



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 09:16 AM UTC

PDB ID : 5T0V / pdb_00005t0v
EMDB ID : EMD-8341
Title : Architecture of the Yeast Mitochondrial Iron-Sulfur Cluster Assembly Machinery: the Sub-Complex Formed by the Iron Donor, Yfh1, and the Scaffold, Isu1
Authors : Ranatunga, W.; Gakh, O.; Galeano, B.K.; Smith IV, D.Y.; Soderberg, C.A.; Al-Karadaghi, S.; Thompson, J.R.; Isaya, G.
Deposited on : 2016-08-16
Resolution : 17.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

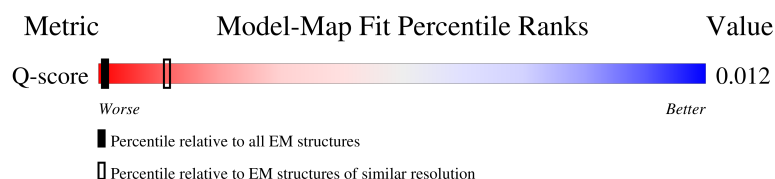
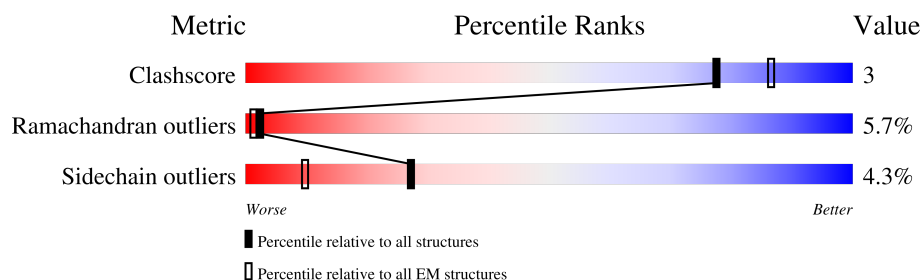
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 17.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	45 (17.00 - 18.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	38% 80% 19% .
1	b	142	38% 76% 21% .
1	c	142	36% 80% 18% .
1	d	142	37% 85% 14% .

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Mol	Chain	Length	Quality of chain
1	e	142	38% 80% 18% .
1	f	142	37% 81% 18% .
1	g	142	36% 84% 14% .
1	h	142	38% 78% 19% .
1	i	142	42% 80% 18% .
1	j	142	38% 80% 20% .
1	k	142	37% 85% 11% 5%
1	l	142	35% 77% 19% .
1	m	142	38% 84% 15% .
1	n	142	38% 73% 27% .
1	o	142	37% 77% 20% ..
1	p	142	37% 79% 18% .
1	q	142	42% 80% 20%
1	r	142	37% 73% 23% .
1	s	142	37% 81% 18% .
1	t	142	39% 78% 17% 5%
1	u	142	41% 79% 20% .
1	v	142	35% 82% 16% .
1	w	142	37% 83% 15% .
1	x	142	37% 82% 15% ..
2	A	121	37% 74% 21% 5% .
2	B	121	33% 74% 25% .
2	C	121	33% 69% 27% .
2	D	121	36% 72% 26% ..
2	E	121	31% 74% 24% ..

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Mol	Chain	Length	Quality of chain
2	F	121	36% 79% 20% .
2	G	121	35% 74% 25% ..
2	H	121	31% 69% 26% .
2	I	121	34% 83% 17% .
2	J	121	36% 72% 26% .
2	K	121	31% 74% 25% .
2	L	121	33% 75% 21% ..
2	M	121	36% 81% 17% .
2	N	121	31% 70% 23% 6% .
2	O	121	36% 77% 22% .
2	P	121	36% 78% 21% .
2	Q	121	34% 74% 22% ..
2	R	121	35% 74% 25% .
2	S	121	36% 75% 17% 7% .
2	T	121	33% 82% 16% .
2	U	121	39% 69% 26% 6%
2	V	121	34% 70% 24% 5% .
2	W	121	35% 70% 26% .
2	X	121	33% 82% 16% .

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

There are 24 discrepancies between the modelled and reference sequences:

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

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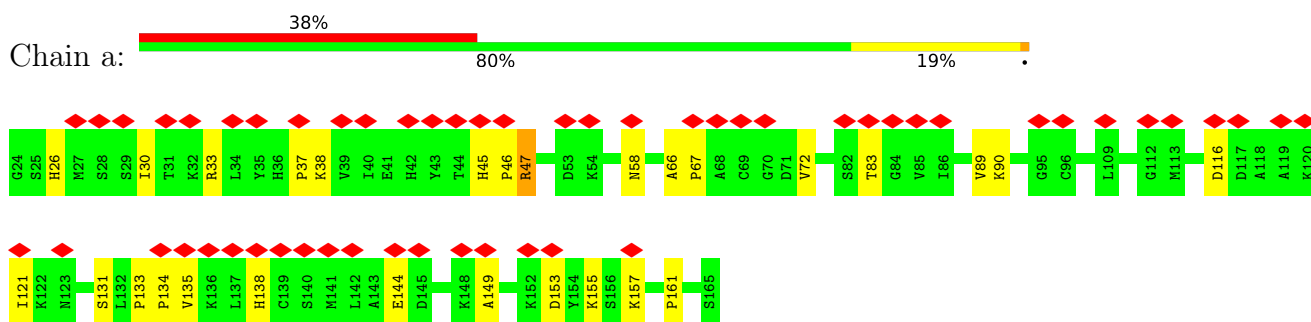
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Chain	Residue	Modelled	Actual	Comment	Reference
B	73	ALA	TYR	conflict	UNP Q07540
C	73	ALA	TYR	conflict	UNP Q07540
D	73	ALA	TYR	conflict	UNP Q07540
E	73	ALA	TYR	conflict	UNP Q07540
F	73	ALA	TYR	conflict	UNP Q07540
G	73	ALA	TYR	conflict	UNP Q07540
H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

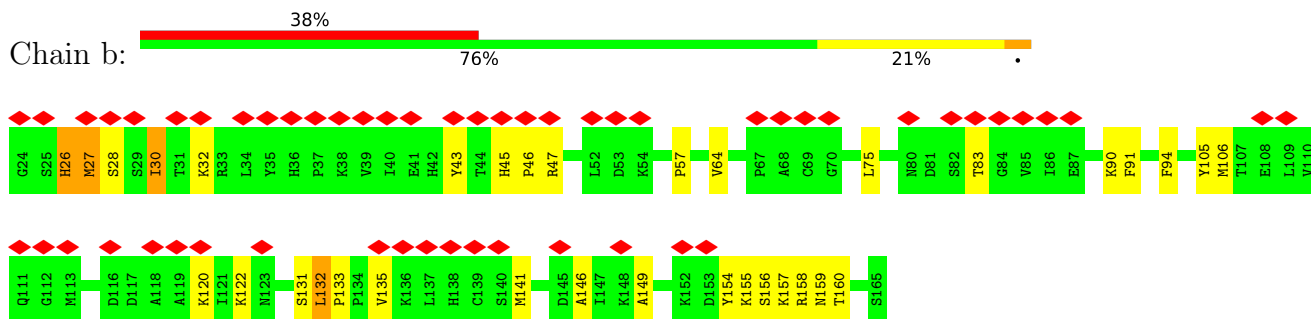
3 Residue-property plots [i](#)

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.

