ALA	C-N-CA	6.08	128.75	120.54
1	h	122	LYS	CA-C-N	6.08	132.65	121.70
1	h	122	LYS	C-N-CA	6.08	132.65	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	104	LEU	N-CA-C	-6.08	98.99	108.90
1	x	123	ASN	N-CA-CB	6.08	120.83	110.50
2	B	71	GLU	CA-C-N	6.08	128.42	120.28
2	B	71	GLU	C-N-CA	6.08	128.42	120.28
2	K	113	ILE	N-CA-C	-6.07	95.76	108.88
1	j	123	ASN	CA-C-N	6.07	128.41	120.28
1	j	123	ASN	C-N-CA	6.07	128.41	120.28
2	O	77	ALA	CA-C-N	6.07	128.41	120.28
2	O	77	ALA	C-N-CA	6.07	128.41	120.28
2	A	124	GLN	CA-C-N	6.06	126.62	120.38
2	A	124	GLN	C-N-CA	6.06	126.62	120.38
2	O	125	PRO	CA-C-N	6.06	127.41	119.84
2	O	125	PRO	C-N-CA	6.06	127.41	119.84
1	v	44	THR	CA-C-N	6.05	132.59	121.70
1	v	44	THR	C-N-CA	6.05	132.59	121.70
1	l	27	MET	CA-C-N	6.05	132.59	121.70
1	l	27	MET	C-N-CA	6.05	132.59	121.70
2	F	102	VAL	N-CA-C	-6.04	99.42	108.12
2	K	113	ILE	CA-C-N	6.04	126.83	120.12
2	K	113	ILE	C-N-CA	6.04	126.83	120.12
2	P	102	VAL	N-CA-C	-6.04	99.35	108.17
1	n	142	LEU	CA-C-N	6.04	128.98	120.28
1	n	142	LEU	C-N-CA	6.04	128.98	120.28
1	o	117	ASP	CA-CB-CG	6.04	118.64	112.60
1	d	129	GLU	N-CA-CB	6.04	118.76	110.01
2	E	170	ILE	N-CA-CB	6.04	118.75	110.54
1	g	30	ILE	CA-C-N	6.03	133.06	121.54
1	g	30	ILE	C-N-CA	6.03	133.06	121.54
2	F	79	ASP	CA-C-N	6.03	128.36	120.28
2	F	79	ASP	C-N-CA	6.03	128.36	120.28
1	g	44	THR	CA-C-N	6.02	132.54	121.70
1	g	44	THR	C-N-CA	6.02	132.54	121.70
1	u	122	LYS	N-CA-C	-6.02	100.60	109.81
1	w	48	ASN	CA-C-N	6.01	132.52	121.70
1	w	48	ASN	C-N-CA	6.01	132.52	121.70
2	U	140	ASN	CA-C-N	6.01	133.01	121.54
2	U	140	ASN	C-N-CA	6.01	133.01	121.54
1	f	48	ASN	CA-C-N	6.00	132.51	121.70
1	f	48	ASN	C-N-CA	6.00	132.51	121.70
1	r	47	ARG	CA-C-N	6.00	132.51	121.70
1	r	47	ARG	C-N-CA	6.00	132.51	121.70
2	F	68	LEU	CA-C-N	6.00	126.31	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	68	LEU	C-N-CA	6.00	126.31	119.83
1	l	42	HIS	CE1-NE2-CD2	-6.00	103.00	109.00
1	b	147	ILE	N-CA-CB	6.00	119.58	110.58
1	f	114	THR	CA-C-N	5.99	128.31	120.28
1	f	114	THR	C-N-CA	5.99	128.31	120.28
1	f	27	MET	CA-C-N	5.99	132.47	121.70
1	f	27	MET	C-N-CA	5.99	132.47	121.70
1	q	38	LYS	N-CA-CB	5.98	120.59	110.49
1	x	116	ASP	CA-C-N	5.98	128.57	120.38
1	x	116	ASP	C-N-CA	5.98	128.57	120.38
2	O	77	ALA	N-CA-C	-5.97	106.00	113.28
1	j	45	HIS	CE1-NE2-CD2	-5.96	103.04	109.00
2	N	56	THR	CA-C-N	5.96	132.43	121.70
2	N	56	THR	C-N-CA	5.96	132.43	121.70
1	e	39	VAL	CA-C-N	5.96	128.58	120.77
1	e	39	VAL	C-N-CA	5.96	128.58	120.77
2	I	78	ASP	CA-C-N	5.96	128.58	120.54
2	I	78	ASP	C-N-CA	5.96	128.58	120.54
1	l	48	ASN	CA-C-N	5.96	132.42	121.70
1	l	48	ASN	C-N-CA	5.96	132.42	121.70
1	j	48	ASN	CA-CB-CG	5.96	118.56	112.60
1	k	30	ILE	CA-C-N	5.95	130.62	122.34
1	k	30	ILE	C-N-CA	5.95	130.62	122.34
1	m	48	ASN	CA-C-N	5.95	132.42	121.70
1	m	48	ASN	C-N-CA	5.95	132.42	121.70
2	Q	74	HIS	CE1-NE2-CD2	-5.95	103.05	109.00
1	b	30	ILE	CA-C-N	5.95	131.31	122.74
1	b	30	ILE	C-N-CA	5.95	131.31	122.74
1	i	35	TYR	CA-C-N	5.95	132.41	121.70
1	i	35	TYR	C-N-CA	5.95	132.41	121.70
1	k	48	ASN	CA-CB-CG	5.95	118.55	112.60
1	v	143	ALA	CA-C-N	5.95	128.17	120.44
1	v	143	ALA	C-N-CA	5.95	128.17	120.44
1	w	26	HIS	CA-C-N	5.94	128.56	120.54
1	w	26	HIS	C-N-CA	5.94	128.56	120.54
2	A	86	ASP	CA-C-N	5.94	128.24	120.28
2	A	86	ASP	C-N-CA	5.94	128.24	120.28
2	K	85	LEU	CA-C-N	5.93	128.16	120.44
2	K	85	LEU	C-N-CA	5.93	128.16	120.44
1	o	154	TYR	CA-C-N	5.93	128.22	120.28
1	o	154	TYR	C-N-CA	5.93	128.22	120.28
2	Q	57	ASP	CA-CB-CG	5.92	118.52	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	169	ALA	CA-C-N	5.92	130.32	120.62
2	S	169	ALA	C-N-CA	5.92	130.32	120.62
2	T	135	PRO	N-CA-C	-5.92	107.88	114.92
1	f	127	ALA	CA-C-N	5.92	128.21	120.28
1	f	127	ALA	C-N-CA	5.92	128.21	120.28
2	H	75	GLU	CA-C-N	5.91	132.34	121.70
2	H	75	GLU	C-N-CA	5.91	132.34	121.70
1	w	139	CYS	N-CA-C	-5.91	104.61	112.94
2	F	116	PHE	CA-CB-CG	5.91	119.71	113.80
2	O	59	GLN	N-CA-C	-5.91	107.31	114.75
1	a	114	THR	CA-C-N	5.91	128.19	120.28
1	a	114	THR	C-N-CA	5.91	128.19	120.28
1	g	129	GLU	N-CA-C	5.91	117.72	111.28
1	i	163	MET	N-CA-C	-5.90	106.05	113.72
2	X	93	GLU	CA-C-N	5.90	132.81	121.54
2	X	93	GLU	C-N-CA	5.90	132.81	121.54
2	N	125	PRO	CA-C-N	5.90	127.22	119.84
2	N	125	PRO	C-N-CA	5.90	127.22	119.84
1	x	132	LEU	N-CA-C	-5.90	101.08	110.10
1	b	35	TYR	CA-C-N	5.89	132.31	121.70
1	b	35	TYR	C-N-CA	5.89	132.31	121.70
2	X	56	THR	CA-C-N	5.89	132.31	121.70
2	X	56	THR	C-N-CA	5.89	132.31	121.70
2	I	153	ARG	N-CA-C	-5.89	105.34	113.18
1	e	125	GLU	CA-C-N	5.88	128.78	120.42
1	e	125	GLU	C-N-CA	5.88	128.78	120.42
2	S	60	VAL	N-CA-C	-5.88	107.00	112.83
1	k	42	HIS	ND1-CE1-NE2	5.88	114.28	108.40
1	m	134	PRO	CA-C-N	5.88	132.56	121.97
1	m	134	PRO	C-N-CA	5.88	132.56	121.97
1	i	26	HIS	CA-C-N	5.88	128.44	120.44
1	i	26	HIS	C-N-CA	5.88	128.44	120.44
2	M	83	HIS	CA-C-N	5.88	128.08	120.44
2	M	83	HIS	C-N-CA	5.88	128.08	120.44
2	G	125	PRO	CA-C-N	5.88	127.18	119.84
2	G	125	PRO	C-N-CA	5.88	127.18	119.84
1	f	138	HIS	CE1-NE2-CD2	-5.87	103.13	109.00
2	Q	143	ASP	CA-C-N	5.87	129.05	120.71
2	Q	143	ASP	C-N-CA	5.87	129.05	120.71
2	V	64	GLU	N-CA-C	-5.87	107.93	114.62
2	M	66	LEU	N-CA-C	-5.87	106.03	112.72
2	H	92	SER	CA-C-N	5.86	132.73	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	92	SER	C-N-CA	5.86	132.73	121.54
2	M	86	ASP	CA-C-N	5.84	128.04	120.44
2	M	86	ASP	C-N-CA	5.84	128.04	120.44
1	m	35	TYR	CA-C-N	5.84	132.21	121.70
1	m	35	TYR	C-N-CA	5.84	132.21	121.70
2	R	113	ILE	N-CA-C	-5.84	101.35	107.60
2	B	96	PRO	N-CA-C	-5.84	106.51	114.80
2	J	124	GLN	N-CA-C	-5.84	102.26	110.31
1	f	67	PRO	N-CA-C	-5.83	106.39	114.27
1	a	122	LYS	N-CA-C	-5.83	101.10	110.14
2	B	128	LYS	N-CA-C	-5.83	99.83	108.99
1	e	27	MET	CA-C-N	5.83	132.20	121.70
1	e	27	MET	C-N-CA	5.83	132.20	121.70
1	u	37	PRO	CA-C-N	5.83	132.66	121.54
1	u	37	PRO	C-N-CA	5.83	132.66	121.54
1	v	30	ILE	CA-C-N	5.82	132.66	121.54
1	v	30	ILE	C-N-CA	5.82	132.66	121.54
2	S	75	GLU	CA-C-N	5.82	132.17	121.70
2	S	75	GLU	C-N-CA	5.82	132.17	121.70
1	a	125	GLU	CA-C-N	5.82	128.43	120.46
1	a	125	GLU	C-N-CA	5.82	128.43	120.46
1	l	108	GLU	CA-C-N	5.82	128.00	120.44
1	l	108	GLU	C-N-CA	5.82	128.00	120.44
2	B	125	PRO	CA-C-O	-5.81	116.71	120.90
1	q	31	THR	N-CA-CB	5.81	120.31	110.49
2	X	87	SER	CA-C-N	5.81	127.99	120.44
2	X	87	SER	C-N-CA	5.81	127.99	120.44
2	D	142	PHE	CA-CB-CG	-5.80	108.00	113.80
2	J	77	ALA	N-CA-C	-5.80	106.55	113.97
1	q	126	ILE	CA-C-N	5.79	128.04	120.28
1	q	126	ILE	C-N-CA	5.79	128.04	120.28
2	V	124	GLN	CA-C-N	5.79	126.34	120.38
2	V	124	GLN	C-N-CA	5.79	126.34	120.38
1	h	27	MET	CA-C-N	5.79	132.12	121.70
1	h	27	MET	C-N-CA	5.79	132.12	121.70
1	w	69	CYS	N-CA-C	-5.79	106.19	113.72
2	N	106	HIS	CE1-NE2-CD2	-5.79	103.22	109.00
2	V	153	ARG	N-CA-C	5.79	117.59	111.28
1	f	44	THR	CA-C-N	5.78	132.11	121.70
1	f	44	THR	C-N-CA	5.78	132.11	121.70
1	e	127	ALA	CA-C-N	5.78	128.02	120.28
1	e	127	ALA	C-N-CA	5.78	128.02	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	s	114	THR	CA-C-N	5.78	128.02	120.28
1	s	114	THR	C-N-CA	5.78	128.02	120.28
1	e	109	LEU	CA-C-N	5.78	128.37	120.46
1	e	109	LEU	C-N-CA	5.78	128.37	120.46
2	H	95	HIS	CE1-NE2-CD2	-5.77	103.23	109.00
1	r	109	LEU	CA-C-N	5.77	128.37	120.46
1	r	109	LEU	C-N-CA	5.77	128.37	120.46
1	j	48	ASN	CA-C-N	5.77	132.08	121.70
1	j	48	ASN	C-N-CA	5.77	132.08	121.70
2	L	113	ILE	CA-C-N	5.77	127.05	119.84
2	L	113	ILE	C-N-CA	5.77	127.05	119.84
2	H	157	LYS	CA-C-N	5.76	128.00	120.28
2	H	157	LYS	C-N-CA	5.76	128.00	120.28
1	r	153	ASP	CA-C-N	5.76	127.93	120.44
1	r	153	ASP	C-N-CA	5.76	127.93	120.44
2	B	158	LEU	N-CA-C	5.76	117.56	111.28
1	q	119	ALA	CA-C-N	5.76	130.30	122.07
1	q	119	ALA	C-N-CA	5.76	130.30	122.07
2	W	89	GLU	CA-C-N	5.76	127.92	120.44
2	W	89	GLU	C-N-CA	5.76	127.92	120.44
1	c	27	MET	CA-C-N	5.75	132.04	121.70
1	c	27	MET	C-N-CA	5.75	132.04	121.70
2	B	90	GLU	CA-C-N	5.74	128.55	120.28
2	B	90	GLU	C-N-CA	5.74	128.55	120.28
1	t	136	LYS	N-CA-C	-5.74	98.57	110.80
2	G	134	SER	N-CA-C	-5.74	101.30	109.62
1	o	35	TYR	CA-C-N	5.74	132.03	121.70
1	o	35	TYR	C-N-CA	5.74	132.03	121.70
2	I	60	VAL	N-CA-C	-5.73	106.72	112.17
1	p	109	LEU	CA-C-N	5.73	128.32	120.46
1	p	109	LEU	C-N-CA	5.73	128.32	120.46
1	t	44	THR	CA-C-N	5.73	132.01	121.70
1	t	44	THR	C-N-CA	5.73	132.01	121.70
1	w	102	SER	CA-C-N	5.73	127.96	120.28
1	w	102	SER	C-N-CA	5.73	127.96	120.28
2	W	159	THR	CA-C-N	5.73	128.23	120.38
2	W	159	THR	C-N-CA	5.73	128.23	120.38
2	X	68	LEU	N-CA-C	-5.71	102.91	110.40
2	W	158	LEU	CA-C-N	5.71	127.93	120.28
2	W	158	LEU	C-N-CA	5.71	127.93	120.28
2	D	89	GLU	N-CA-CB	5.70	118.50	110.12
2	H	82	ASP	CA-C-N	5.70	127.92	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	82	ASP	C-N-CA	5.70	127.92	120.28
1	p	115	LEU	CA-C-N	5.70	127.92	120.28
1	p	115	LEU	C-N-CA	5.70	127.92	120.28
2	X	127	ASN	N-CA-CB	5.70	120.12	110.49
2	U	78	ASP	CA-C-N	5.69	127.90	120.28
2	U	78	ASP	C-N-CA	5.69	127.90	120.28
2	W	83	HIS	CE1-NE2-CD2	-5.69	103.31	109.00
2	Q	62	PRO	CA-C-N	5.68	130.24	122.34
2	Q	62	PRO	C-N-CA	5.68	130.24	122.34
2	Q	122	ASN	N-CA-C	-5.68	100.71	109.52
1	r	45	HIS	CE1-NE2-CD2	-5.68	103.32	109.00
1	b	131	SER	N-CA-CB	5.67	120.08	110.49
1	d	149	ALA	CA-C-N	5.66	127.80	120.44
1	d	149	ALA	C-N-CA	5.66	127.80	120.44
1	j	83	THR	N-CA-C	-5.66	106.21	113.23
2	T	78	ASP	CA-CB-CG	-5.66	106.94	112.60
1	p	42	HIS	CE1-NE2-CD2	-5.66	103.34	109.00
1	j	45	HIS	ND1-CE1-NE2	5.65	114.05	108.40
2	R	65	VAL	N-CA-C	-5.65	106.30	112.80
1	b	159	ASN	CA-CB-CG	-5.65	106.95	112.60
2	B	92	SER	N-CA-C	5.65	117.11	111.07
2	R	95	HIS	ND1-CE1-NE2	5.64	114.04	108.40
2	J	146	ASN	N-CA-C	-5.63	105.83	114.16
2	V	163	THR	CA-C-N	5.63	128.13	120.54
2	V	163	THR	C-N-CA	5.63	128.13	120.54
1	p	36	HIS	CE1-NE2-CD2	-5.62	103.38	109.00
1	c	136	LYS	CA-C-N	5.62	129.68	121.31
1	c	136	LYS	C-N-CA	5.62	129.68	121.31
2	A	79	ASP	N-CA-C	5.62	117.40	111.28
1	e	103	SER	CA-C-N	5.62	127.74	120.44
1	e	103	SER	C-N-CA	5.62	127.74	120.44
1	q	117	ASP	CA-C-N	5.62	127.80	120.28
1	q	117	ASP	C-N-CA	5.62	127.80	120.28
2	U	138	GLY	CA-C-N	5.62	125.38	119.76
2	U	138	GLY	C-N-CA	5.62	125.38	119.76
1	g	133	PRO	N-CA-C	-5.61	103.85	110.70
2	U	54	SER	CA-C-N	5.61	131.80	121.70
2	U	54	SER	C-N-CA	5.61	131.80	121.70
1	g	114	THR	CA-C-N	5.61	128.36	120.28
1	g	114	THR	C-N-CA	5.61	128.36	120.28
2	P	121	ILE	N-CA-C	-5.61	97.82	107.24
2	L	83	HIS	CE1-NE2-CD2	-5.61	103.39	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	125	GLU	CA-C-N	5.60	128.13	120.46
1	d	125	GLU	C-N-CA	5.60	128.13	120.46
2	L	135	PRO	N-CA-C	-5.60	105.23	114.75
1	l	128	LYS	CA-C-N	5.60	127.78	120.28
1	l	128	LYS	C-N-CA	5.60	127.78	120.28
1	b	139	CYS	N-CA-C	-5.59	106.50	113.38
1	m	138	HIS	N-CA-C	5.59	117.84	111.02
1	v	135	VAL	N-CA-CB	5.59	120.45	111.23
2	E	95	HIS	CE1-NE2-CD2	-5.58	103.42	109.00
1	p	113	MET	CA-C-N	5.58	132.19	121.54
1	p	113	MET	C-N-CA	5.58	132.19	121.54
1	n	127	ALA	CA-C-N	5.57	127.69	120.44
1	n	127	ALA	C-N-CA	5.57	127.69	120.44
1	s	45	HIS	CE1-NE2-CD2	-5.57	103.43	109.00
1	h	99	ALA	CA-C-N	5.57	128.09	120.46
1	h	99	ALA	C-N-CA	5.57	128.09	120.46
2	S	121	ILE	N-CA-C	-5.57	99.79	108.81
1	u	38	LYS	CA-C-N	5.57	128.33	120.42
1	u	38	LYS	C-N-CA	5.57	128.33	120.42
2	D	70	LEU	CA-C-N	5.57	128.62	120.71
2	D	70	LEU	C-N-CA	5.57	128.62	120.71
1	s	122	LYS	N-CA-C	-5.57	99.23	108.75
1	c	35	TYR	CA-C-N	5.56	131.71	121.70
1	c	35	TYR	C-N-CA	5.56	131.71	121.70
2	H	66	LEU	CA-C-N	5.56	132.16	121.54
2	H	66	LEU	C-N-CA	5.56	132.16	121.54
1	n	161	PRO	CA-C-N	5.56	128.19	120.29
1	n	161	PRO	C-N-CA	5.56	128.19	120.29
2	G	159	THR	CA-C-N	5.56	127.73	120.28
2	G	159	THR	C-N-CA	5.56	127.73	120.28
1	c	127	ALA	CA-C-N	5.56	127.73	120.28
1	c	127	ALA	C-N-CA	5.56	127.73	120.28
2	N	119	TYR	N-CA-C	-5.56	100.86	109.14
1	c	96	CYS	CA-C-N	5.55	126.14	119.98
1	c	96	CYS	C-N-CA	5.55	126.14	119.98
2	D	148	GLU	CA-C-N	5.55	128.73	120.90
2	D	148	GLU	C-N-CA	5.55	128.73	120.90
2	P	61	VAL	N-CA-C	-5.55	102.74	109.01
2	Q	161	ILE	CB-CA-C	-5.55	104.65	112.14
1	b	151	ILE	CA-C-N	5.55	127.65	120.44
1	b	151	ILE	C-N-CA	5.55	127.65	120.44
1	q	30	ILE	N-CA-C	-5.54	106.00	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	x	59	VAL	N-CA-C	-5.54	107.34	112.83
2	M	148	GLU	N-CA-C	-5.54	99.90	108.42
1	g	113	MET	CA-C-N	5.53	128.57	120.71
1	g	113	MET	C-N-CA	5.53	128.57	120.71
1	f	38	LYS	CA-C-N	5.53	128.04	120.46
1	f	38	LYS	C-N-CA	5.53	128.04	120.46
2	Q	77	ALA	CA-C-N	5.53	127.69	120.28
2	Q	77	ALA	C-N-CA	5.53	127.69	120.28
1	u	42	HIS	CE1-NE2-CD2	-5.53	103.47	109.00
2	C	82	ASP	CA-CB-CG	-5.52	107.08	112.60
1	e	130	LEU	N-CA-C	5.52	117.38	111.36
1	t	27	MET	CA-C-N	5.52	131.63	121.70
1	t	27	MET	C-N-CA	5.52	131.63	121.70
1	x	138	HIS	CA-C-N	5.51	130.19	122.36
1	x	138	HIS	C-N-CA	5.51	130.19	122.36
1	n	51	SER	N-CA-C	-5.51	104.81	112.03
1	k	72	VAL	N-CA-C	-5.51	101.08	108.35
1	h	123	ASN	CA-C-N	5.51	127.66	120.28
1	h	123	ASN	C-N-CA	5.51	127.66	120.28
2	B	106	HIS	ND1-CE1-NE2	5.50	113.90	108.40
2	D	53	GLU	CA-C-N	5.50	132.05	121.54
2	D	53	GLU	C-N-CA	5.50	132.05	121.54
2	D	145	LEU	N-CA-C	-5.50	107.82	114.75
1	e	29	SER	CA-C-N	5.50	127.49	120.56
1	e	29	SER	C-N-CA	5.50	127.49	120.56
1	l	113	MET	CA-C-N	5.50	128.58	120.82
1	l	113	MET	C-N-CA	5.50	128.58	120.82
1	l	126	ILE	CA-C-N	5.50	127.65	120.28
1	l	126	ILE	C-N-CA	5.50	127.65	120.28
1	g	109	LEU	CA-C-N	5.50	128.00	120.46
1	g	109	LEU	C-N-CA	5.50	128.00	120.46
2	V	90	GLU	CA-C-N	5.50	127.65	120.28
2	V	90	GLU	C-N-CA	5.50	127.65	120.28
1	t	123	ASN	N-CA-CB	5.49	119.84	110.50
1	a	102	SER	CA-C-N	5.49	127.58	120.44
1	a	102	SER	C-N-CA	5.49	127.58	120.44
1	r	39	VAL	N-CA-C	-5.49	107.40	112.83
1	i	102	SER	CA-C-N	5.49	127.63	120.28
1	i	102	SER	C-N-CA	5.49	127.63	120.28
1	m	67	PRO	CA-C-N	5.49	127.63	120.28
1	m	67	PRO	C-N-CA	5.49	127.63	120.28
1	r	83	THR	N-CA-C	-5.49	107.84	114.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	58	GLY	N-CA-C	-5.48	107.75	115.32
1	m	161	PRO	N-CA-C	-5.48	107.02	114.80
1	t	108	GLU	CA-C-N	5.48	127.57	120.44
1	t	108	GLU	C-N-CA	5.48	127.57	120.44
1	o	42	HIS	CE1-NE2-CD2	-5.48	103.52	109.00
1	t	115	LEU	CA-C-N	5.48	129.04	120.82
1	t	115	LEU	C-N-CA	5.48	129.04	120.82
1	q	44	THR	O-C-N	-5.48	117.21	123.40
2	W	106	HIS	CE1-NE2-CD2	-5.48	103.52	109.00
1	d	114	THR	CA-C-N	5.48	128.16	120.28
1	d	114	THR	C-N-CA	5.48	128.16	120.28
2	U	122	ASN	CA-C-N	5.47	129.02	120.75
2	U	122	ASN	C-N-CA	5.47	129.02	120.75
1	p	161	PRO	N-CA-C	-5.47	106.99	114.98
2	R	90	GLU	CA-C-N	5.47	127.61	120.28
2	R	90	GLU	C-N-CA	5.47	127.61	120.28
1	k	98	SER	CA-C-N	5.46	128.62	120.31
1	k	98	SER	C-N-CA	5.46	128.62	120.31
1	m	142	LEU	CA-C-N	5.46	128.15	120.28
1	m	142	LEU	C-N-CA	5.46	128.15	120.28
1	f	119	ALA	CA-C-N	5.46	131.12	122.61
1	f	119	ALA	C-N-CA	5.46	131.12	122.61
1	f	125	GLU	CA-C-N	5.46	127.64	120.60
1	f	125	GLU	C-N-CA	5.46	127.64	120.60
1	k	35	TYR	CA-C-O	-5.46	115.08	120.70
1	c	109	LEU	CA-C-N	5.46	127.93	120.46
1	c	109	LEU	C-N-CA	5.46	127.93	120.46
1	g	108	GLU	CA-C-N	5.46	127.85	120.65
1	g	108	GLU	C-N-CA	5.46	127.85	120.65
1	t	35	TYR	CA-C-N	5.46	131.52	121.70
1	t	35	TYR	C-N-CA	5.46	131.52	121.70
1	l	96	CYS	CA-C-N	5.46	127.21	120.34
1	l	96	CYS	C-N-CA	5.46	127.21	120.34
2	R	124	GLN	CA-C-O	-5.46	115.01	120.63
1	e	43	TYR	N-CA-C	5.45	117.03	111.14
2	O	83	HIS	CA-C-N	5.45	127.53	120.44
2	O	83	HIS	C-N-CA	5.45	127.53	120.44
1	r	27	MET	CA-C-N	5.45	131.51	121.70
1	r	27	MET	C-N-CA	5.45	131.51	121.70
2	D	106	HIS	CE1-NE2-CD2	-5.45	103.55	109.00
1	t	106	MET	N-CA-CB	5.45	118.22	110.16
1	x	36	HIS	CA-CB-CG	-5.45	108.35	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	158	LEU	CA-C-N	5.45	127.89	120.54
2	C	158	LEU	C-N-CA	5.45	127.89	120.54
2	L	65	VAL	N-CA-CB	-5.45	106.22	112.21
1	c	48	ASN	CA-C-N	5.44	131.50	121.70
1	c	48	ASN	C-N-CA	5.44	131.50	121.70
2	B	61	VAL	O-C-N	-5.44	114.90	121.10
2	J	54	SER	CA-C-N	5.43	131.48	121.70
2	J	54	SER	C-N-CA	5.43	131.48	121.70
2	T	125	PRO	CA-C-N	5.43	125.75	119.93
2	T	125	PRO	C-N-CA	5.43	125.75	119.93
2	C	113	ILE	CB-CA-C	-5.43	104.67	110.16
2	L	67	ASN	N-CA-CB	5.43	119.67	110.49
1	r	97	GLY	CA-C-N	5.43	127.56	120.28
1	r	97	GLY	C-N-CA	5.43	127.56	120.28
2	A	59	GLN	CA-C-N	5.43	127.90	120.46
2	A	59	GLN	C-N-CA	5.43	127.90	120.46
2	U	106	HIS	CG-CD2-NE2	5.43	112.63	107.20
2	X	99	ILE	N-CA-C	-5.43	97.15	108.88
2	L	83	HIS	ND1-CE1-NE2	5.43	113.83	108.40
2	N	64	GLU	N-CA-C	-5.43	105.36	112.41
2	J	86	ASP	CA-CB-CG	5.42	118.03	112.60
1	t	127	ALA	CA-C-N	5.42	127.54	120.28
1	t	127	ALA	C-N-CA	5.42	127.54	120.28
2	L	102	VAL	N-CA-C	-5.42	99.90	108.90
2	C	124	GLN	CA-C-O	-5.42	114.40	120.25
1	g	51	SER	CA-C-N	5.41	128.40	120.71
1	g	51	SER	C-N-CA	5.41	128.40	120.71
1	h	42	HIS	CE1-NE2-CD2	-5.41	103.59	109.00
1	d	159	ASN	N-CA-CB	5.41	119.64	110.49
2	A	84	LEU	CA-C-N	5.41	127.47	120.44
2	A	84	LEU	C-N-CA	5.41	127.47	120.44
1	g	43	TYR	N-CA-C	5.41	117.25	111.36
1	s	27	MET	N-CA-C	5.41	116.85	111.07
2	E	74	HIS	CE1-NE2-CD2	-5.40	103.60	109.00
1	i	27	MET	CA-C-N	5.40	131.43	121.70