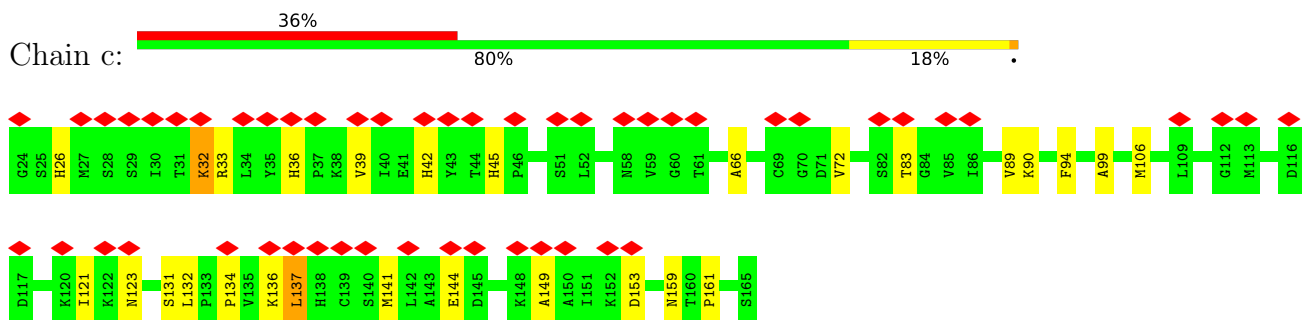
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



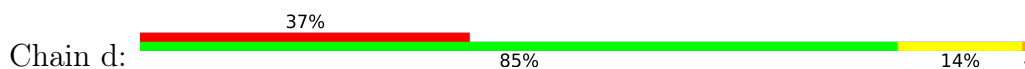
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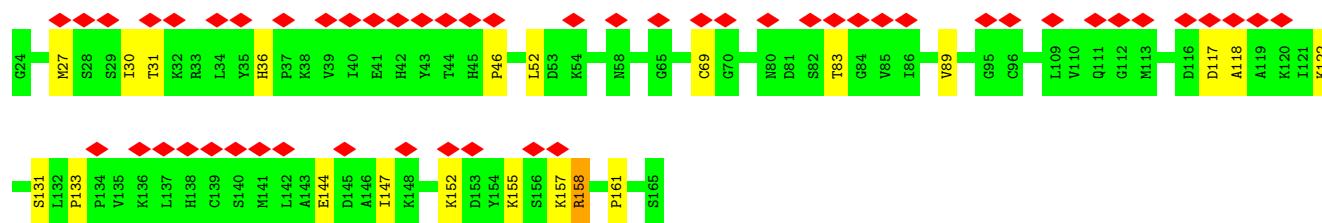


- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

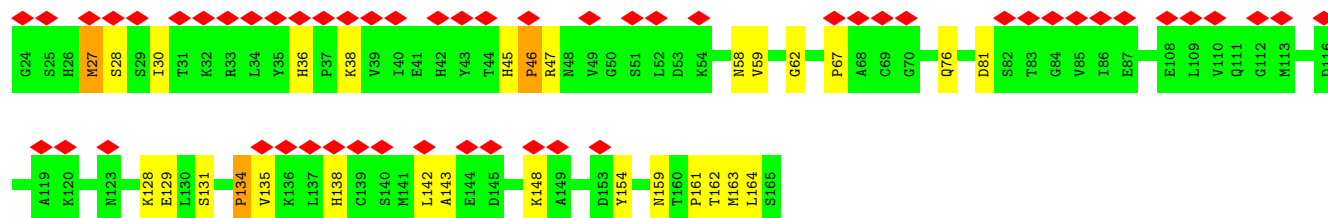
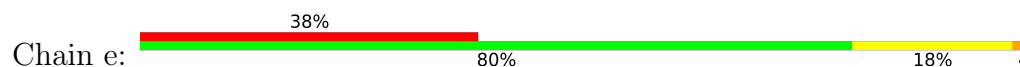


- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

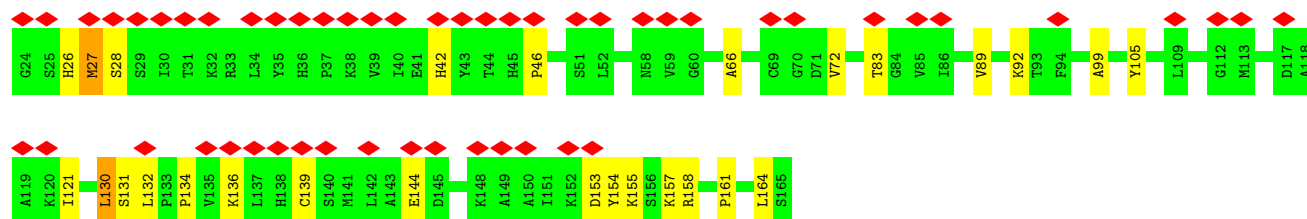
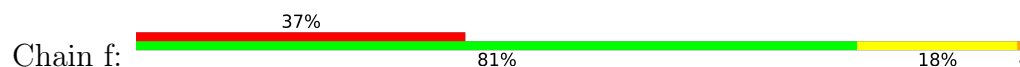




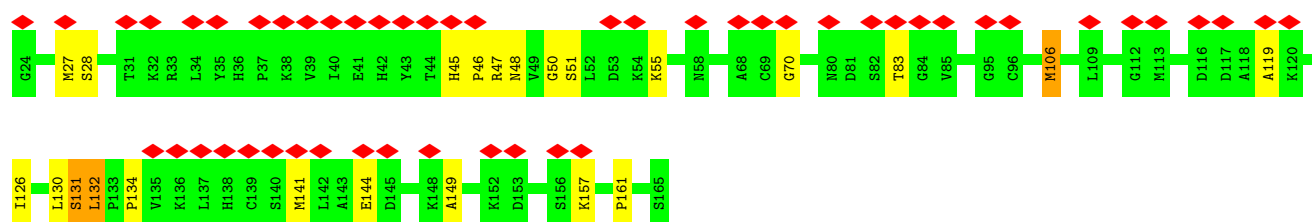
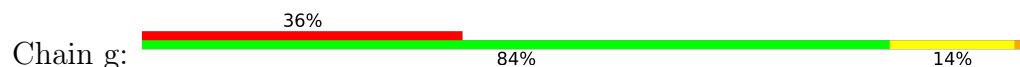
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



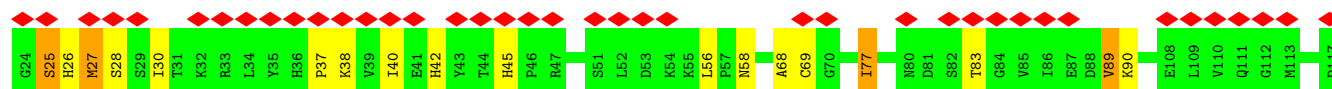
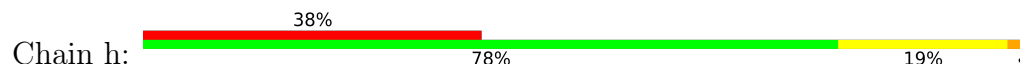
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

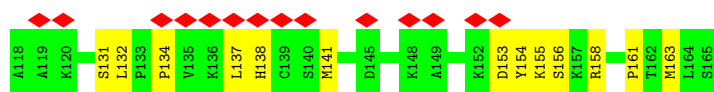


- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

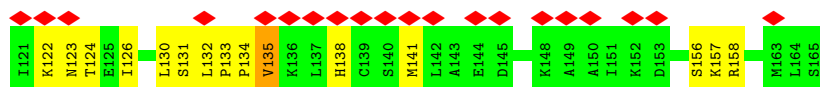
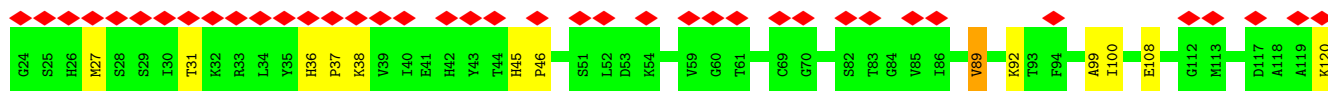
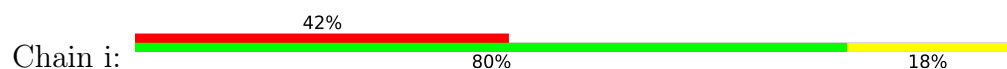


- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

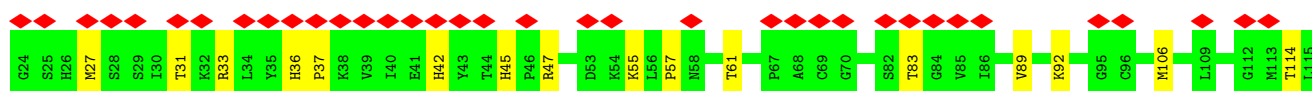
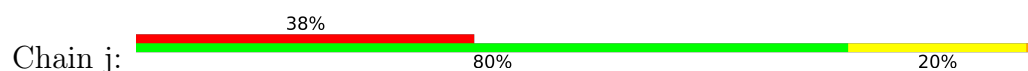




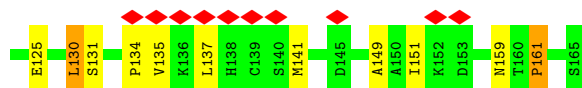
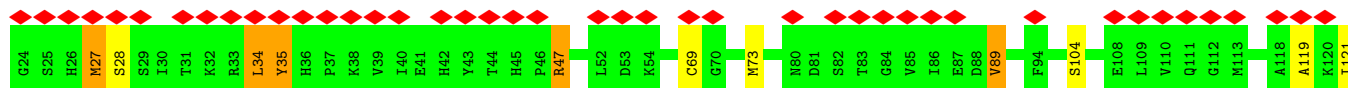
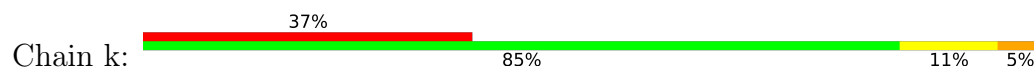
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



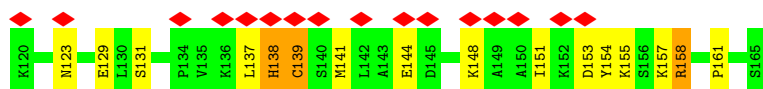
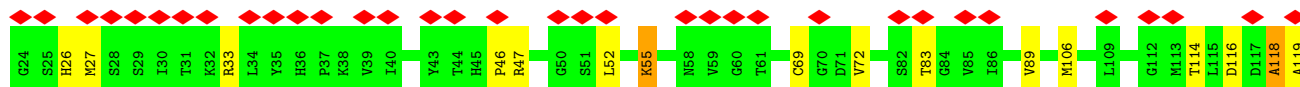
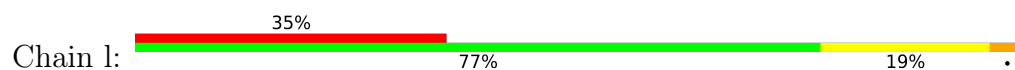
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



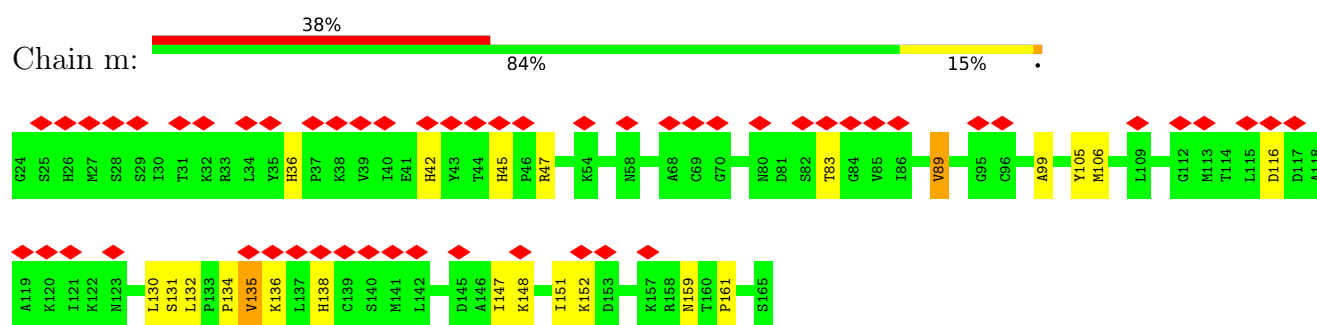
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



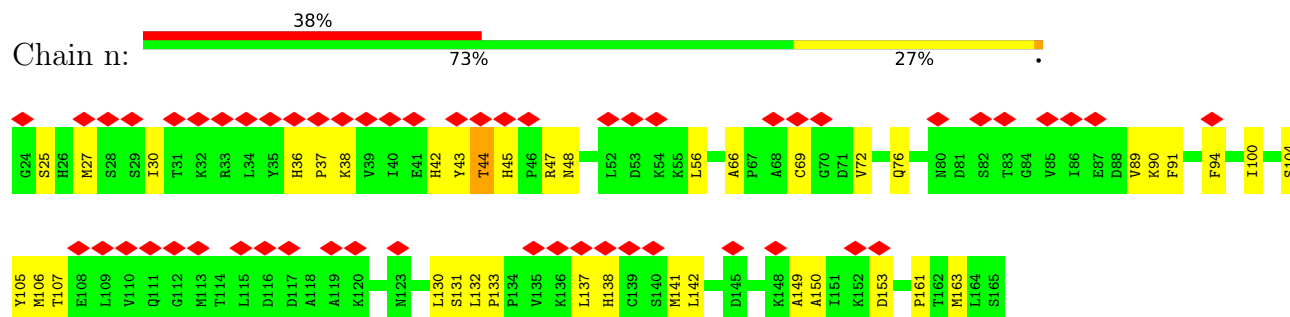
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



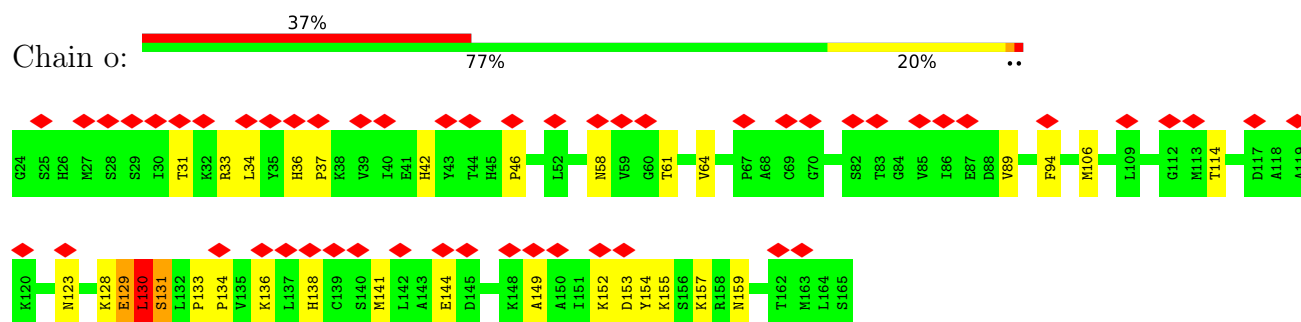
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



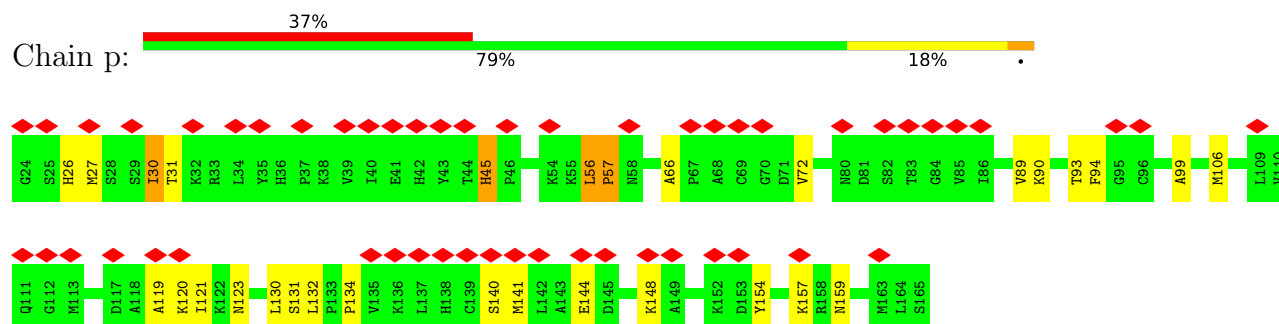
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



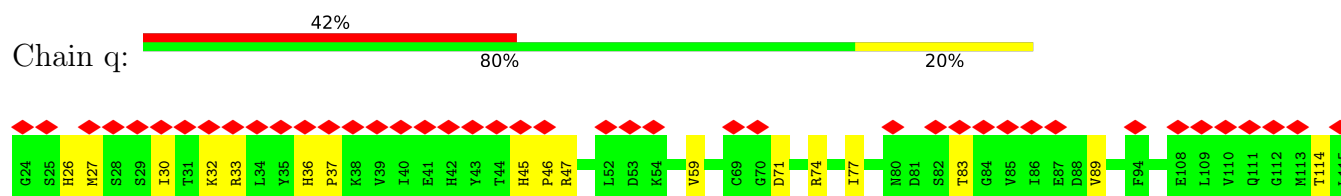
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

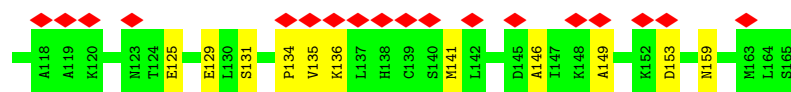


- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

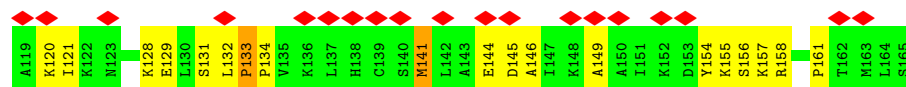
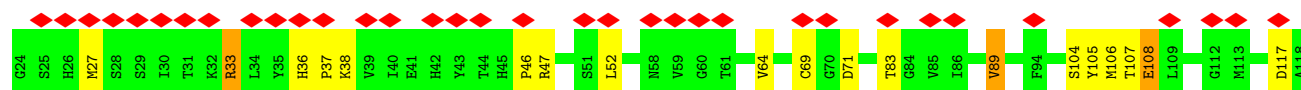


- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

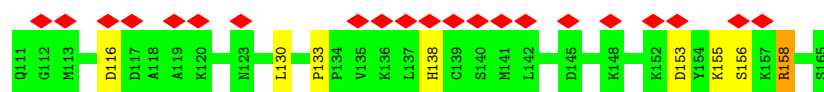
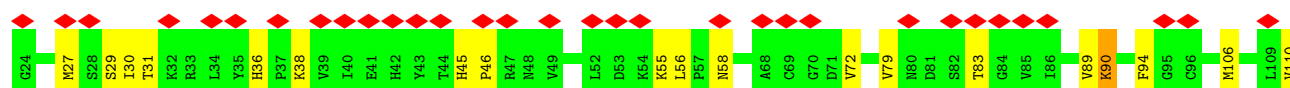
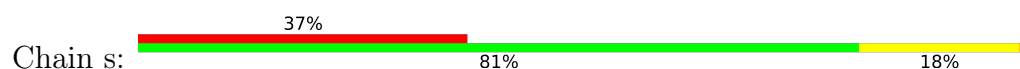




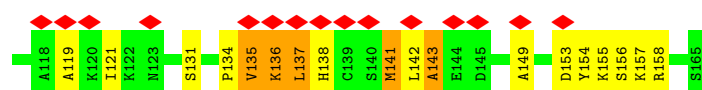
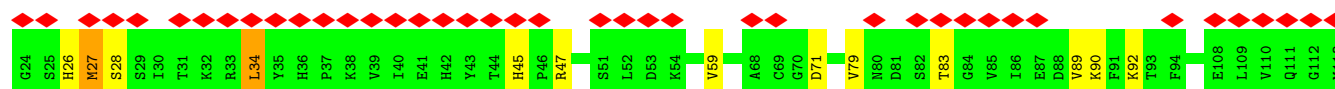
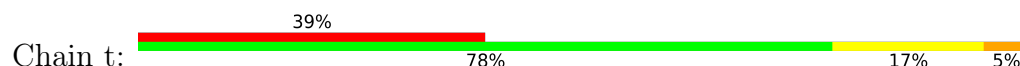
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



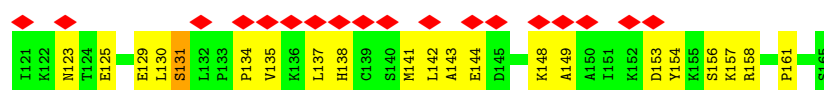
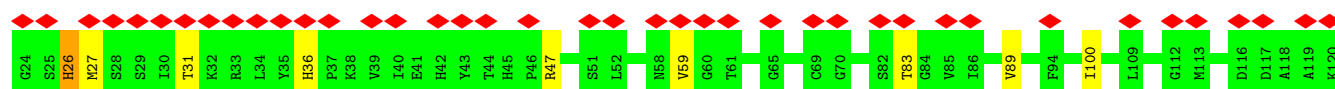
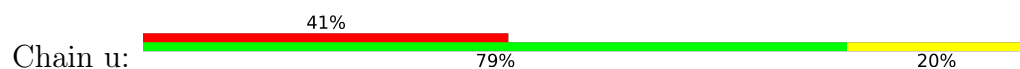
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



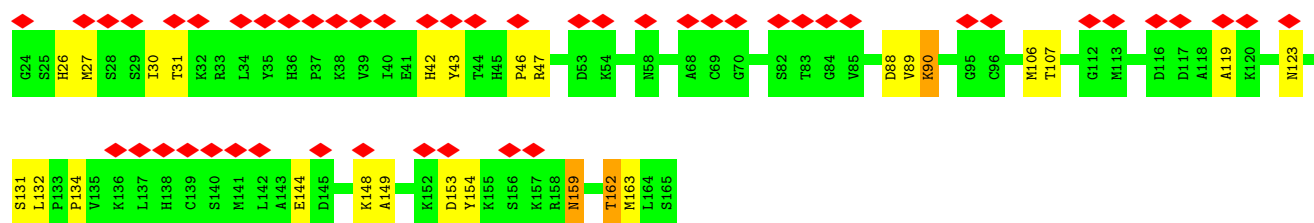
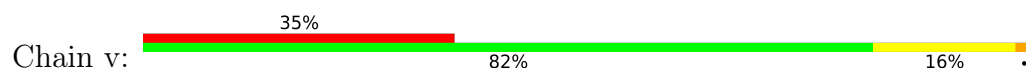
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



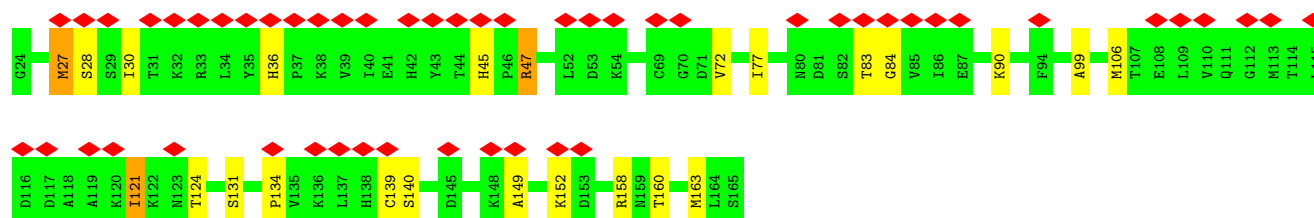
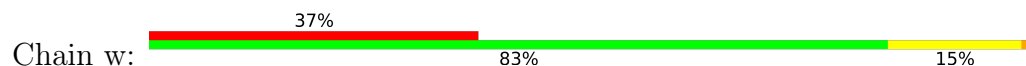
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



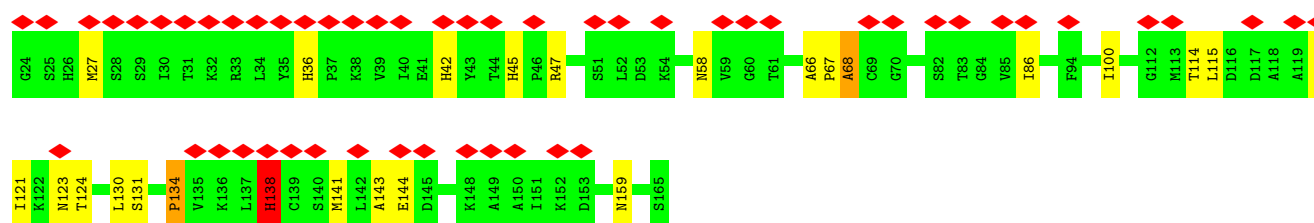
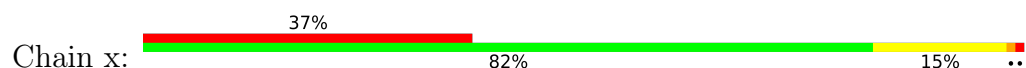
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



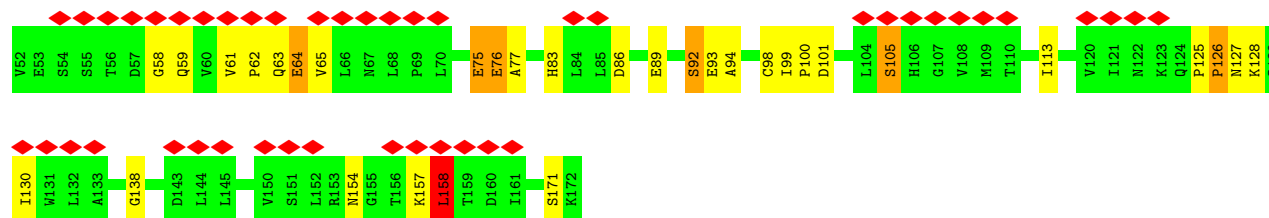
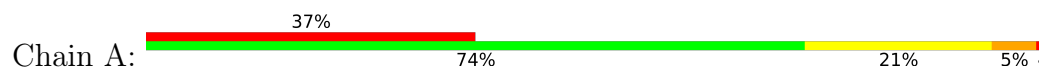
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