1	i	27	MET	C-N-CA	5.40	131.43	121.70
1	b	55	LYS	CA-C-N	5.40	131.43	121.70
1	b	55	LYS	C-N-CA	5.40	131.43	121.70
2	J	111	LEU	N-CA-C	-5.40	100.10	108.90
1	n	36	HIS	CA-CB-CG	5.40	119.20	113.80
2	R	85	LEU	CA-C-N	5.40	127.46	120.44
2	R	85	LEU	C-N-CA	5.40	127.46	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	n	121	ILE	CA-C-N	5.39	129.35	121.31
1	n	121	ILE	C-N-CA	5.39	129.35	121.31
1	l	138	HIS	ND1-CE1-NE2	5.39	113.79	108.40
1	c	30	ILE	CA-C-N	5.39	129.79	122.19
1	c	30	ILE	C-N-CA	5.39	129.79	122.19
2	K	74	HIS	CE1-NE2-CD2	-5.39	103.61	109.00
1	j	114	THR	CA-C-N	5.39	128.04	120.28
1	j	114	THR	C-N-CA	5.39	128.04	120.28
1	t	120	LYS	N-CA-C	5.38	119.15	112.47
2	D	158	LEU	CA-C-N	5.38	127.81	120.54
2	D	158	LEU	C-N-CA	5.38	127.81	120.54
1	x	96	CYS	CA-C-N	5.38	125.92	120.00
1	x	96	CYS	C-N-CA	5.38	125.92	120.00
2	R	95	HIS	CE1-NE2-CD2	-5.38	103.62	109.00
1	t	64	VAL	N-CA-C	-5.38	100.72	108.42
2	I	124	GLN	N-CA-C	-5.38	100.07	109.48
2	S	85	LEU	CA-C-N	5.38	127.43	120.44
2	S	85	LEU	C-N-CA	5.38	127.43	120.44
1	e	115	LEU	CA-C-N	5.38	127.80	120.54
1	e	115	LEU	C-N-CA	5.38	127.80	120.54
1	p	154	TYR	CA-C-N	5.38	127.48	120.28
1	p	154	TYR	C-N-CA	5.38	127.48	120.28
2	P	56	THR	CA-C-N	5.38	131.38	121.70
2	P	56	THR	C-N-CA	5.38	131.38	121.70
1	m	97	GLY	CA-C-N	5.37	128.23	120.38
1	m	97	GLY	C-N-CA	5.37	128.23	120.38
1	p	116	ASP	CA-C-N	5.37	127.79	120.54
1	p	116	ASP	C-N-CA	5.37	127.79	120.54
1	k	33	ARG	NE-CZ-NH1	-5.36	116.14	121.50
1	c	42	HIS	CE1-NE2-CD2	-5.36	103.64	109.00
2	H	95	HIS	CG-CD2-NE2	5.36	112.56	107.20
1	d	42	HIS	CE1-NE2-CD2	-5.36	103.64	109.00
1	l	132	LEU	CA-C-O	-5.36	114.44	119.91
1	d	35	TYR	CA-C-N	5.35	131.34	121.70
1	d	35	TYR	C-N-CA	5.35	131.34	121.70
2	L	148	GLU	N-CA-C	-5.35	100.60	108.79
2	U	101	ASP	CA-CB-CG	-5.35	107.25	112.60
1	q	89	VAL	N-CA-C	-5.35	100.94	108.27
1	p	107	THR	N-CA-CB	5.35	117.98	110.12
2	X	95	HIS	CE1-NE2-CD2	-5.35	103.65	109.00
2	I	75	GLU	CA-C-N	5.34	131.32	121.70
2	I	75	GLU	C-N-CA	5.34	131.32	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	r	45	HIS	ND1-CE1-NE2	5.34	113.74	108.40
2	U	106	HIS	CE1-NE2-CD2	-5.34	103.66	109.00
2	Q	56	THR	CA-C-N	5.34	131.31	121.70
2	Q	56	THR	C-N-CA	5.34	131.31	121.70
2	S	78	ASP	CA-C-N	5.34	127.69	120.38
2	S	78	ASP	C-N-CA	5.34	127.69	120.38
1	l	117	ASP	CA-C-N	5.34	127.43	120.28
1	l	117	ASP	C-N-CA	5.34	127.43	120.28
2	V	54	SER	CA-C-N	5.34	131.31	121.70
2	V	54	SER	C-N-CA	5.34	131.31	121.70
2	F	106	HIS	CE1-NE2-CD2	-5.33	103.67	109.00
1	v	27	MET	CA-C-N	5.33	131.30	121.70
1	v	27	MET	C-N-CA	5.33	131.30	121.70
2	E	159	THR	CA-C-N	5.33	127.86	120.29
2	E	159	THR	C-N-CA	5.33	127.86	120.29
1	n	94	PHE	CA-CB-CG	-5.33	108.47	113.80
2	R	74	HIS	CE1-NE2-CD2	-5.33	103.67	109.00
2	W	116	PHE	CB-CA-C	-5.33	102.16	110.37
2	X	74	HIS	CE1-NE2-CD2	-5.33	103.67	109.00
2	W	143	ASP	CA-C-N	5.33	128.28	120.71
2	W	143	ASP	C-N-CA	5.33	128.28	120.71
1	i	148	LYS	CB-CA-C	-5.33	102.52	110.88
1	x	66	ALA	CA-C-O	-5.33	114.44	119.55
1	m	27	MET	CA-C-N	5.32	131.28	121.70
1	m	27	MET	C-N-CA	5.32	131.28	121.70
1	s	27	MET	CA-C-N	5.32	131.28	121.70
1	s	27	MET	C-N-CA	5.32	131.28	121.70
2	E	143	ASP	CA-C-N	5.32	128.26	120.71
2	E	143	ASP	C-N-CA	5.32	128.26	120.71
1	d	138	HIS	CA-C-N	5.32	131.70	121.54
1	d	138	HIS	C-N-CA	5.32	131.70	121.54
2	J	143	ASP	N-CA-C	-5.32	99.47	110.80
2	J	80	TYR	CA-C-N	5.32	127.40	120.28
2	J	80	TYR	C-N-CA	5.32	127.40	120.28
1	l	138	HIS	CE1-NE2-CD2	-5.32	103.69	109.00
1	j	125	GLU	N-CA-C	5.31	117.07	111.28
2	N	98	CYS	CA-C-N	5.31	131.96	122.13
2	N	98	CYS	C-N-CA	5.31	131.96	122.13
1	c	44	THR	O-C-N	-5.31	116.98	123.30
1	f	26	HIS	CE1-NE2-CD2	-5.31	103.69	109.00
1	f	97	GLY	CA-C-N	5.31	127.65	120.38
1	f	97	GLY	C-N-CA	5.31	127.65	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	143	ALA	CA-C-N	5.31	127.34	120.44
1	f	143	ALA	C-N-CA	5.31	127.34	120.44
1	n	80	ASN	N-CA-C	-5.31	100.08	108.73
1	m	119	ALA	CA-C-N	5.31	129.67	122.19
1	m	119	ALA	C-N-CA	5.31	129.67	122.19
1	e	120	LYS	CA-C-N	5.30	127.68	120.63
1	e	120	LYS	C-N-CA	5.30	127.68	120.63
2	M	95	HIS	CE1-NE2-CD2	-5.30	103.70	109.00
1	m	79	VAL	N-CA-C	-5.30	101.35	108.35
2	N	148	GLU	N-CA-C	-5.30	101.02	109.07
1	s	48	ASN	CA-C-N	5.30	131.24	121.70
1	s	48	ASN	C-N-CA	5.30	131.24	121.70
2	T	126	PRO	CA-C-N	5.30	131.66	121.54
2	T	126	PRO	C-N-CA	5.30	131.66	121.54
1	w	142	LEU	CA-C-N	5.30	127.38	120.28
1	w	142	LEU	C-N-CA	5.30	127.38	120.28
2	Q	87	SER	CA-C-N	5.29	127.32	120.44
2	Q	87	SER	C-N-CA	5.29	127.32	120.44
1	e	31	THR	N-CA-CB	5.29	119.43	110.49
1	t	102	SER	CA-C-N	5.29	127.31	120.44
1	t	102	SER	C-N-CA	5.29	127.31	120.44
2	L	83	HIS	CA-C-N	5.28	127.36	120.28
2	L	83	HIS	C-N-CA	5.28	127.36	120.28
2	M	95	HIS	CA-C-N	5.28	124.97	119.64
2	M	95	HIS	C-N-CA	5.28	124.97	119.64
1	i	55	LYS	CA-C-N	5.28	131.21	121.70
1	i	55	LYS	C-N-CA	5.28	131.21	121.70
2	M	102	VAL	N-CA-C	-5.28	100.46	108.17
2	V	162	LEU	CA-C-N	5.28	129.58	121.19
2	V	162	LEU	C-N-CA	5.28	129.58	121.19
1	e	51	SER	N-CA-C	-5.28	104.49	112.99
2	P	89	GLU	N-CA-C	5.28	116.72	111.07
1	s	35	TYR	CA-C-N	5.28	131.19	121.70
1	s	35	TYR	C-N-CA	5.28	131.19	121.70
1	x	36	HIS	CE1-NE2-CD2	-5.28	103.72	109.00
2	U	124	GLN	N-CA-C	-5.27	102.18	110.14
1	n	27	MET	CA-C-O	-5.27	114.96	120.55
1	h	122	LYS	O-C-N	-5.27	117.01	122.96
2	T	114	PRO	CA-C-N	5.27	129.62	122.19
2	T	114	PRO	C-N-CA	5.27	129.62	122.19
1	g	123	ASN	CA-C-N	5.27	128.72	120.82
1	g	123	ASN	C-N-CA	5.27	128.72	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	116	PHE	CA-CB-CG	-5.27	108.53	113.80
1	x	37	PRO	CA-C-N	5.27	131.60	121.54
1	x	37	PRO	C-N-CA	5.27	131.60	121.54
2	S	99	ILE	N-CA-C	-5.26	99.39	107.71
2	I	73	ALA	N-CA-CB	5.26	119.38	110.49
1	k	147	ILE	N-CA-CB	5.26	117.69	110.54
2	I	129	GLN	N-CA-C	5.25	117.92	111.82
2	G	124	GLN	CA-C-N	5.25	125.79	120.38
2	G	124	GLN	C-N-CA	5.25	125.79	120.38
1	v	39	VAL	CA-C-N	5.25	131.42	121.97
1	v	39	VAL	C-N-CA	5.25	131.42	121.97
1	k	115	LEU	CA-C-N	5.25	127.31	120.28
1	k	115	LEU	C-N-CA	5.25	127.31	120.28
2	L	56	THR	CA-C-N	5.25	131.15	121.70
2	L	56	THR	C-N-CA	5.25	131.15	121.70
2	X	168	LYS	N-CA-CB	5.25	118.30	110.22
1	k	144	GLU	CA-C-N	5.25	127.31	120.28
1	k	144	GLU	C-N-CA	5.25	127.31	120.28
1	g	28	SER	CA-C-N	5.24	127.26	120.44
1	g	28	SER	C-N-CA	5.24	127.26	120.44
1	b	27	MET	CA-C-N	5.24	131.12	121.70
1	b	27	MET	C-N-CA	5.24	131.12	121.70
2	R	127	ASN	N-CA-CB	5.24	119.34	110.49
1	n	134	PRO	CA-N-CD	-5.23	104.67	112.00
1	x	44	THR	O-C-N	-5.23	117.15	123.27
1	j	128	LYS	CA-C-N	5.22	127.28	120.28
1	j	128	LYS	C-N-CA	5.22	127.28	120.28
2	Q	67	ASN	N-CA-C	-5.22	106.49	112.92
1	f	138	HIS	ND1-CE1-NE2	5.22	113.62	108.40
1	h	110	VAL	N-CA-CB	5.22	117.64	110.54
1	k	138	HIS	N-CA-C	-5.22	99.68	110.80
1	f	152	LYS	CA-C-N	5.22	127.27	120.28
1	f	152	LYS	C-N-CA	5.22	127.27	120.28
2	T	91	LEU	CA-C-N	5.22	127.59	120.54
2	T	91	LEU	C-N-CA	5.22	127.59	120.54
1	i	121	ILE	CA-C-N	5.22	128.63	120.75
1	i	121	ILE	C-N-CA	5.22	128.63	120.75
1	t	48	ASN	CA-CB-CG	5.22	117.82	112.60
1	n	35	TYR	CA-C-N	5.22	131.09	121.70
1	n	35	TYR	C-N-CA	5.22	131.09	121.70
2	L	54	SER	CA-C-N	5.21	131.09	121.70
2	L	54	SER	C-N-CA	5.21	131.09	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	40	ILE	CA-C-N	5.21	127.69	120.29
1	e	40	ILE	C-N-CA	5.21	127.69	120.29
1	h	133	PRO	N-CA-C	-5.21	104.34	110.70
2	W	124	GLN	CA-C-N	5.21	125.75	120.38
2	W	124	GLN	C-N-CA	5.21	125.75	120.38
1	l	42	HIS	ND1-CE1-NE2	5.21	113.61	108.40
2	T	166	VAL	N-CA-CB	5.21	117.23	110.57
2	K	157	LYS	N-CA-C	5.21	117.01	110.24
1	a	56	LEU	CA-C-N	5.20	125.20	119.90
1	a	56	LEU	C-N-CA	5.20	125.20	119.90
2	I	96	PRO	N-CA-C	-5.20	107.42	114.80
2	A	143	ASP	CA-C-N	5.20	128.23	120.90
2	A	143	ASP	C-N-CA	5.20	128.23	120.90
1	w	85	VAL	N-CA-C	-5.20	100.37	107.75
2	O	71	GLU	CA-C-N	5.20	127.24	120.28
2	O	71	GLU	C-N-CA	5.20	127.24	120.28
1	r	89	VAL	N-CA-C	-5.20	101.15	108.27
2	F	116	PHE	N-CA-CB	5.19	119.27	110.49
1	u	113	MET	CA-C-N	5.19	131.46	121.54
1	u	113	MET	C-N-CA	5.19	131.46	121.54
2	U	125	PRO	CA-C-O	-5.19	113.03	120.56
1	c	127	ALA	N-CA-C	5.19	116.94	111.28
2	I	106	HIS	N-CA-C	-5.19	105.94	113.21
1	x	149	ALA	CA-C-N	5.19	127.19	120.44
1	x	149	ALA	C-N-CA	5.19	127.19	120.44
2	J	90	GLU	CA-C-N	5.19	127.23	120.28
2	J	90	GLU	C-N-CA	5.19	127.23	120.28
2	A	116	PHE	N-CA-C	-5.18	106.26	112.59
2	M	65	VAL	N-CA-CB	5.18	119.78	111.23
1	r	42	HIS	CE1-NE2-CD2	-5.18	103.82	109.00
1	k	27	MET	CA-C-N	5.18	131.03	121.70
1	k	27	MET	C-N-CA	5.18	131.03	121.70