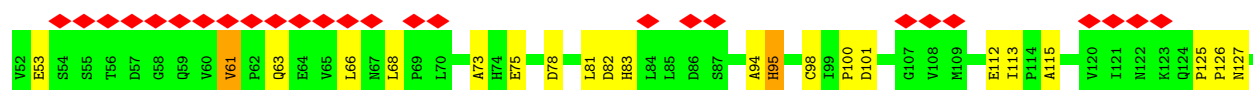
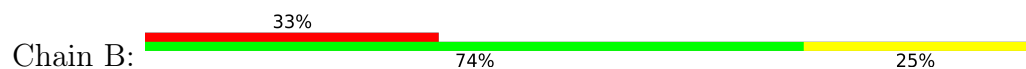
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial



- Molecule 2: Frataxin homolog, mitochondrial

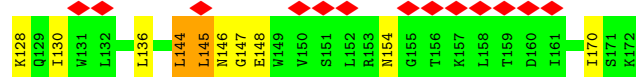
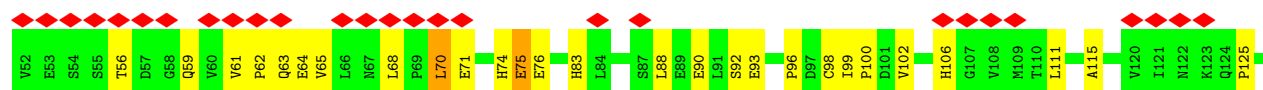


- Molecule 2: Frataxin homolog, mitochondrial

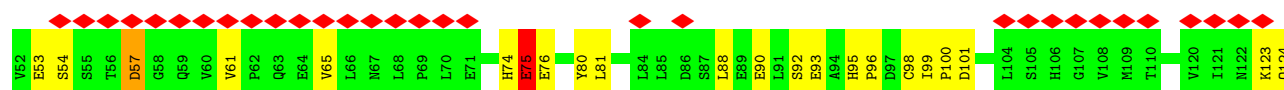
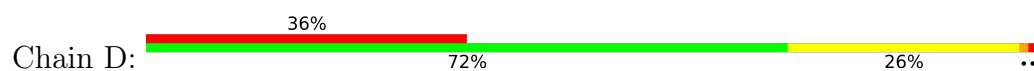




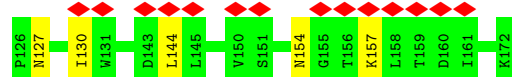
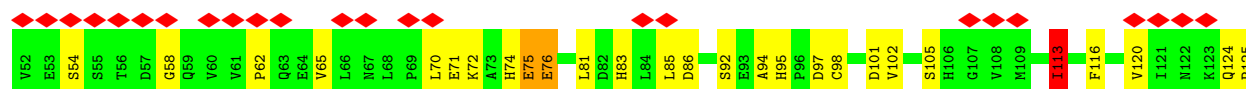
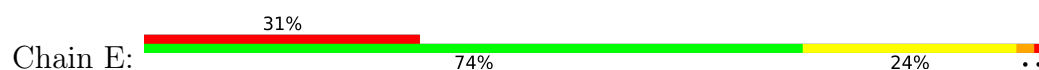
- Molecule 2: Frataxin homolog, mitochondrial



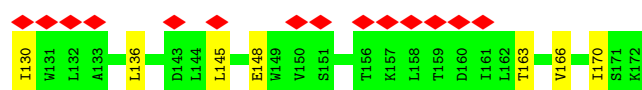
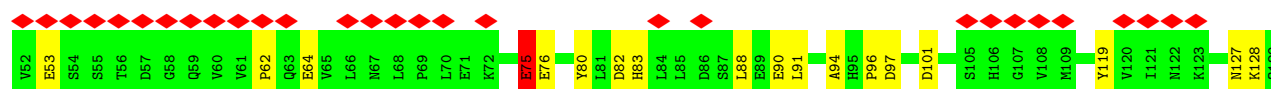
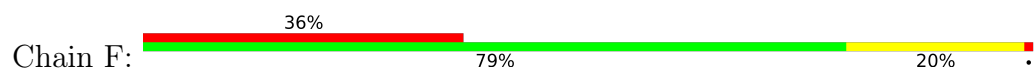
- Molecule 2: Frataxin homolog, mitochondrial



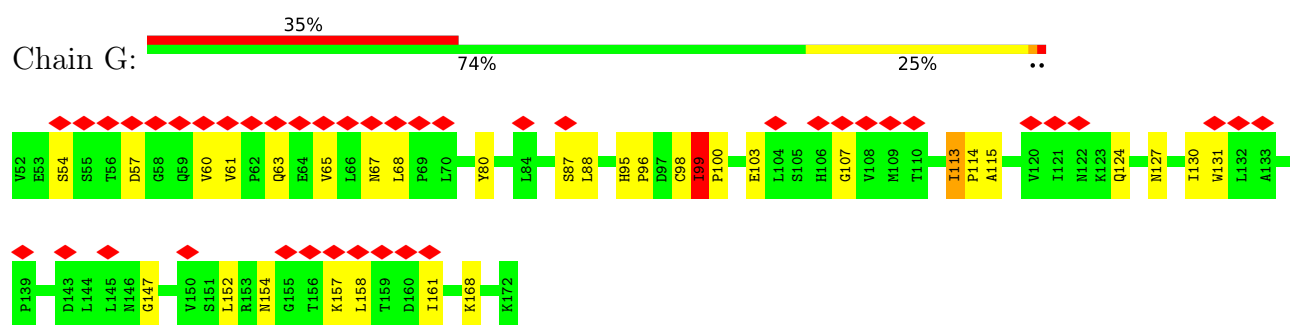
- Molecule 2: Frataxin homolog, mitochondrial



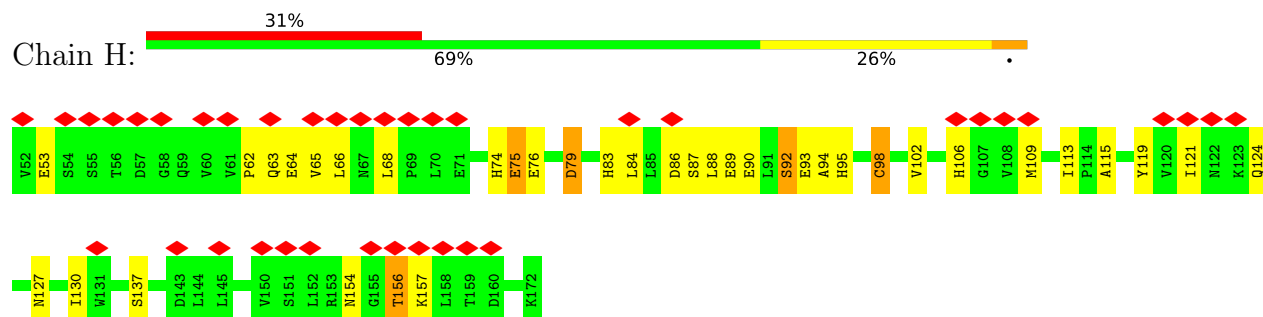
- Molecule 2: Frataxin homolog, mitochondrial



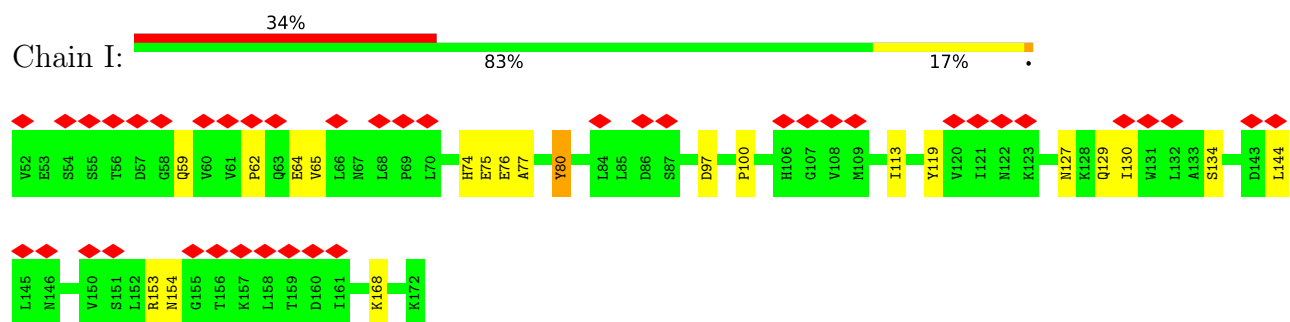
- Molecule 2: Frataxin homolog, mitochondrial



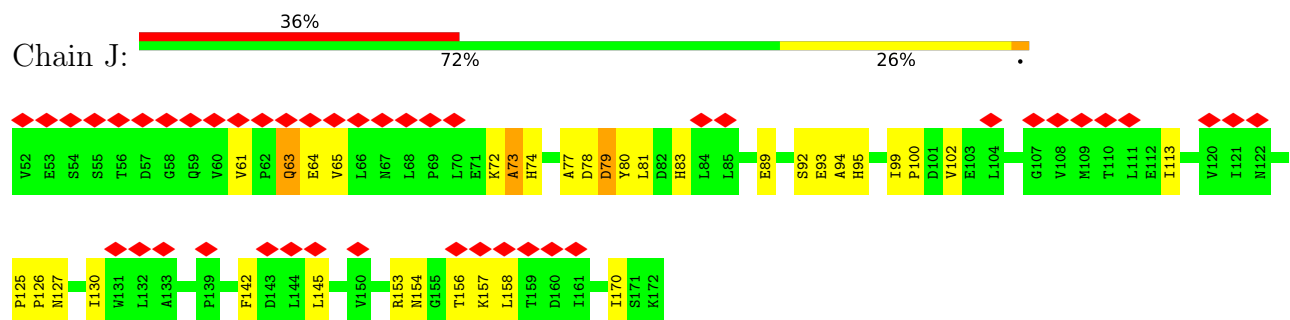
- Molecule 2: Frataxin homolog, mitochondrial



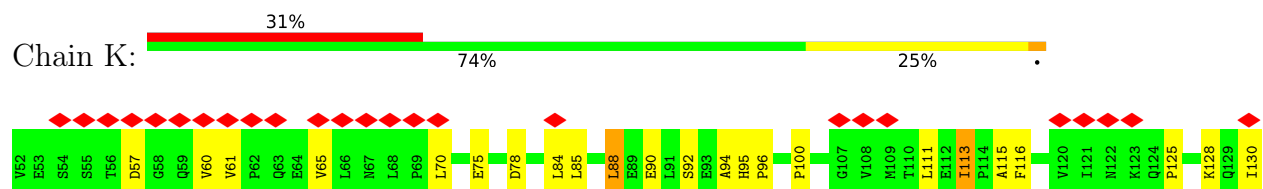
- Molecule 2: Frataxin homolog, mitochondrial

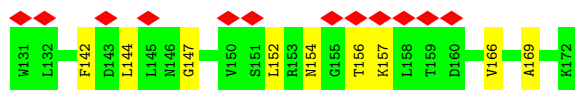


- Molecule 2: Frataxin homolog, mitochondrial

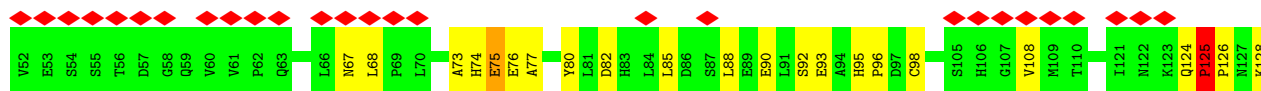
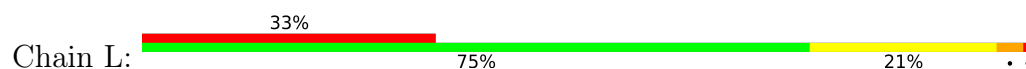


- Molecule 2: Frataxin homolog, mitochondrial

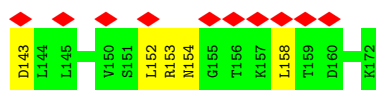
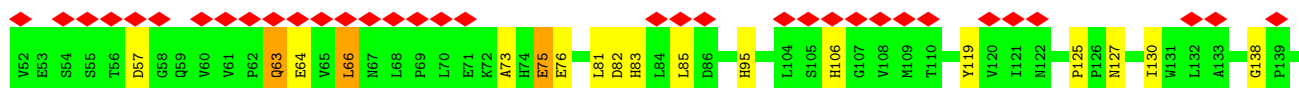
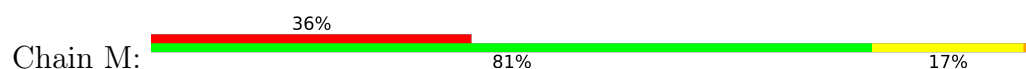




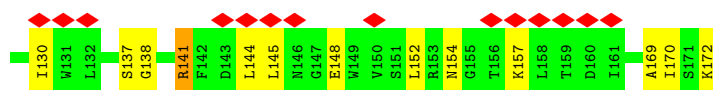
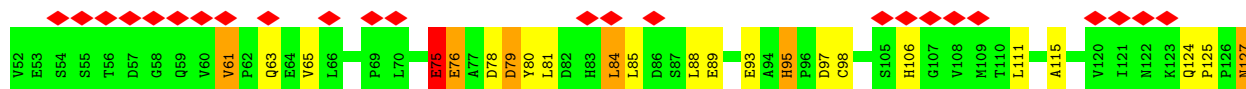
- Molecule 2: Frataxin homolog, mitochondrial



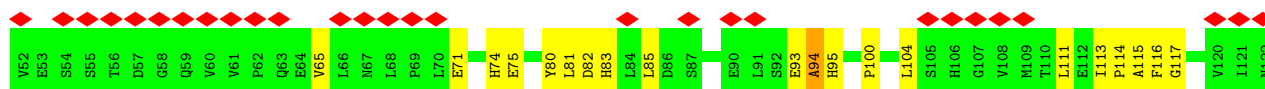
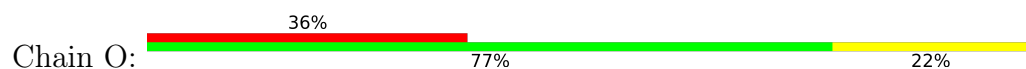
- Molecule 2: Frataxin homolog, mitochondrial



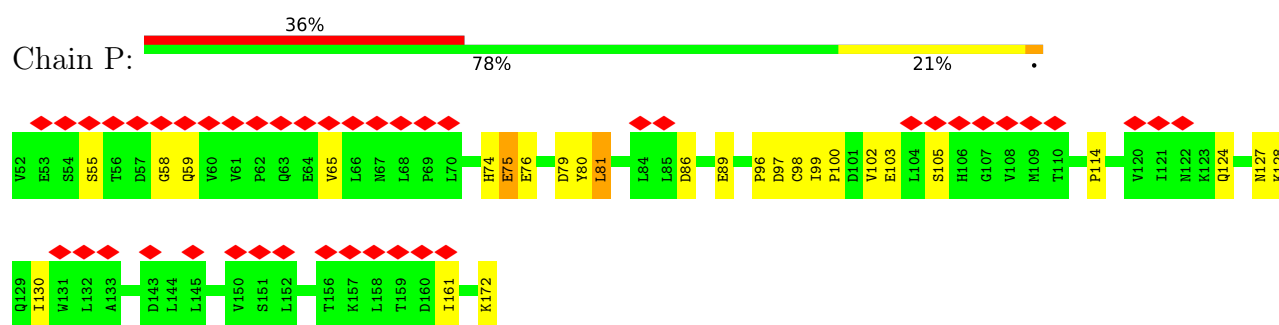
- Molecule 2: Frataxin homolog, mitochondrial



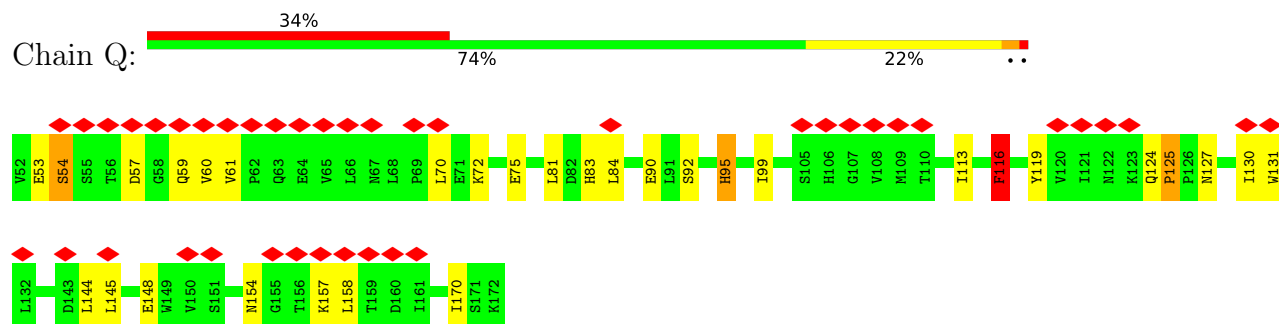
- Molecule 2: Frataxin homolog, mitochondrial