1	h	33	ARG	CA-C-N	5.18	129.70	122.08
1	h	33	ARG	C-N-CA	5.18	129.70	122.08
2	M	95	HIS	CG-CD2-NE2	5.18	112.38	107.20
2	R	142	PHE	N-CA-C	-5.18	100.59	109.24
1	v	139	CYS	N-CA-CB	5.18	119.25	110.49
1	w	159	ASN	CA-CB-CG	-5.18	107.42	112.60
1	m	38	LYS	CA-C-N	5.18	127.77	120.42
1	m	38	LYS	C-N-CA	5.18	127.77	120.42
1	d	157	LYS	CA-C-N	5.17	127.21	120.28
1	d	157	LYS	C-N-CA	5.17	127.21	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	85	LEU	CA-C-N	5.17	127.17	120.44
2	J	85	LEU	C-N-CA	5.17	127.17	120.44
2	O	159	THR	CA-C-N	5.17	127.64	120.29
2	O	159	THR	C-N-CA	5.17	127.64	120.29
1	x	117	ASP	CA-C-N	5.17	127.22	120.28
1	x	117	ASP	C-N-CA	5.17	127.22	120.28
2	D	83	HIS	CA-C-N	5.17	127.16	120.44
2	D	83	HIS	C-N-CA	5.17	127.16	120.44
2	I	169	ALA	CA-C-N	5.17	127.82	120.53
2	I	169	ALA	C-N-CA	5.17	127.82	120.53
2	A	105	SER	N-CA-C	-5.17	100.97	109.40
2	I	90	GLU	CA-C-N	5.17	127.72	120.28
2	I	90	GLU	C-N-CA	5.17	127.72	120.28
1	n	29	SER	CA-C-N	5.17	127.54	120.46
1	n	29	SER	C-N-CA	5.17	127.54	120.46
2	K	164	GLU	N-CA-C	5.16	116.59	111.07
1	w	27	MET	CA-C-N	5.16	130.99	121.70
1	w	27	MET	C-N-CA	5.16	130.99	121.70
2	L	80	TYR	N-CA-CB	5.16	117.50	110.01
1	t	128	LYS	CA-C-N	5.16	127.15	120.44
1	t	128	LYS	C-N-CA	5.16	127.15	120.44
2	V	106	HIS	CE1-NE2-CD2	-5.16	103.84	109.00
1	u	42	HIS	ND1-CE1-NE2	5.16	113.56	108.40
1	v	118	ALA	N-CA-C	5.16	116.91	111.28
1	p	164	LEU	N-CA-C	-5.16	105.74	111.36
2	U	128	LYS	CA-C-N	5.16	128.17	120.95
2	U	128	LYS	C-N-CA	5.16	128.17	120.95
2	X	172	LYS	N-CA-CB	5.16	119.27	110.50
1	c	128	LYS	CB-CA-C	-5.16	102.23	110.79
1	x	27	MET	CA-C-N	5.16	130.98	121.70
1	x	27	MET	C-N-CA	5.16	130.98	121.70
1	e	147	ILE	N-CA-CB	5.15	118.31	110.58
1	a	51	SER	N-CA-C	-5.15	105.01	113.50
1	n	67	PRO	N-CA-C	-5.15	107.32	114.27
2	B	125	PRO	CA-C-N	5.14	126.27	119.84
2	B	125	PRO	C-N-CA	5.14	126.27	119.84
2	E	82	ASP	CA-CB-CG	-5.14	107.46	112.60
1	k	35	TYR	CA-C-N	5.14	130.96	121.70
1	k	35	TYR	C-N-CA	5.14	130.96	121.70
1	t	93	THR	N-CA-C	-5.14	100.52	108.90
2	W	157	LYS	CA-C-N	5.14	127.17	120.28
2	W	157	LYS	C-N-CA	5.14	127.17	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	67	PRO	CA-C-N	5.13	127.58	120.29
1	c	67	PRO	C-N-CA	5.13	127.58	120.29
1	g	117	ASP	CA-C-N	5.13	127.16	120.28
1	g	117	ASP	C-N-CA	5.13	127.16	120.28
2	G	83	HIS	CA-C-N	5.13	127.11	120.44
2	G	83	HIS	C-N-CA	5.13	127.11	120.44
1	l	35	TYR	CA-C-N	5.13	130.94	121.70
1	l	35	TYR	C-N-CA	5.13	130.94	121.70
1	t	36	HIS	CE1-NE2-CD2	-5.13	103.87	109.00
2	W	135	PRO	N-CA-C	-5.13	108.81	114.92
1	p	138	HIS	CE1-NE2-CD2	-5.13	103.87	109.00
2	R	160	ASP	CA-CB-CG	-5.13	107.47	112.60
2	E	127	ASN	N-CA-CB	5.13	119.15	110.49
1	u	36	HIS	CA-C-O	-5.12	112.09	120.80
1	m	120	LYS	CA-C-N	5.12	131.19	121.97
1	m	120	LYS	C-N-CA	5.12	131.19	121.97
1	u	128	LYS	CB-CA-C	-5.12	102.28	110.79
1	b	44	THR	CA-C-N	5.12	130.91	121.70
1	b	44	THR	C-N-CA	5.12	130.91	121.70
2	E	157	LYS	N-CA-C	5.12	117.31	110.35
2	M	152	LEU	N-CA-C	-5.12	106.62	112.92
1	h	86	ILE	N-CA-C	-5.12	99.89	107.51
2	T	59	GLN	N-CA-C	-5.12	105.73	112.94
1	w	123	ASN	CA-C-N	5.11	127.13	120.28
1	w	123	ASN	C-N-CA	5.11	127.13	120.28
1	w	159	ASN	N-CA-CB	5.11	119.13	110.49
1	b	94	PHE	N-CA-C	-5.11	100.71	109.24
1	p	26	HIS	ND1-CE1-NE2	5.11	113.51	108.40
2	R	169	ALA	CA-C-N	5.11	127.73	120.53
2	R	169	ALA	C-N-CA	5.11	127.73	120.53
1	k	134	PRO	N-CA-C	-5.11	101.95	112.47
1	n	42	HIS	CE1-NE2-CD2	-5.11	103.89	109.00
1	u	45	HIS	CE1-NE2-CD2	-5.11	103.89	109.00
1	q	156	SER	CA-C-N	5.10	127.12	120.28
1	q	156	SER	C-N-CA	5.10	127.12	120.28
1	p	159	ASN	CA-CB-CG	-5.10	107.50	112.60
2	W	73	ALA	N-CA-C	5.10	115.55	108.00
1	d	142	LEU	CA-C-N	5.10	127.37	120.38
1	d	142	LEU	C-N-CA	5.10	127.37	120.38
2	K	90	GLU	CA-C-N	5.10	127.11	120.28
2	K	90	GLU	C-N-CA	5.10	127.11	120.28
1	t	38	LYS	CA-C-N	5.10	127.45	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	t	38	LYS	C-N-CA	5.10	127.45	120.46
1	e	114	THR	CA-C-N	5.10	127.11	120.28
1	e	114	THR	C-N-CA	5.10	127.11	120.28
1	j	143	ALA	CA-C-N	5.10	127.07	120.44
1	j	143	ALA	C-N-CA	5.10	127.07	120.44
2	K	158	LEU	CA-C-N	5.10	127.36	120.38
2	K	158	LEU	C-N-CA	5.10	127.36	120.38
1	t	39	VAL	N-CA-C	5.10	115.82	110.62
2	W	92	SER	N-CA-C	5.10	116.84	111.28
1	g	33	ARG	CA-C-N	5.10	129.38	122.19
1	g	33	ARG	C-N-CA	5.10	129.38	122.19
2	J	79	ASP	CA-C-N	5.10	127.06	120.44
2	J	79	ASP	C-N-CA	5.10	127.06	120.44
1	a	29	SER	N-CA-C	-5.09	99.95	110.80
1	o	159	ASN	N-CA-CB	5.09	119.10	110.49
1	m	33	ARG	N-CA-CB	5.09	119.16	110.50
1	m	133	PRO	CA-C-N	5.09	126.20	119.84
1	m	133	PRO	C-N-CA	5.09	126.20	119.84
1	r	113	MET	CA-C-N	5.09	129.47	120.87
1	r	113	MET	C-N-CA	5.09	129.47	120.87
2	B	106	HIS	CE1-NE2-CD2	-5.08	103.92	109.00
2	N	131	TRP	CA-CB-CG	5.08	123.25	113.60
1	p	35	TYR	N-CA-C	-5.08	106.22	112.72
1	p	42	HIS	ND1-CE1-NE2	5.08	113.48	108.40
1	t	119	ALA	CA-C-N	5.08	130.53	122.61
1	t	119	ALA	C-N-CA	5.08	130.53	122.61
1	d	113	MET	CA-C-N	5.08	128.41	120.75
1	d	113	MET	C-N-CA	5.08	128.41	120.75
1	j	42	HIS	CE1-NE2-CD2	-5.07	103.93	109.00
2	K	102	VAL	N-CA-C	-5.07	101.01	108.11
2	K	142	PHE	CA-CB-CG	-5.07	108.73	113.80
1	i	134	PRO	N-CA-C	-5.07	106.14	114.75
1	l	142	LEU	CA-C-N	5.06	127.57	120.28
1	l	142	LEU	C-N-CA	5.06	127.57	120.28
1	o	34	LEU	CA-C-N	5.06	127.02	120.44
1	o	34	LEU	C-N-CA	5.06	127.02	120.44
2	R	163	THR	CA-C-N	5.06	127.37	120.54
2	R	163	THR	C-N-CA	5.06	127.37	120.54
1	b	51	SER	N-CA-C	-5.06	104.85	112.99
2	P	127	ASN	N-CA-CB	5.06	119.04	110.49
1	r	116	ASP	CA-C-N	5.06	127.06	120.28
1	r	116	ASP	C-N-CA	5.06	127.06	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	64	GLU	N-CA-CB	5.06	119.03	110.49
2	C	147	GLY	N-CA-C	-5.05	107.84	115.32
1	k	122	LYS	N-CA-C	-5.05	101.40	109.23
2	M	127	ASN	N-CA-CB	5.05	119.03	110.49
2	R	54	SER	CA-C-N	5.05	130.80	121.70
2	R	54	SER	C-N-CA	5.05	130.80	121.70
1	n	73	MET	CG-SD-CE	-5.05	89.78	100.90
1	g	128	LYS	CA-C-N	5.05	127.05	120.28
1	g	128	LYS	C-N-CA	5.05	127.05	120.28
1	i	107	THR	N-CA-CB	5.05	117.55	110.12
1	h	151	ILE	CA-CB-CG1	5.04	118.98	110.40
1	r	48	ASN	CA-C-N	5.04	130.78	121.70
1	r	48	ASN	C-N-CA	5.04	130.78	121.70
1	x	94	PHE	N-CA-C	-5.04	100.81	109.24
1	k	123	ASN	N-CA-C	-5.04	96.88	111.00
1	t	163	MET	CA-C-N	5.04	127.45	120.29
1	t	163	MET	C-N-CA	5.04	127.45	120.29
2	N	59	GLN	N-CA-C	-5.04	106.38	112.88
2	L	122	ASN	N-CA-C	-5.04	102.03	109.18
1	m	26	HIS	ND1-CE1-NE2	5.04	113.44	108.40
1	a	128	LYS	N-CA-CB	5.04	117.53	110.12
2	G	148	GLU	N-CA-C	-5.04	101.08	108.99
1	o	42	HIS	ND1-CE1-NE2	5.04	113.44	108.40
1	e	45	HIS	CE1-NE2-CD2	-5.03	103.97	109.00
2	F	143	ASP	CA-C-N	5.03	127.86	120.71
2	F	143	ASP	C-N-CA	5.03	127.86	120.71
1	k	116	ASP	CA-C-N	5.03	128.37	120.82
1	k	116	ASP	C-N-CA	5.03	128.37	120.82
2	O	95	HIS	CE1-NE2-CD2	-5.03	103.97	109.00
1	s	42	HIS	CE1-NE2-CD2	-5.03	103.97	109.00
2	Q	74	HIS	ND1-CE1-NE2	5.03	113.43	108.40
2	J	82	ASP	CA-C-N	5.03	126.98	120.44
2	J	82	ASP	C-N-CA	5.03	126.98	120.44
2	J	155	GLY	N-CA-C	-5.03	101.26	113.18
2	E	74	HIS	CG-CD2-NE2	5.03	112.23	107.20
1	o	72	VAL	N-CA-C	-5.03	101.71	108.35
2	F	157	LYS	CA-C-N	5.03	127.02	120.28
2	F	157	LYS	C-N-CA	5.03	127.02	120.28
2	L	122	ASN	CA-CB-CG	-5.03	107.58	112.60
2	P	151	SER	N-CA-C	-5.03	101.77	109.76
2	X	106	HIS	CE1-NE2-CD2	-5.03	103.97	109.00
2	A	111	LEU	N-CA-C	-5.02	100.98	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	s	113	MET	CA-C-N	5.02	129.36	120.87
1	s	113	MET	C-N-CA	5.02	129.36	120.87
1	c	164	LEU	N-CA-C	-5.02	105.52	111.69
1	k	83	THR	N-CA-C	-5.02	106.57	113.30
1	l	115	LEU	N-CA-C	5.02	116.44	111.07
1	u	126	ILE	CA-C-N	5.02	127.00	120.28
1	u	126	ILE	C-N-CA	5.02	127.00	120.28
1	w	145	ASP	CA-C-N	5.02	127.27	120.44
1	w	145	ASP	C-N-CA	5.02	127.27	120.44
2	X	83	HIS	CE1-NE2-CD2	-5.02	103.98	109.00
2	E	74	HIS	ND1-CE1-NE2	5.02	113.42	108.40
2	D	78	ASP	CA-C-N	5.01	127.25	120.38
2	D	78	ASP	C-N-CA	5.01	127.25	120.38
2	E	102	VAL	N-CA-C	-5.01	101.03	108.45
1	m	44	THR	CA-C-N	5.01	130.73	121.70
1	m	44	THR	C-N-CA	5.01	130.73	121.70
1	p	35	TYR	CA-C-N	5.01	130.73	121.70
1	p	35	TYR	C-N-CA	5.01	130.73	121.70
1	s	120	LYS	N-CA-CB	5.01	118.96	110.49
2	D	150	VAL	N-CA-C	-5.01	101.00	108.46
1	p	124	THR	CA-C-N	5.01	127.24	120.38
1	p	124	THR	C-N-CA	5.01	127.24	120.38
1	t	114	THR	CA-C-N	5.00	126.99	120.28
1	t	114	THR	C-N-CA	5.00	126.99	120.28
1	h	145	ASP	CA-C-N	5.00	127.25	120.44
1	h	145	ASP	C-N-CA	5.00	127.25	120.44
1	j	127	ALA	CA-C-N	5.00	126.98	120.28
1	j	127	ALA	C-N-CA	5.00	126.98	120.28

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

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Mol	Chain	Res	Type	Group
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	5	0
1	b	1072	0	1106	2	0
1	c	1072	0	1106	3	0
1	d	1072	0	1106	2	0
1	e	1072	0	1108	5	0
1	f	1072	0	1106	3	0
1	g	1072	0	1108	3	0
1	h	1072	0	1106	3	0
1	i	1072	0	1108	4	0
1	j	1072	0	1106	4	0
1	k	1072	0	1108	3	0
1	l	1072	0	1108	3	0
1	m	1072	0	1108	9	0
1	n	1072	0	1106	4	0
1	o	1072	0	1106	3	0
1	p	1072	0	1108	3	0
1	q	1072	0	1108	1	0
1	r	1072	0	1106	2	0
1	s	1072	0	1108	2	0
1	t	1072	0	1108	7	0
1	u	1072	0	1108	18	0
1	v	1072	0	1106	2	0
1	w	1072	0	1108	3	0
1	x	1072	0	1108	3	0
2	A	947	0	921	7	0
2	B	947	0	921	3	0
2	C	947	0	921	17	0
2	D	947	0	921	1	0
2	E	947	0	921	0	0
2	F	947	0	921	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	947	0	921	3	0
2	H	947	0	921	8	0
2	I	947	0	921	16	0
2	J	947	0	921	19	0
2	K	947	0	921	1	0
2	L	947	0	921	34	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	30	0
2	Q	947	0	921	4	0
2	R	947	0	921	6	0
2	S	947	0	921	28	0
2	T	947	0	921	2	0
2	U	947	0	921	1	0
2	V	947	0	921	47	0
2	W	947	0	921	37	0
2	X	947	0	921	1	0
All	All	48456	0	48674	381	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 (381) 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
1:u:30:ILE:HD11	1:u:98:SER:CA	1.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:u:30:ILE:CD1	1:u:98:SER:HA	1.78	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:L:121:ILE:HA	2:L:132:LEU:HD23	1.20	1.10
2:W:132:LEU:HD11	2:W:158:LEU:HB2	1.25	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:F:121:ILE:CG1	2:F:132:LEU:CD2	2.31	1.08
2:J:132:LEU:HD22	2:J:158:LEU:HG	1.31	1.08
1:u:30:ILE:HG12	1:u:97:GLY:C	1.78	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:I:95:HIS:CE1	2:I:170:ILE:HD11	1.93	1.03
2:V:131:TRP:CD1	2:V:142:PHE:HB2	1.93	1.03
2:I:95:HIS:HD1	2:I:170:ILE:HG12	1.21	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:131:TRP:HE1	2:L:133:ALA:HB2	1.23	1.02
2:L:121:ILE:CB	2:L:132:LEU:CD2	2.36	1.02
2:V:131:TRP:NE1	2:V:142:PHE:H	1.56	1.01
2:P:73:ALA:HB1	2:P:80:TYR:CE1	1.94	1.01
2:L:121:ILE:CA	2:L:132:LEU:CD2	2.38	1.00
1:u:30:ILE:CD1	1:u:98:SER:CA	2.35	1.00
2:V:130:ILE:O	2:V:131:TRP:HD1	1.41	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
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:A:76:GLU:CD	2:C:131:TRP:CZ3	2.46	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
1:u:30:ILE:CG1	1:u:97:GLY:C	2.41	0.93
2:A:76:GLU:CD	2:C:131:TRP:HZ3	1.77	0.93
2:P:73:ALA:O	2:P:80:TYR:OH	1.86	0.92
2:P:130:ILE:HD11	2:P:149:TRP:HE1	1.10	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
1:u:30:ILE:HD11	1:u:98:SER:N	1.85	0.91
2:V:131:TRP:CE3	2:V:141:ARG:HA	2.06	0.90
2:V:131:TRP:HE1	2:V:142:PHE:C	1.79	0.90
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
1:u:30:ILE:CD1	1:u:98:SER:N	2.36	0.88
2:V:130:ILE:O	2:V:131:TRP:CD1	2.26	0.88
2:J:132:LEU:HD21	2:J:158:LEU:CG	2.04	0.88
1:m:81:ASP:CB	1:m:154:TYR:OH	2.21	0.88
2:F:121:ILE:HG12	2:F:132:LEU:HD22	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:m:81:ASP:CG	1:m:154:TYR:OH	2.23	0.81
2:M:132:LEU:HD12	2:M:158:LEU:HB2	1.63	0.81
1:u:30:ILE:HD11	1:u:98:SER:HA	0.84	0.81
1:u:30:ILE:HG12	1:u:97:GLY:CA	2.11	0.80
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:V:131:TRP:NE1	2:V:142:PHE:C	2.39	0.79
2:V:131:TRP:CD1	2:V:142:PHE:H	2.00	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:u:30:ILE:HG12	1:u:98:SER:N	2.05	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:W:132:LEU:HD11	2:W:158:LEU:C	2.18	0.69
1:u:30:ILE:CG1	1:u:98:SER:N	2.56	0.68
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
1:m:81:ASP:CG	1:m:154:TYR:CZ	2.74	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
2:M:75:GLU:H	2:M:76:GLU:HA	1.61	0.64
1:p:35:TYR:H	1:p:36:HIS:HA	1.62	0.63
1:u:30:ILE:HG12	1:u:97:GLY:HA3	1.80	0.63
1:u:30:ILE:HD13	1:u:98:SER:OG	1.99	0.63
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
1:j:35:TYR:H	1:j:36:HIS:HA	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG1	2:L:132:LEU:HD22	2.04	0.61
2:L:121:ILE:HD13	2:L:132:LEU:HD11	1.83	0.61
2:V:132:LEU:HD12	2:V:132:LEU:O	2.02	0.60
2:V:132:LEU:HD12	2:V:132:LEU:C	2.27	0.59
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:V:131:TRP:CG	2:V:142:PHE:H	2.21	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
1:d:122:LYS:HB3	1:d:124:THR:H	1.67	0.58
2:I:95:HIS:CE1	2:I:170:ILE:CG1	2.87	0.57
2:V:130:ILE:C	2:V:131:TRP:CD1	2.81	0.57
2:I:95:HIS:CE1	2:I:170:ILE:HG12	2.40	0.57
1:m:121:ILE:HD12	1:m:121:ILE:H	1.69	0.57
2:P:131:TRP:CD1	2:P:132:LEU:N	2.73	0.57
2:G:68:LEU:HD13	1:i:149:ALA:HB2	1.87	0.56
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
1:t:36:HIS:CD2	1:t:37:PRO:HD3	2.42	0.55
2:V:131:TRP:NE1	2:V:142:PHE:CB	2.70	0.55
1:w:36:HIS:H	1:w:37:PRO:CD	2.20	0.55
2:S:55:SER:H	2:S:59:GLN:HB2	1.72	0.54
2:C:131:TRP:C	2:C:131:TRP:CD1	2.86	0.54
1:n:36:HIS:CG	1:n:37:PRO:HD3	2.43	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:S:131:TRP:CD1	2:S:131:TRP:C	2.86	0.54
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:W:131:TRP:CD1	2:W:132:LEU:C	2.86	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
1:n:122:LYS:HB3	1:n:124:THR:H	1.74	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: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
1:t:161:PRO:HD3	1:u:158:ARG:HE	1.74	0.52
2:S:132:LEU:HD11	2:S:158:LEU:HB2	1.92	0.52
1:h:56:LEU:H	1:h:57:PRO:HD2	1.75	0.51
1:a:56:LEU:H	1:a:56:LEU:HD22	1.75	0.51
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:P:131:TRP:CD1	2:P:131:TRP:C	2.88	0.51
2:J:150:VAL:HG22	2:J:151:SER:H	1.75	0.51
1:n:36:HIS:CD2	1:n:37:PRO:HD3	2.46	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
1:u:35:TYR:H	1:u:36:HIS:HA	1.76	0.50
1:i:56:LEU:H	1:i:57:PRO:HD2	1.75	0.50
1:t:40:ILE:HD12	1:t:40:ILE:H	1.76	0.50
1:o:36:HIS:CG	1:o:37:PRO:HD3	2.47	0.50
2:P:121:ILE:HG12	2:P:132:LEU:HD21	1.93	0.50
2:I:92:SER:O	2:I:95:HIS:NE2	2.45	0.50
1:x:122:LYS:HB3	1:x:124:THR:H	1.76	0.50
1:t:36:HIS:CG	1:t:37:PRO:HD3	2.46	0.49
2:L:131:TRP:CD1	2:L:131:TRP:C	2.90	0.49
1:e:121:ILE:HD13	1:e:147:ILE:HG23	1.93	0.49
2:V:131:TRP:HZ3	2:V:141:ARG:CG	2.18	0.49
1:a:39:VAL:HG13	1:a:40:ILE:H	1.78	0.49
1:l:56:LEU:H	1:l:57:PRO:HD2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:c:30:ILE:HG23	1:c:97:GLY:H	1.78	0.48
2:I:144:LEU:HD12	2:I:144:LEU:H	1.77	0.48
1:m:81:ASP:CG	1:m:154:TYR:HH	2.13	0.48
1:m:81:ASP:HB2	1:m:154:TYR:OH	2.07	0.48
1:w:110:VAL:HG13	1:w:118:ALA:HB2	1.94	0.48
1:w:66:ALA:HB1	2:X:63:GLN:HE21	1.78	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
1:k:36:HIS:CG	1:k:37:PRO:HD3	2.49	0.47
1:u:45:HIS:CG	1:u:46:PRO:HA	2.48	0.47
1:s:122:LYS:HA	1:s:123:ASN:HB2	1.96	0.47
1:c:56:LEU:H	1:c:57:PRO:HD2	1.79	0.47
2:W:131:TRP:CZ3	2:W:140:ASN:HB2	2.50	0.47
2:R:71:GLU:HB3	2:R:74:HIS:CE1	2.50	0.46
1:m:73:MET:HE1	1:m:94:PHE:H	1.79	0.46
1:m:81:ASP:HB3	1:m:154:TYR:OH	2.11	0.46
2:W:131:TRP:HE1	2:W:133:ALA:HA	1.80	0.46
1:a:79:VAL:HG11	1:a:154:TYR:CE2	2.50	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
1:r:56:LEU:H	1:r:57:PRO:HD2	1.80	0.46
2:W:131:TRP:HE3	2:W:142:PHE:CD1	2.32	0.46
1:h:138:HIS:CG	1:h:139:CYS:H	2.34	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
2:W:157:LYS:H	2:W:157:LYS:HD2	1.81	0.46
1:e:122:LYS:HB3	1:e:125:GLU:H	1.80	0.45
1:e:122:LYS:HA	1:e:123:ASN:HB2	1.98	0.45
1:g:36:HIS:CG	1:g:37:PRO:HD3	2.51	0.45
1:h:119:ALA:HB3	2:H:156:THR:HG21	1.99	0.45
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:P:131:TRP:CH2	2:Q:76:GLU:CD	2.80	0.45
2:C:129:GLN:O	2:C:130:ILE:HB	2.16	0.45
1:g:132:LEU:C	1:g:132:LEU:HD22	2.41	0.45
1:s:36:HIS:CD2	1:s:37:PRO:HD3	2.52	0.45
1:e:56:LEU:H	1:e:57:PRO:HD2	1.81	0.45
1:j:64:VAL:HA	2:K:67:ASN:HD21	1.82	0.45
2:J:132:LEU:HD21	2:J:142:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:l:124:THR:HG23	1:l:125:GLU:H	1.82	0.44
2:W:131:TRP:CG	2:W:132:LEU:N	2.85	0.44
1:x:32:LYS:HB3	1:x:33:ARG:HH21	1.83	0.44
1:a:122:LYS:HA	1:a:123:ASN:HB2	2.00	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
1:k:36:HIS:CD2	1:k:37:PRO:HD3	2.53	0.44
1:n:66:ALA:HB1	2:O:62:PRO:HB3	1.99	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
1:b:52:LEU:HD23	1:b:52:LEU:H	1.83	0.44
2:G:74:HIS:CE1	2:G:144:LEU:HD22	2.52	0.43
1:o:36:HIS:CD2	1:o:37:PRO:HD3	2.53	0.43
1:u:36:HIS:CG	1:u:37:PRO:HD3	2.52	0.43
2:O:93:GLU:HG2	1:v:132:LEU:H	1.84	0.43
2:P:131:TRP:CD1	2:P:132:LEU:C	2.96	0.43
2:V:131:TRP:CD2	2:V:142:PHE:N	2.70	0.43
1:f:123:ASN:H	1:f:126:ILE:HD12	1.83	0.43
2:S:129:GLN:O	2:S:130:ILE:HB	2.19	0.43
2:T:76:GLU:CD	2:T:76:GLU:H	2.26	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
1:k:127:ALA:HB1	1:k:133:PRO:HA	2.01	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
1:t:31:THR:HA	1:t:38:LYS:H	1.84	0.42
2:A:75:GLU:HB3	2:A:76:GLU:HA	2.00	0.42
1:g:122:LYS:HD3	1:g:144:GLU:H	1.84	0.42
1:a:120:LYS:HZ2	2:A:151:SER:HB3	1.84	0.42
2:S:121:ILE:HG22	2:S:132:LEU:HD23	2.02	0.42
1:f:127:ALA:HB1	1:f:133:PRO:HA	2.00	0.42
1:e:36:HIS:CG	1:e:37:PRO:HD3	2.55	0.42
2:L:131:TRP:HZ2	2:L:139:PRO:CG	2.32	0.42
2:F:157:LYS:H	2:F:157:LYS:HD2	1.84	0.42
1:r:122:LYS:HB3	1:r:123:ASN:HB2	2.00	0.42
1:t:52:LEU:H	1:t:52:LEU:HD23	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:68:LEU:CD1	1:i:149:ALA:HB2	2.49	0.42
1:j:138:HIS:CG	1:j:139:CYS:N	2.88	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
1:q:56:LEU:H	1:q:57:PRO:HD2	1.83	0.42
1:v:73:MET:HE3	1:v:142:LEU:H	1.84	0.42
2:V:131:TRP:CZ2	2:V:142:PHE:O	2.73	0.42
1:d:124:THR:HG23	2:D:136:LEU:HD12	2.01	0.41
2:O:72:LYS:H	2:O:72:LYS:HD2	1.84	0.41
2:W:113:ILE:H	2:W:118:THR:HG22	1.85	0.41
2:B:93:GLU:HB2	1:o:132:LEU:HD23	2.01	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
1:p:49:VAL:HG23	1:p:51:SER:H	1.84	0.41
2:M:158:LEU:H	2:M:158:LEU:HD23	1.86	0.41
2:C:94:ALA:H	1:l:132:LEU:HB2	1.85	0.41
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
1:c:127:ALA:HB1	1:c:133:PRO:HA	2.03	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
1:b:110:VAL:HG12	1:b:118:ALA:HA	2.03	0.41
1:p:122:LYS:HA	1:p:123:ASN:HB2	2.02	0.41
2:S:130:ILE:HG21	2:S:158:LEU:HD22	2.02	0.41
1:t:138:HIS:CD2	2:U:54:SER:H	2.38	0.41
1:i:35:TYR:N	1:i:36:HIS:HA	2.36	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:V:68:LEU:HD13	1:x:64:VAL:HG23	2.02	0.40
2:C:75:GLU:N	2:C:76:GLU:HA	2.36	0.40
1:f:138:HIS:CD2	1:f:138:HIS:H	2.38	0.40
1:j:56:LEU:H	1:j:57:PRO:HD2	1.86	0.40
1:m:81:ASP:OD2	1:m:154:TYR:OH	2.31	0.40
2:M:76:GLU:CD	2:M:76:GLU:H	2.29	0.40
1:u:30:ILE:CD1	1:u:98:SER:OG	2.68	0.40
2:F:121:ILE:CG2	2:F:132:LEU:CD2	2.99	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%)	1	16
1	b	140/142 (99%)	124 (89%)	11 (8%)	5 (4%)	2	20
1	c	140/142 (99%)	122 (87%)	10 (7%)	8 (6%)	1	14
1	d	140/142 (99%)	123 (88%)	9 (6%)	8 (6%)	1	14
1	e	140/142 (99%)	123 (88%)	11 (8%)	6 (4%)	2	17
1	f	140/142 (99%)	120 (86%)	14 (10%)	6 (4%)	2	17
1	g	140/142 (99%)	118 (84%)	20 (14%)	2 (1%)	9	40
1	h	140/142 (99%)	118 (84%)	15 (11%)	7 (5%)	1	16
1	i	140/142 (99%)	124 (89%)	10 (7%)	6 (4%)	2	17
1	j	140/142 (99%)	118 (84%)	12 (9%)	10 (7%)	1	11
1	k	140/142 (99%)	120 (86%)	13 (9%)	7 (5%)	1	16
1	l	140/142 (99%)	122 (87%)	12 (9%)	6 (4%)	2	17
1	m	140/142 (99%)	118 (84%)	17 (12%)	5 (4%)	2	20
1	n	140/142 (99%)	118 (84%)	19 (14%)	3 (2%)	5	30
1	o	140/142 (99%)	121 (86%)	14 (10%)	5 (4%)	2	20
1	p	140/142 (99%)	123 (88%)	11 (8%)	6 (4%)	2	17
1	q	140/142 (99%)	122 (87%)	12 (9%)	6 (4%)	2	17
1	r	140/142 (99%)	118 (84%)	14 (10%)	8 (6%)	1	14
1	s	140/142 (99%)	125 (89%)	7 (5%)	8 (6%)	1	14
1	t	140/142 (99%)	120 (86%)	13 (9%)	7 (5%)	1	16
1	u	140/142 (99%)	122 (87%)	11 (8%)	7 (5%)	1	16
1	v	140/142 (99%)	119 (85%)	12 (9%)	9 (6%)	1	12
1	w	140/142 (99%)	118 (84%)	18 (13%)	4 (3%)	3	23
1	x	140/142 (99%)	124 (89%)	11 (8%)	5 (4%)	2	20
2	A	119/121 (98%)	93 (78%)	24 (20%)	2 (2%)	7	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	119/121 (98%)	95 (80%)	14 (12%)	10 (8%)	0	9
2	C	119/121 (98%)	96 (81%)	18 (15%)	5 (4%)	2	17
2	D	119/121 (98%)	102 (86%)	11 (9%)	6 (5%)	1	16
2	E	119/121 (98%)	92 (77%)	20 (17%)	7 (6%)	1	13
2	F	119/121 (98%)	92 (77%)	20 (17%)	7 (6%)	1	13
2	G	119/121 (98%)	99 (83%)	14 (12%)	6 (5%)	1	16
2	H	119/121 (98%)	98 (82%)	18 (15%)	3 (2%)	4	26
2	I	119/121 (98%)	101 (85%)	11 (9%)	7 (6%)	1	13
2	J	119/121 (98%)	94 (79%)	20 (17%)	5 (4%)	2	17
2	K	119/121 (98%)	97 (82%)	15 (13%)	7 (6%)	1	13
2	L	119/121 (98%)	95 (80%)	15 (13%)	9 (8%)	1	10
2	M	119/121 (98%)	97 (82%)	14 (12%)	8 (7%)	1	12
2	N	119/121 (98%)	98 (82%)	16 (13%)	5 (4%)	2	17
2	O	119/121 (98%)	94 (79%)	21 (18%)	4 (3%)	3	21
2	P	119/121 (98%)	99 (83%)	13 (11%)	7 (6%)	1	13
2	Q	119/121 (98%)	90 (76%)	22 (18%)	7 (6%)	1	13
2	R	119/121 (98%)	97 (82%)	18 (15%)	4 (3%)	3	21
2	S	119/121 (98%)	95 (80%)	19 (16%)	5 (4%)	2	17
2	T	119/121 (98%)	100 (84%)	8 (7%)	11 (9%)	0	8
2	U	119/121 (98%)	97 (82%)	16 (13%)	6 (5%)	1	16
2	V	119/121 (98%)	100 (84%)	13 (11%)	6 (5%)	1	16
2	W	119/121 (98%)	93 (78%)	21 (18%)	5 (4%)	2	17
2	X	119/121 (98%)	98 (82%)	12 (10%)	9 (8%)	1	10
All	All	6216/6312 (98%)	5213 (84%)	701 (11%)	302 (5%)	3	16