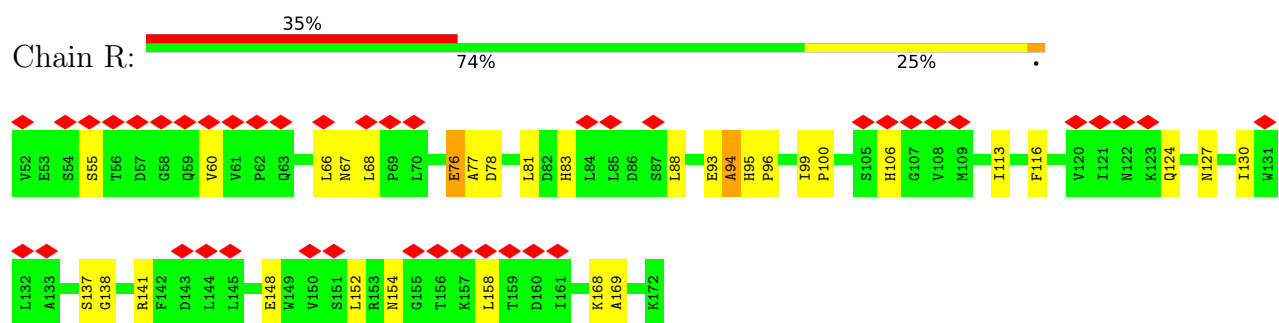
- Molecule 2: Frataxin homolog, mitochondrial



- Molecule 2: Frataxin homolog, mitochondrial



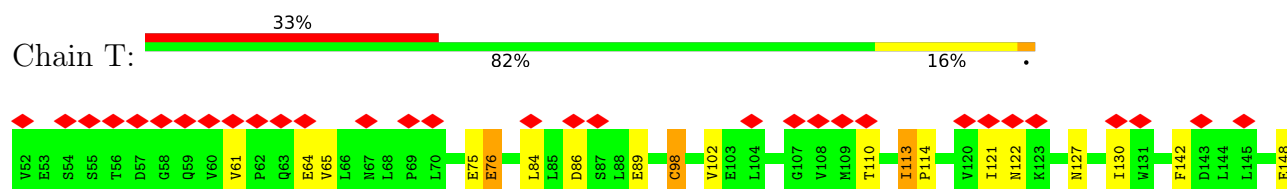
- Molecule 2: Frataxin homolog, mitochondrial

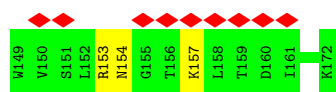


- Molecule 2: Frataxin homolog, mitochondrial

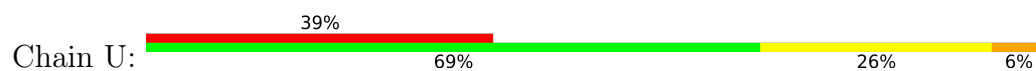


- Molecule 2: Frataxin homolog, mitochondrial

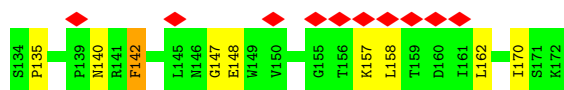
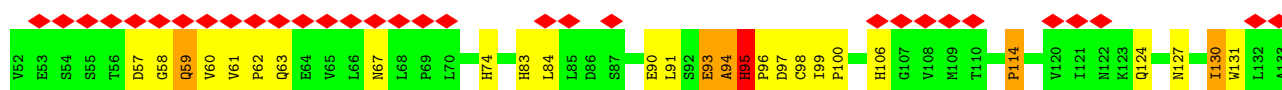




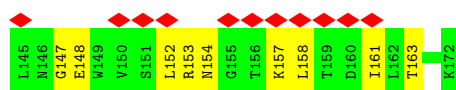
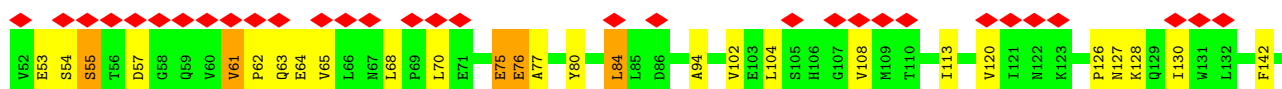
- Molecule 2: Frataxin homolog, mitochondrial



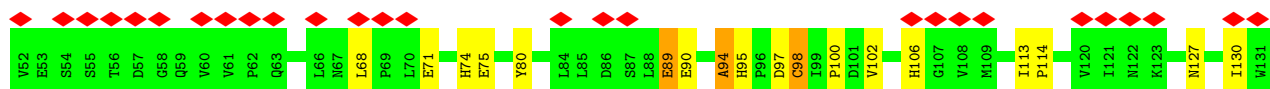
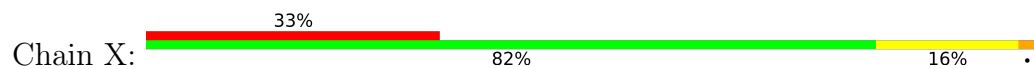
- Molecule 2: Frataxin homolog, mitochondrial



- 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	4153	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; The ctf.auto function from EMAN2 was applied.	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	12.440	Depositor
Minimum map value	-8.726	Depositor
Average map value	0.043	Depositor
Map value standard deviation	0.800	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	297.79202, 297.79202, 297.79202	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.034, 1.034, 1.034	Depositor

5 Model quality ⓘ

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	1.44	1/1089 (0.1%)	1.81	25/1466 (1.7%)
1	b	1.47	0/1089	1.88	33/1466 (2.3%)
1	c	1.40	1/1089 (0.1%)	1.86	18/1466 (1.2%)
1	d	1.42	0/1089	1.77	25/1466 (1.7%)
1	e	1.46	2/1089 (0.2%)	1.91	29/1466 (2.0%)
1	f	1.47	0/1089	1.80	26/1466 (1.8%)
1	g	1.43	1/1089 (0.1%)	1.79	17/1466 (1.2%)
1	h	1.41	2/1089 (0.2%)	1.80	28/1466 (1.9%)
1	i	1.41	1/1089 (0.1%)	1.77	25/1466 (1.7%)
1	j	1.40	3/1089 (0.3%)	1.88	27/1466 (1.8%)
1	k	1.43	1/1089 (0.1%)	1.84	19/1466 (1.3%)
1	l	1.43	2/1089 (0.2%)	1.87	28/1466 (1.9%)
1	m	1.39	0/1089	1.74	21/1466 (1.4%)
1	n	1.39	1/1089 (0.1%)	1.79	22/1466 (1.5%)
1	o	1.37	1/1089 (0.1%)	1.75	25/1466 (1.7%)
1	p	1.45	2/1089 (0.2%)	1.83	23/1466 (1.6%)
1	q	1.44	3/1089 (0.3%)	1.82	19/1466 (1.3%)
1	r	1.40	2/1089 (0.2%)	1.85	32/1466 (2.2%)
1	s	1.45	3/1089 (0.3%)	1.81	23/1466 (1.6%)
1	t	1.45	2/1089 (0.2%)	1.81	24/1466 (1.6%)
1	u	1.46	0/1089	1.78	28/1466 (1.9%)
1	v	1.39	1/1089 (0.1%)	1.80	24/1466 (1.6%)
1	w	1.46	1/1089 (0.1%)	1.73	16/1466 (1.1%)
1	x	1.47	0/1089	1.84	30/1466 (2.0%)
2	A	1.37	1/967 (0.1%)	1.77	19/1319 (1.4%)
2	B	1.39	1/967 (0.1%)	1.81	25/1319 (1.9%)
2	C	1.37	2/967 (0.2%)	1.77	21/1319 (1.6%)
2	D	1.41	2/967 (0.2%)	1.78	21/1319 (1.6%)
2	E	1.40	3/967 (0.3%)	1.79	23/1319 (1.7%)
2	F	1.41	1/967 (0.1%)	1.76	14/1319 (1.1%)
2	G	1.38	0/967	1.77	17/1319 (1.3%)
2	H	1.36	1/967 (0.1%)	1.76	25/1319 (1.9%)
2	I	1.36	0/967	1.69	11/1319 (0.8%)
2	J	1.39	1/967 (0.1%)	1.77	21/1319 (1.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	K	1.36	1/967 (0.1%)	1.74	12/1319 (0.9%)
2	L	1.40	0/967	1.75	23/1319 (1.7%)
2	M	1.36	0/967	1.73	17/1319 (1.3%)
2	N	1.36	0/967	1.84	24/1319 (1.8%)
2	O	1.37	0/967	1.70	16/1319 (1.2%)
2	P	1.41	1/967 (0.1%)	1.84	25/1319 (1.9%)
2	Q	1.36	0/967	1.80	28/1319 (2.1%)
2	R	1.37	0/967	1.75	32/1319 (2.4%)
2	S	1.40	2/967 (0.2%)	1.83	21/1319 (1.6%)
2	T	1.43	0/967	1.71	11/1319 (0.8%)
2	U	1.37	0/967	1.83	24/1319 (1.8%)
2	V	1.42	1/967 (0.1%)	1.86	30/1319 (2.3%)
2	W	1.45	1/967 (0.1%)	1.79	21/1319 (1.6%)
2	X	1.36	1/967 (0.1%)	1.74	17/1319 (1.3%)
All	All	1.41	49/49344 (0.1%)	1.80	1085/66840 (1.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	1
1	n	0	1
1	r	0	2
1	t	0	1
2	I	0	1
2	M	0	1
All	All	0	7