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	118 (98%)	3 (2%)	42	63
1	b	121/121 (100%)	119 (98%)	2 (2%)	53	69
1	c	121/121 (100%)	116 (96%)	5 (4%)	27	49
1	d	121/121 (100%)	117 (97%)	4 (3%)	33	55
1	e	121/121 (100%)	118 (98%)	3 (2%)	42	63
1	f	121/121 (100%)	117 (97%)	4 (3%)	33	55
1	g	121/121 (100%)	112 (93%)	9 (7%)	13	33
1	h	121/121 (100%)	113 (93%)	8 (7%)	15	37
1	i	121/121 (100%)	116 (96%)	5 (4%)	27	49
1	j	121/121 (100%)	113 (93%)	8 (7%)	15	37
1	k	121/121 (100%)	120 (99%)	1 (1%)	73	80
1	l	121/121 (100%)	113 (93%)	8 (7%)	15	37
1	m	121/121 (100%)	113 (93%)	8 (7%)	15	37
1	n	121/121 (100%)	115 (95%)	6 (5%)	22	43
1	o	121/121 (100%)	117 (97%)	4 (3%)	33	55
1	p	121/121 (100%)	110 (91%)	11 (9%)	9	27
1	q	121/121 (100%)	118 (98%)	3 (2%)	42	63
1	r	121/121 (100%)	117 (97%)	4 (3%)	33	55
1	s	121/121 (100%)	113 (93%)	8 (7%)	15	37
1	t	121/121 (100%)	116 (96%)	5 (4%)	27	49
1	u	121/121 (100%)	119 (98%)	2 (2%)	53	69
1	v	121/121 (100%)	112 (93%)	9 (7%)	13	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	w	121/121 (100%)	113 (93%)	8 (7%)	15	37
1	x	121/121 (100%)	116 (96%)	5 (4%)	27	49
2	A	109/109 (100%)	106 (97%)	3 (3%)	38	60
2	B	109/109 (100%)	105 (96%)	4 (4%)	30	51
2	C	109/109 (100%)	101 (93%)	8 (7%)	13	34
2	D	109/109 (100%)	105 (96%)	4 (4%)	30	51
2	E	109/109 (100%)	107 (98%)	2 (2%)	51	68
2	F	109/109 (100%)	104 (95%)	5 (5%)	24	45
2	G	109/109 (100%)	104 (95%)	5 (5%)	24	45
2	H	109/109 (100%)	105 (96%)	4 (4%)	30	51
2	I	109/109 (100%)	103 (94%)	6 (6%)	19	41
2	J	109/109 (100%)	107 (98%)	2 (2%)	51	68
2	K	109/109 (100%)	105 (96%)	4 (4%)	30	51
2	L	109/109 (100%)	107 (98%)	2 (2%)	51	68
2	M	109/109 (100%)	105 (96%)	4 (4%)	30	51
2	N	109/109 (100%)	107 (98%)	2 (2%)	51	68
2	O	109/109 (100%)	107 (98%)	2 (2%)	51	68
2	P	109/109 (100%)	105 (96%)	4 (4%)	30	51
2	Q	109/109 (100%)	102 (94%)	7 (6%)	16	37
2	R	109/109 (100%)	107 (98%)	2 (2%)	51	68
2	S	109/109 (100%)	104 (95%)	5 (5%)	24	45
2	T	109/109 (100%)	102 (94%)	7 (6%)	16	37
2	U	109/109 (100%)	107 (98%)	2 (2%)	51	68
2	V	109/109 (100%)	106 (97%)	3 (3%)	38	60
2	W	109/109 (100%)	105 (96%)	4 (4%)	30	51
2	X	109/109 (100%)	105 (96%)	4 (4%)	30	51
All	All	5520/5520 (100%)	5292 (96%)	228 (4%)	28	49

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	38	LYS
1	a	83	THR

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Mol	Chain	Res	Type
1	a	89	VAL
2	A	89	GLU
2	A	99	ILE
2	A	140	ASN
1	b	33	ARG
1	b	71	ASP
2	B	128	LYS
2	B	132	LEU
2	B	158	LEU
2	B	164	GLU
1	c	48	ASN
1	c	71	ASP
1	c	89	VAL
1	c	120	LYS
1	c	154	TYR
2	C	56	THR
2	C	59	GLN
2	C	64	GLU
2	C	93	GLU
2	C	111	LEU
2	C	112	GLU
2	C	113	ILE
2	C	158	LEU
1	d	33	ARG
1	d	120	LYS
1	d	125	GLU
1	d	132	LEU
2	D	76	GLU
2	D	85	LEU
2	D	140	ASN
2	D	144	LEU
1	e	33	ARG
1	e	38	LYS
1	e	89	VAL
2	E	108	VAL
2	E	136	LEU
1	f	33	ARG
1	f	89	VAL
1	f	120	LYS
1	f	138	HIS
2	F	67	ASN
2	F	89	GLU

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Mol	Chain	Res	Type
2	F	111	LEU
2	F	145	LEU
2	F	157	LYS
1	g	33	ARG
1	g	34	LEU
1	g	52	LEU
1	g	63	LEU
1	g	89	VAL
1	g	120	LYS
1	g	126	ILE
1	g	128	LYS
1	g	132	LEU
2	G	76	GLU
2	G	88	LEU
2	G	132	LEU
2	G	157	LYS
2	G	170	ILE
1	h	33	ARG
1	h	38	LYS
1	h	47	ARG
1	h	48	ASN
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	125	PRO
2	H	168	LYS
1	i	33	ARG
1	i	89	VAL
1	i	122	LYS
1	i	129	GLU
1	i	137	LEU
2	I	64	GLU
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	64	VAL

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Mol	Chain	Res	Type
1	j	89	VAL
1	j	120	LYS
1	j	128	LYS
1	j	129	GLU
1	j	132	LEU
1	j	148	LYS
2	J	136	LEU
2	J	152	LEU
1	k	49	VAL
2	K	75	GLU
2	K	119	TYR
2	K	126	PRO
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	131	SER
2	L	76	GLU
2	L	157	LYS
1	m	33	ARG
1	m	49	VAL
1	m	76	GLN
1	m	79	VAL
1	m	87	GLU
1	m	120	LYS
1	m	125	GLU
1	m	132	LEU
2	M	111	LEU
2	M	130	ILE
2	M	157	LYS
2	M	168	LYS
1	n	38	LYS
1	n	122	LYS
1	n	132	LEU
1	n	134	PRO
1	n	135	VAL
1	n	148	LYS
2	N	84	LEU

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Mol	Chain	Res	Type
2	N	125	PRO
1	o	48	ASN
1	o	89	VAL
1	o	132	LEU
1	o	148	LYS
2	O	118	THR
2	O	157	LYS
1	p	30	ILE
1	p	33	ARG
1	p	38	LYS
1	p	49	VAL
1	p	63	LEU
1	p	71	ASP
1	p	89	VAL
1	p	124	THR
1	p	125	GLU
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	89	VAL
2	Q	53	GLU
2	Q	89	GLU
2	Q	102	VAL
2	Q	113	ILE
2	Q	132	LEU
2	Q	153	ARG
2	Q	154	ASN
1	r	33	ARG
1	r	49	VAL
1	r	126	ILE
1	r	135	VAL
2	R	136	LEU
2	R	141	ARG
1	s	33	ARG
1	s	36	HIS
1	s	71	ASP
1	s	89	VAL

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Mol	Chain	Res	Type
1	s	121	ILE
1	s	130	LEU
1	s	135	VAL
1	s	148	LYS
2	S	63	GLN
2	S	76	GLU
2	S	85	LEU
2	S	111	LEU
2	S	136	LEU
1	t	33	ARG
1	t	89	VAL
1	t	120	LYS
1	t	128	LYS
1	t	142	LEU
2	T	56	THR
2	T	70	LEU
2	T	76	GLU
2	T	120	VAL
2	T	136	LEU
2	T	158	LEU
2	T	168	LYS
1	u	132	LEU
1	u	137	LEU
2	U	61	VAL
2	U	102	VAL
1	v	33	ARG
1	v	34	LEU
1	v	71	ASP
1	v	89	VAL
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	158	LEU
1	w	33	ARG
1	w	63	LEU
1	w	89	VAL
1	w	106	MET
1	w	120	LYS

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Mol	Chain	Res	Type
1	w	122	LYS
1	w	125	GLU
1	w	148	LYS
2	W	111	LEU
2	W	119	TYR
2	W	150	VAL
2	W	157	LYS
1	x	48	ASN
1	x	71	ASP
1	x	89	VAL
1	x	120	LYS
1	x	164	LEU
2	X	61	VAL
2	X	126	PRO
2	X	136	LEU
2	X	172	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (181) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	36	HIS
1	a	58	ASN
1	a	76	GLN
1	a	80	ASN
2	A	63	GLN
2	A	74	HIS
2	A	127	ASN
1	b	138	HIS
2	B	59	GLN
2	B	67	ASN
2	B	95	HIS
2	B	146	ASN
2	B	154	ASN
1	c	48	ASN
1	c	80	ASN
1	c	138	HIS
2	C	74	HIS
2	C	95	HIS
2	C	106	HIS
2	C	124	GLN
2	C	127	ASN
1	d	76	GLN

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Mol	Chain	Res	Type
1	d	138	HIS
2	D	67	ASN
2	D	95	HIS
2	D	122	ASN
1	e	80	ASN
1	e	111	GLN
2	E	67	ASN
2	E	74	HIS
2	E	83	HIS
2	E	127	ASN
2	E	154	ASN
1	f	58	ASN
1	f	111	GLN
1	f	138	HIS
2	F	63	GLN
2	F	67	ASN
2	F	83	HIS
2	F	122	ASN
2	F	129	GLN
2	F	154	ASN
1	g	48	ASN
1	g	58	ASN
2	G	67	ASN
2	G	74	HIS
2	G	122	ASN
1	h	48	ASN
1	h	138	HIS
1	h	159	ASN
2	H	59	GLN
2	H	74	HIS
2	H	95	HIS
2	H	129	GLN
2	H	140	ASN
1	i	26	HIS
1	i	48	ASN
1	i	76	GLN
2	I	67	ASN
1	j	26	HIS
1	j	48	ASN
1	j	76	GLN
1	j	111	GLN
1	j	159	ASN

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Mol	Chain	Res	Type
2	J	59	GLN
2	J	74	HIS
1	k	123	ASN
1	k	138	HIS
2	K	83	HIS
2	K	95	HIS
2	K	122	ASN
2	K	124	GLN
2	K	127	ASN
2	K	140	ASN
1	l	48	ASN
1	l	58	ASN
1	l	80	ASN
1	l	138	HIS
2	L	63	GLN
2	L	122	ASN
2	L	129	GLN
2	L	140	ASN
2	L	146	ASN
2	L	154	ASN
1	m	36	HIS
1	m	123	ASN
1	m	159	ASN
2	M	95	HIS
2	M	129	GLN
2	M	140	ASN
2	M	146	ASN
1	n	48	ASN
1	n	58	ASN
1	n	76	GLN
1	n	111	GLN
1	n	159	ASN
2	N	67	ASN
2	N	95	HIS
2	N	122	ASN
2	N	124	GLN
2	N	127	ASN
1	o	36	HIS
1	o	48	ASN
1	o	76	GLN
1	o	123	ASN
1	o	138	HIS

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Mol	Chain	Res	Type
2	O	74	HIS
2	O	122	ASN
2	O	129	GLN
1	p	76	GLN
1	p	80	ASN
1	p	111	GLN
2	P	63	GLN
2	P	74	HIS
2	P	106	HIS
2	P	140	ASN
1	q	48	ASN
1	q	76	GLN
1	q	111	GLN
1	q	159	ASN
2	Q	122	ASN
1	r	58	ASN
1	r	76	GLN
1	r	80	ASN
1	r	123	ASN
2	R	74	HIS
2	R	83	HIS
1	s	58	ASN
2	S	59	GLN
2	S	63	GLN
2	S	67	ASN
2	S	74	HIS
2	S	83	HIS
2	S	140	ASN
2	S	154	ASN
1	t	48	ASN
1	t	58	ASN
1	t	80	ASN
1	t	138	HIS
1	t	159	ASN
2	T	63	GLN
2	T	74	HIS
2	T	83	HIS
2	T	106	HIS
2	T	154	ASN
1	u	42	HIS
1	u	45	HIS
1	u	58	ASN

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Mol	Chain	Res	Type
1	u	138	HIS
2	U	106	HIS
1	v	36	HIS
1	v	58	ASN
1	v	76	GLN
1	v	123	ASN
1	v	159	ASN
2	V	74	HIS
2	V	83	HIS
2	V	95	HIS
2	V	124	GLN
2	V	129	GLN
2	V	140	ASN
1	w	26	HIS
1	w	48	ASN
1	w	76	GLN
1	w	159	ASN
2	W	83	HIS
2	W	106	HIS
2	W	122	ASN
2	W	124	GLN
2	W	129	GLN
1	x	48	ASN
1	x	80	ASN
2	X	63	GLN
2	X	67	ASN
2	X	83	HIS
2	X	106	HIS
2	X	127	ASN
2	X	129	GLN
2	X	140	ASN
2	X	146	ASN
2	X	154	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

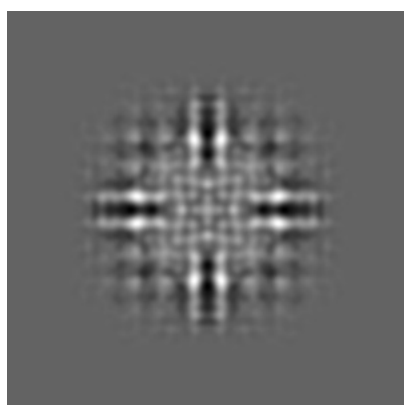
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8458. These allow visual inspection of the internal detail of the map and identification of artifacts.

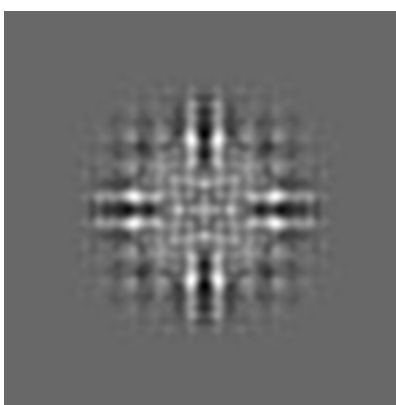
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

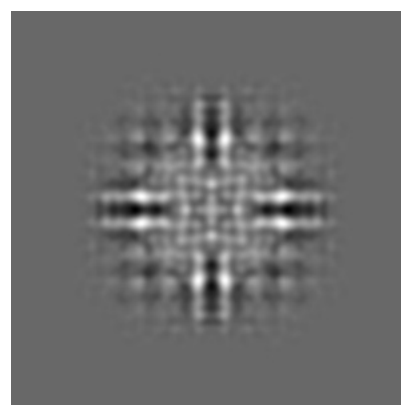
#### 6.1.1 Primary map



X



Y

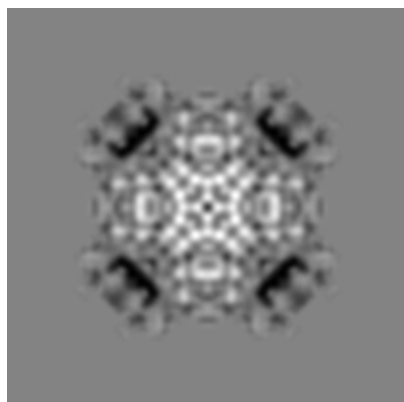


Z

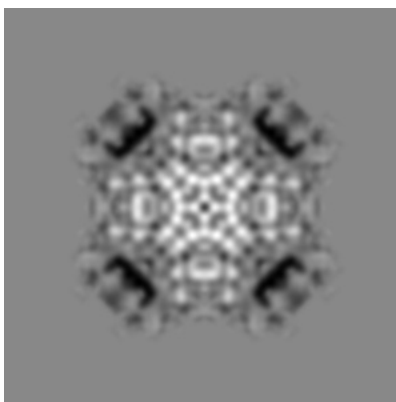
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

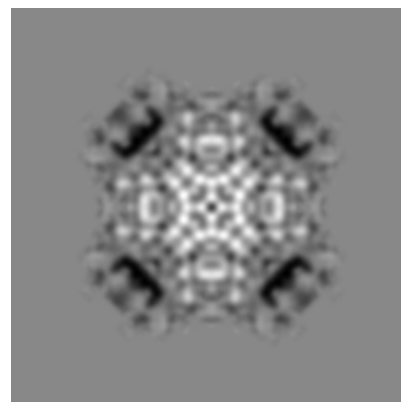
#### 6.2.1 Primary map



X Index: 144



Y Index: 144

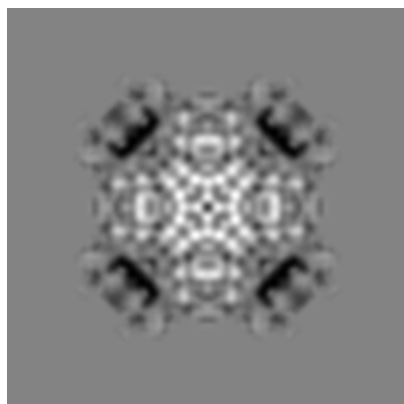


Z Index: 144

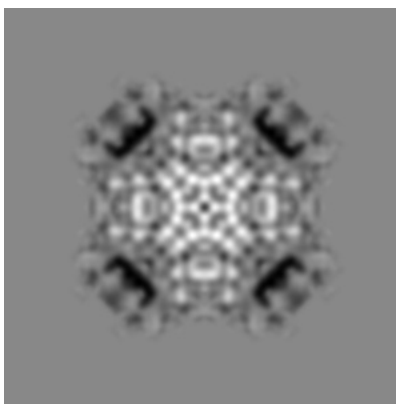
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

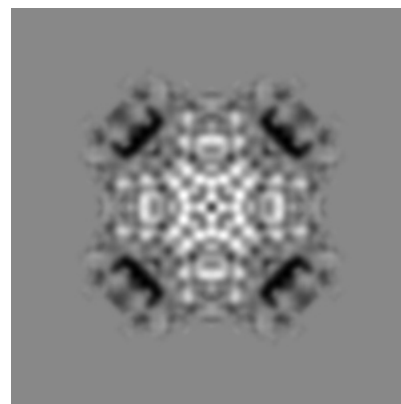
### 6.3.1 Primary map



X Index: 144



Y Index: 144

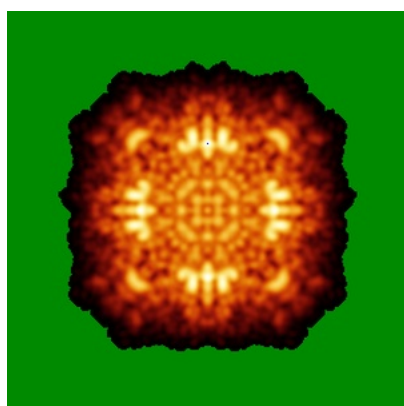


Z Index: 144

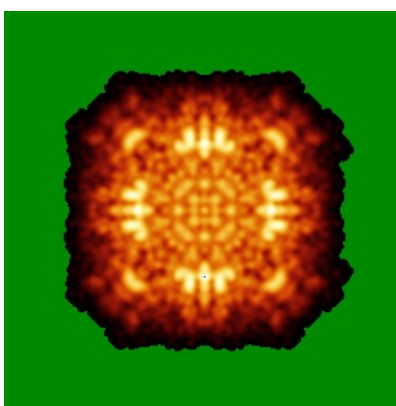
The images above show the largest variance slices of the map in three orthogonal directions.

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

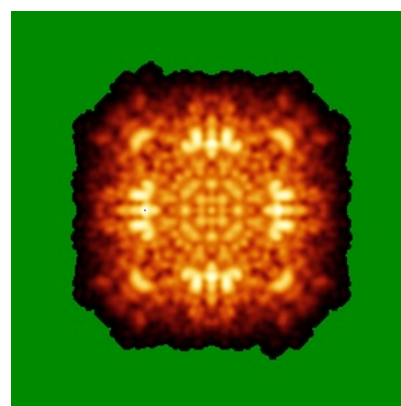
### 6.4.1 Primary map



X



Y



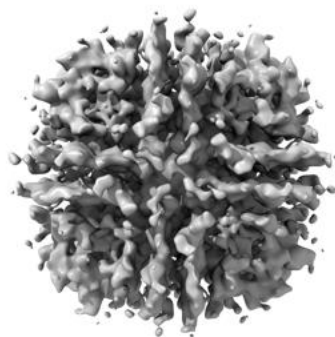
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

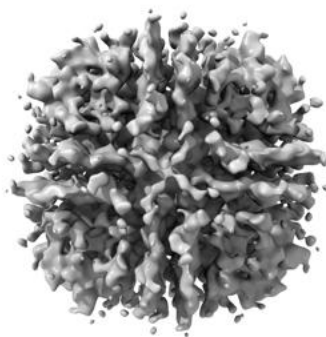


## 6.5 Orthogonal surface views [i](#)

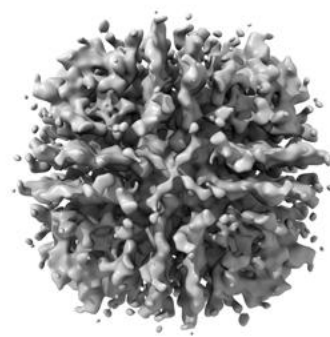
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

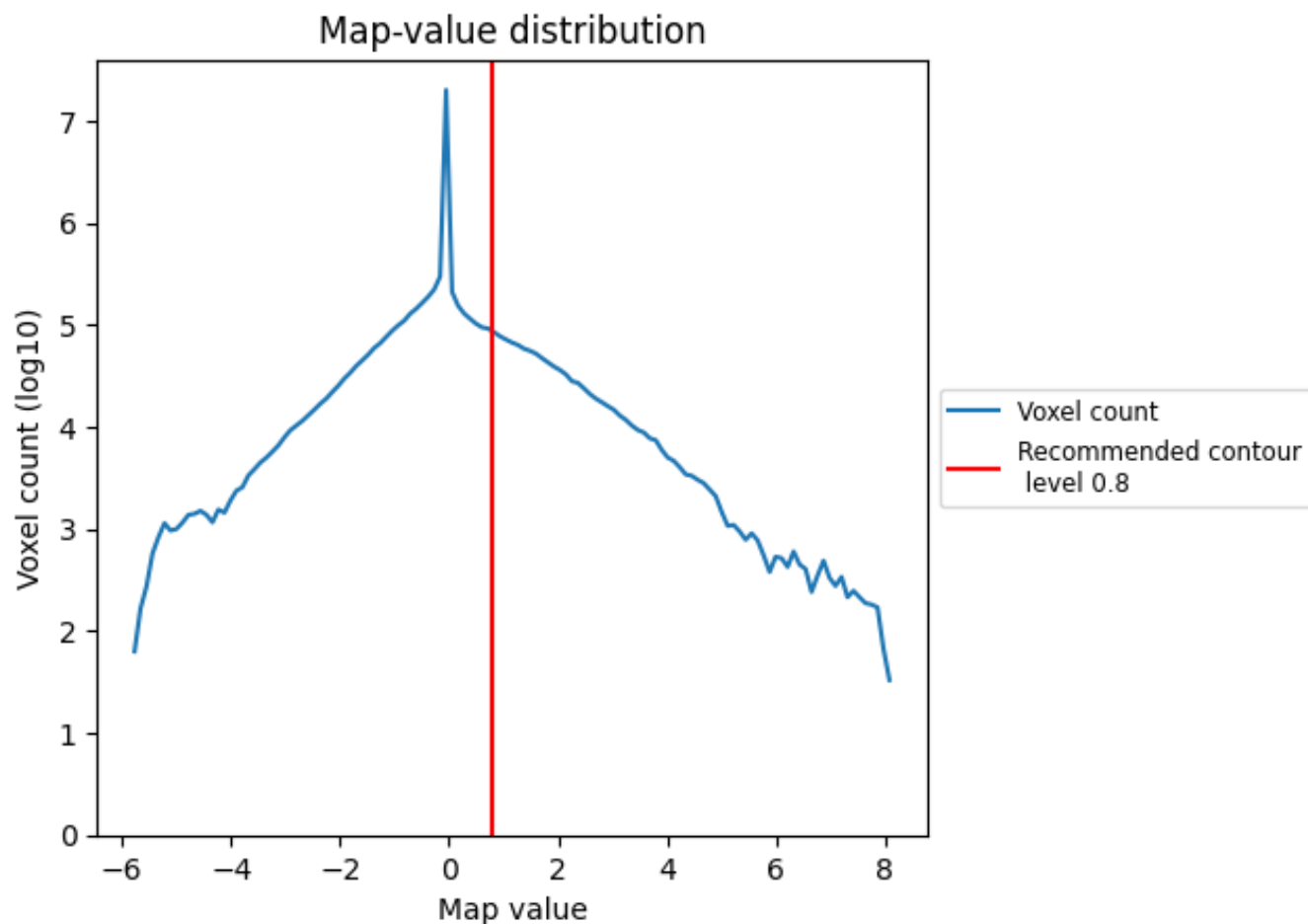
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

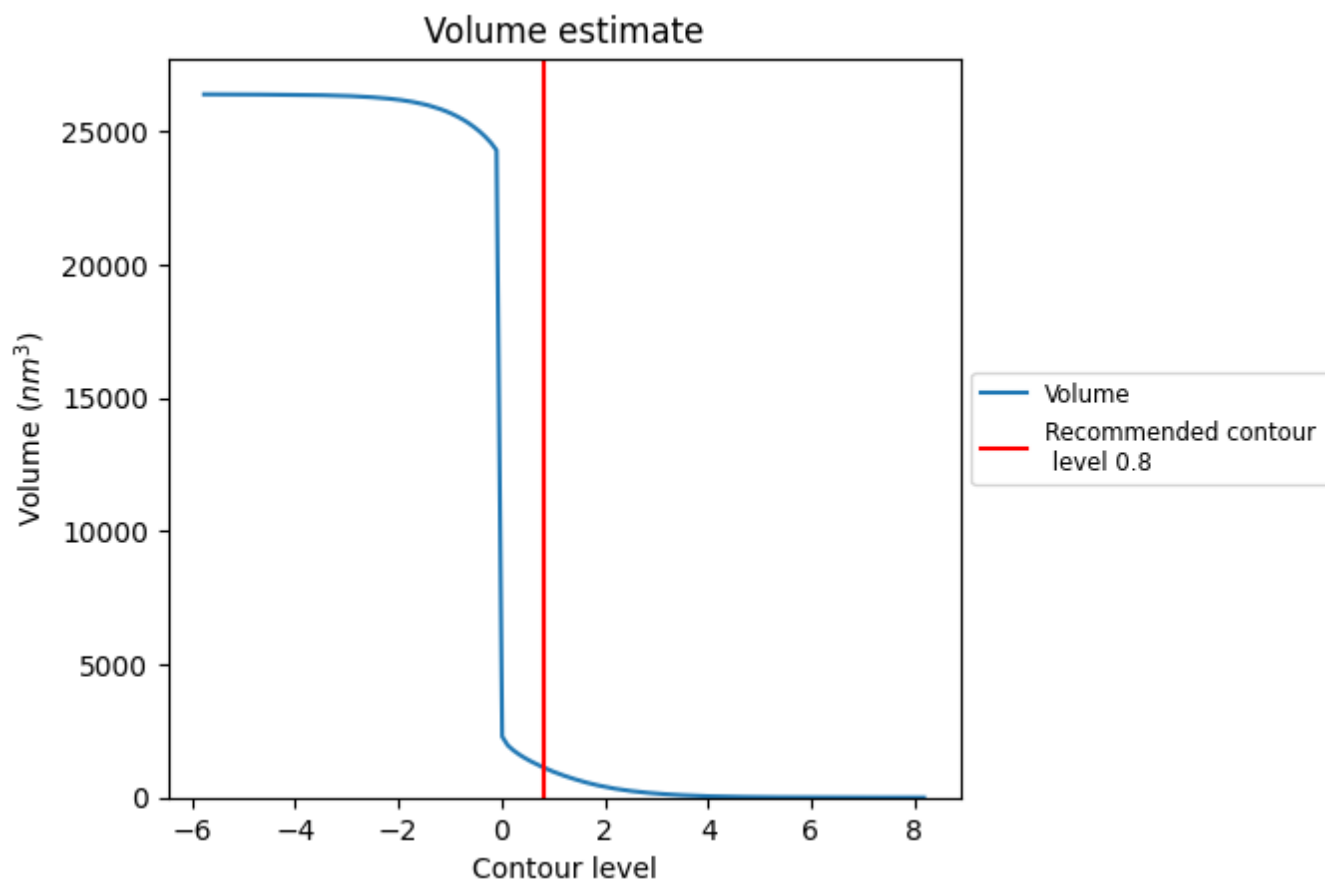
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

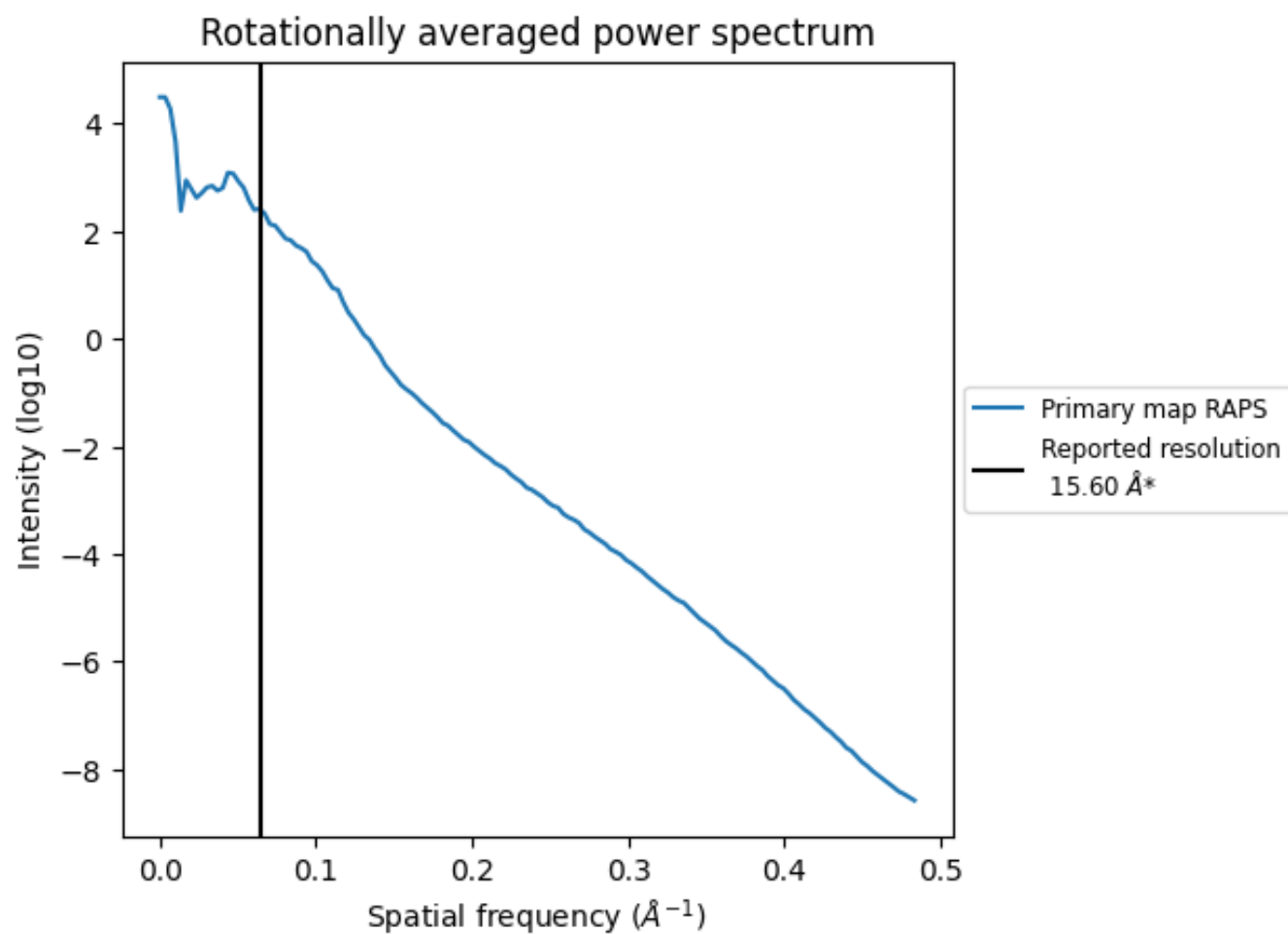
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1142  $\text{nm}^3$ ; this corresponds to an approximate mass of 1031 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

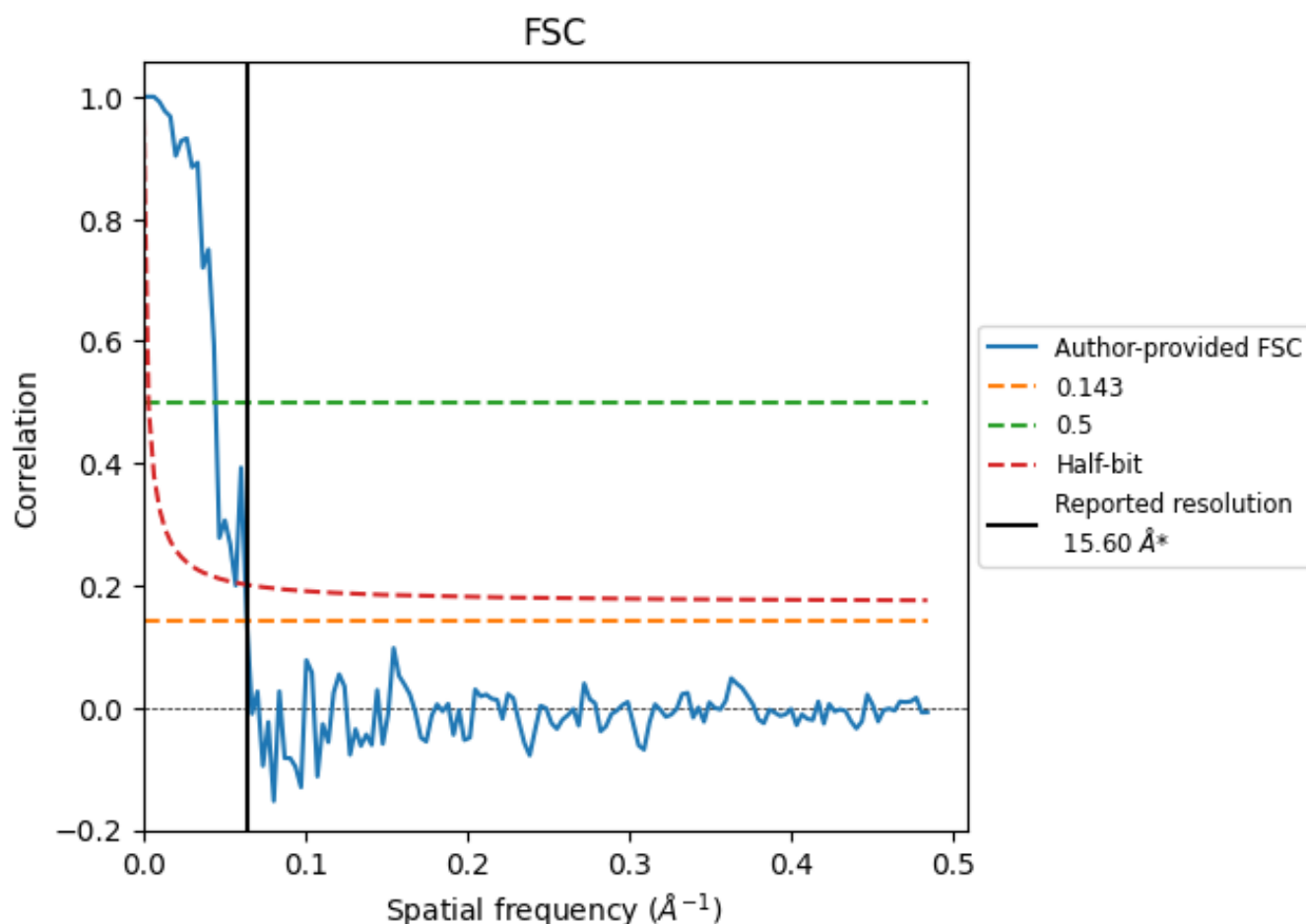


\*Reported resolution corresponds to spatial frequency of 0.064 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.064 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

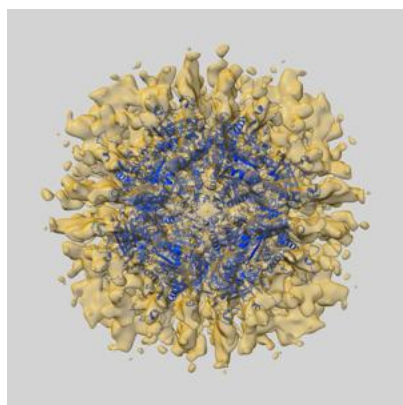
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	15.60	-	-
Author-provided FSC curve	15.65	22.42	17.57
Unmasked-calculated*	-	-	-

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

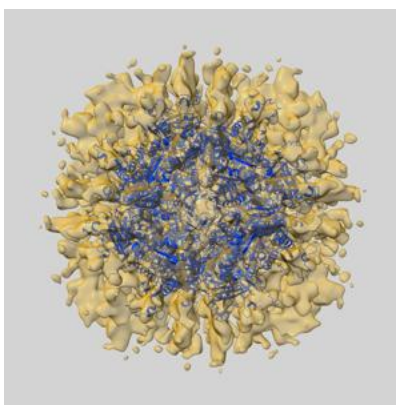
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8458 and PDB model 5TRE. Per-residue inclusion information can be found in section 3 on page 11.

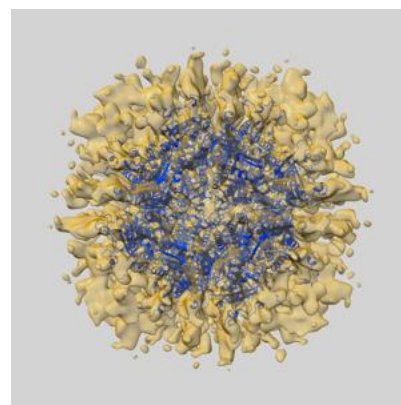
### 9.1 Map-model overlay [i](#)



X



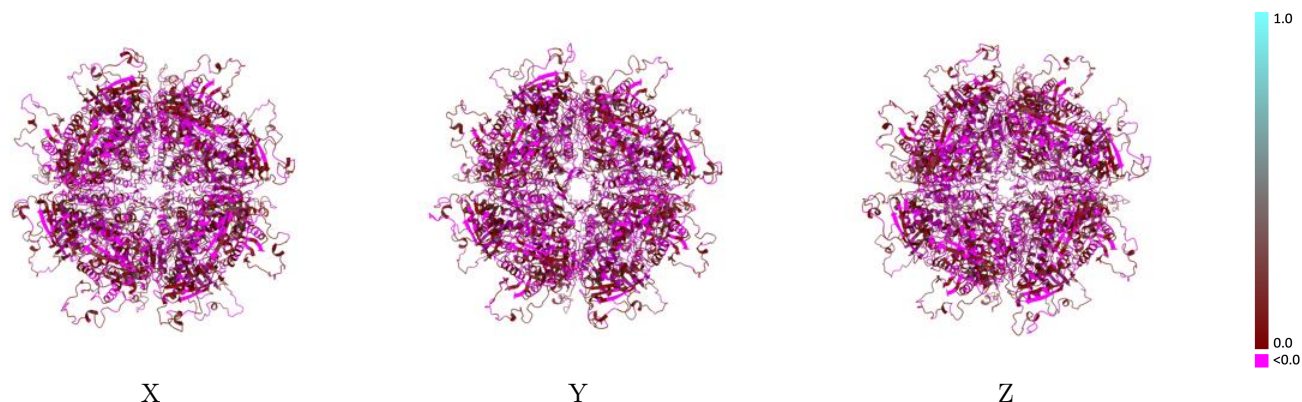
Y



Z

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

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



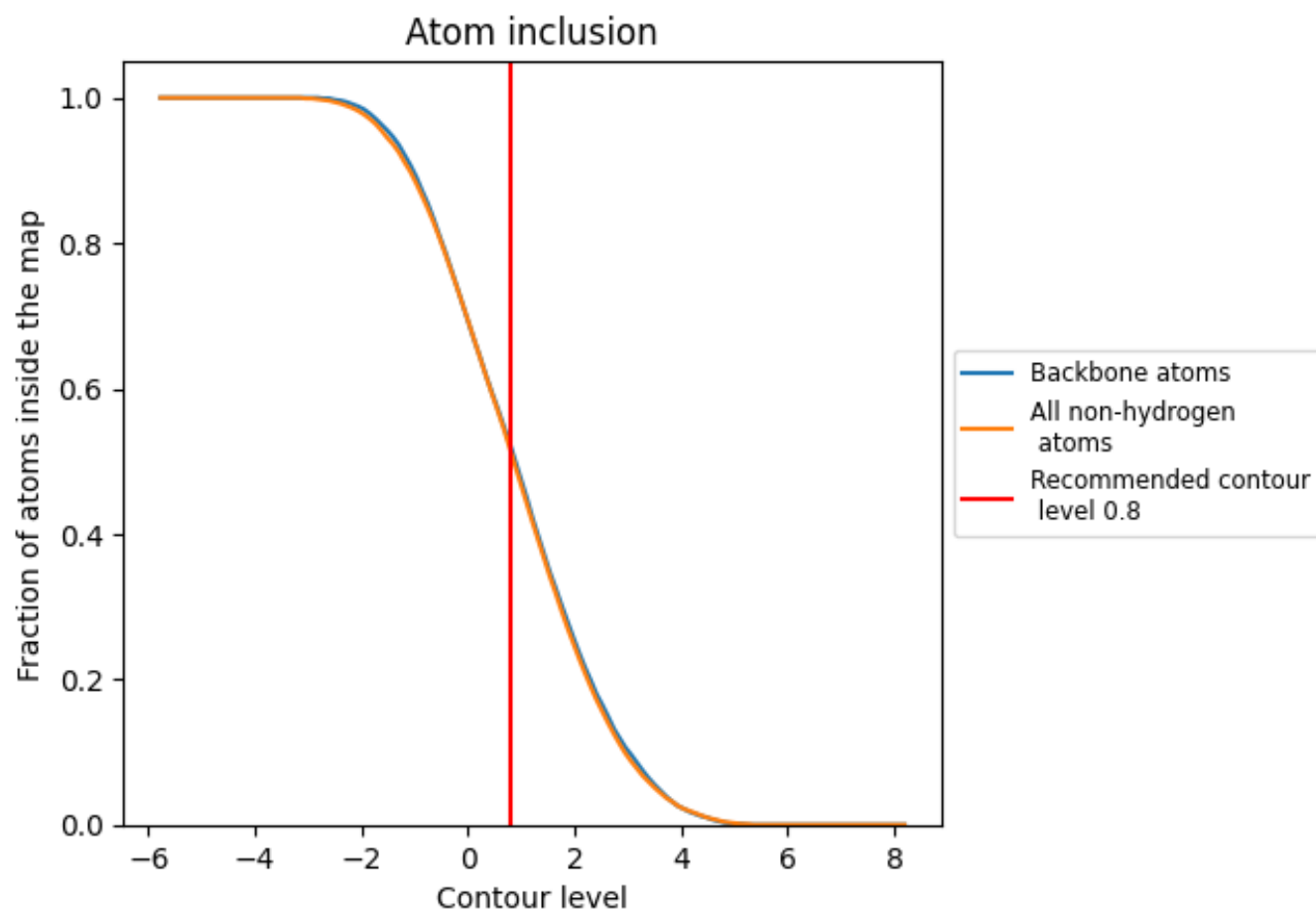
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 51% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ





























The table lists the average atom inclusion at the recommended contour level (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5140	0.0160
A	0.5280	0.0110
B	0.5120	0.0000
C	0.4990	-0.0020
D	0.5310	0.0080
E	0.5020	0.0020
F	0.4870	-0.0090
G	0.5140	0.0020
H	0.5210	-0.0070
I	0.4900	-0.0070
J	0.5140	-0.0000
K	0.4860	-0.0020
L	0.5130	-0.0050
M	0.5090	0.0160
N	0.4950	-0.0070
O	0.5180	0.0000
P	0.5000	0.0050
Q	0.4920	-0.0040
R	0.5070	-0.0020
S	0.5030	-0.0030
T	0.4820	-0.0130
U	0.5360	0.0030
V	0.5150	0.0000
W	0.4910	-0.0060
X	0.5020	-0.0010
a	0.5460	0.0320
b	0.4930	0.0280
c	0.5310	0.0340
d	0.4890	0.0220
e	0.5270	0.0260
f	0.5420	0.0250
g	0.5450	0.0320
h	0.4830	0.0230
i	0.5340	0.0310
j	0.4990	0.0290



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Chain	Atom inclusion	Q-score
k	 0.5270	 0.0340
l	 0.5310	 0.0310
m	 0.5340	 0.0310
n	 0.5460	 0.0410
o	 0.5180	 0.0370
p	 0.5290	 0.0370
q	 0.5470	 0.0310
r	 0.5000	 0.0300
s	 0.5070	 0.0220
t	 0.5410	 0.0320
u	 0.5150	 0.0320
v	 0.4770	 0.0240
w	 0.5120	 0.0330
x	 0.5400	 0.0320