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	p	154	TYR	CA-C	-7.88	1.44	1.52
2	D	92	SER	CA-C	-7.73	1.49	1.53
1	r	108	GLU	CA-C	-7.06	1.46	1.52
1	n	66	ALA	CA-C	-6.73	1.47	1.52
2	E	74	HIS	CA-CB	6.41	1.58	1.53
2	V	60	VAL	C-N	6.37	1.38	1.33
2	S	60	VAL	CA-C	-6.21	1.47	1.52
1	o	138	HIS	ND1-CE1	6.06	1.38	1.32
1	j	47	ARG	NE-CZ	5.88	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	74	HIS	CA-C	-5.83	1.47	1.53
1	e	47	ARG	NE-CZ	5.70	1.39	1.33
2	P	55	SER	CA-C	-5.66	1.45	1.53
1	r	155	LYS	N-CA	-5.64	1.41	1.46
1	a	138	HIS	ND1-CE1	5.63	1.38	1.32
1	j	42	HIS	ND1-CE1	5.58	1.38	1.32
2	W	57	ASP	C-N	5.56	1.38	1.33
1	q	45	HIS	ND1-CE1	5.54	1.38	1.32
1	p	93	THR	N-CA	-5.52	1.39	1.46
2	E	83	HIS	ND1-CE1	5.49	1.38	1.32
1	k	125	GLU	CA-C	-5.41	1.45	1.52
2	J	153	ARG	NE-CZ	5.37	1.39	1.33
1	q	74	ARG	CD-NE	5.34	1.53	1.46
1	s	29	SER	C-N	5.33	1.39	1.33
2	C	74	HIS	ND1-CE1	5.33	1.37	1.32
2	C	106	HIS	ND1-CE1	5.31	1.37	1.32
1	g	45	HIS	ND1-CE1	5.30	1.37	1.32
2	X	74	HIS	ND1-CE1	5.29	1.37	1.32
1	e	45	HIS	C-O	-5.28	1.20	1.25
1	j	92	LYS	CA-C	-5.26	1.46	1.52
1	l	26	HIS	ND1-CE1	5.23	1.37	1.32
1	c	66	ALA	CA-C	-5.21	1.47	1.52
1	t	92	LYS	CA-C	-5.19	1.46	1.52
2	S	148	GLU	CA-C	-5.18	1.46	1.52
1	s	158	ARG	CD-NE	5.16	1.53	1.46
1	i	45	HIS	ND1-CE1	5.14	1.37	1.32
1	q	26	HIS	ND1-CE1	5.12	1.37	1.32
2	B	112	GLU	C-N	5.12	1.38	1.33
1	l	158	ARG	CD-NE	5.12	1.53	1.46
1	s	138	HIS	ND1-CE1	5.11	1.37	1.32
1	w	36	HIS	ND1-CE1	5.09	1.37	1.32
1	h	42	HIS	ND1-CE1	5.08	1.37	1.32
2	F	83	HIS	ND1-CE1	5.06	1.37	1.32
2	A	83	HIS	ND1-CE1	5.05	1.37	1.32
2	H	74	HIS	ND1-CE1	5.05	1.37	1.32
1	t	138	HIS	ND1-CE1	5.03	1.37	1.32
2	D	74	HIS	ND1-CE1	5.01	1.37	1.32
1	v	26	HIS	ND1-CE1	5.01	1.37	1.32
2	K	95	HIS	ND1-CE1	5.01	1.37	1.32
1	h	56	LEU	N-CA	-5.01	1.41	1.46

All (1085) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	131	SER	CA-C-N	11.48	142.36	121.70
1	c	131	SER	C-N-CA	11.48	142.36	121.70
2	N	78	ASP	N-CA-C	11.23	123.27	111.14
1	h	131	SER	CA-C-N	11.05	141.60	121.70
1	h	131	SER	C-N-CA	11.05	141.60	121.70
2	X	113	ILE	N-CA-C	-11.01	100.16	109.19
1	e	131	SER	CA-C-N	10.70	140.97	121.70
1	e	131	SER	C-N-CA	10.70	140.97	121.70
1	t	158	ARG	N-CA-C	-10.66	101.31	114.75
1	l	131	SER	CA-C-N	10.55	140.69	121.70
1	l	131	SER	C-N-CA	10.55	140.69	121.70
1	q	46	PRO	CA-C-N	9.48	138.76	121.70
1	q	46	PRO	C-N-CA	9.48	138.76	121.70
1	h	156	SER	N-CA-C	-9.45	103.85	114.62
2	D	65	VAL	N-CA-C	-9.33	103.60	112.83
2	Q	57	ASP	N-CA-C	-9.21	104.12	114.62
1	x	67	PRO	CA-C-N	9.20	138.25	121.70
1	x	67	PRO	C-N-CA	9.20	138.25	121.70
2	J	78	ASP	CA-C-N	9.18	138.22	121.70
2	J	78	ASP	C-N-CA	9.18	138.22	121.70
2	D	92	SER	N-CA-C	-9.14	101.29	108.78
1	l	83	THR	N-CA-C	-9.11	104.23	114.62
2	J	78	ASP	N-CA-C	9.01	120.71	111.07
1	t	156	SER	N-CA-C	-9.01	104.35	114.62
1	q	83	THR	N-CA-C	-8.92	104.45	114.62
1	v	119	ALA	CA-C-N	8.58	132.11	120.44
1	v	119	ALA	C-N-CA	8.58	132.11	120.44
1	t	131	SER	CA-C-N	8.53	137.06	121.70
1	t	131	SER	C-N-CA	8.53	137.06	121.70
2	C	88	LEU	N-CA-C	-8.48	104.06	114.75
2	B	125	PRO	CA-C-O	-8.47	114.80	120.90
2	N	75	GLU	N-CA-C	8.45	120.26	111.14
1	g	131	SER	CA-C-N	8.40	136.82	121.70
1	g	131	SER	C-N-CA	8.40	136.82	121.70
1	k	27	MET	CA-C-N	8.35	136.72	121.70
1	k	27	MET	C-N-CA	8.35	136.72	121.70
1	x	68	ALA	N-CA-CB	8.30	122.86	110.40
2	I	75	GLU	CA-C-N	8.29	136.63	121.70
2	I	75	GLU	C-N-CA	8.29	136.63	121.70
2	C	125	PRO	CA-C-O	-8.29	114.93	120.90
2	B	81	LEU	N-CA-C	-8.28	101.90	114.16
1	o	131	SER	CA-C-N	8.25	136.55	121.70
1	o	131	SER	C-N-CA	8.25	136.55	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	170	ILE	N-CA-C	-8.21	104.75	112.96
2	F	64	GLU	N-CA-C	-8.19	105.29	114.62
2	V	60	VAL	N-CA-C	-8.14	104.67	111.91
1	t	83	THR	N-CA-C	-8.12	104.52	114.75
1	j	131	SER	CA-C-N	8.08	136.24	121.70
1	j	131	SER	C-N-CA	8.08	136.24	121.70
2	B	152	LEU	N-CA-C	-8.07	101.61	112.26
2	W	102	VAL	N-CA-C	-8.07	97.21	108.27
2	U	75	GLU	CA-C-N	8.03	136.16	121.70
2	U	75	GLU	C-N-CA	8.03	136.16	121.70
2	S	146	ASN	CA-C-N	8.00	136.10	121.70
2	S	146	ASN	C-N-CA	8.00	136.10	121.70
2	R	83	HIS	CA-C-N	7.97	130.96	120.28
2	R	83	HIS	C-N-CA	7.97	130.96	120.28
2	H	75	GLU	CA-C-N	7.96	136.03	121.70
2	H	75	GLU	C-N-CA	7.96	136.03	121.70
2	U	154	ASN	CA-CB-CG	7.94	120.54	112.60
2	J	125	PRO	CA-C-O	-7.90	115.21	120.90
2	T	86	ASP	N-CA-C	7.88	119.50	111.07
2	Q	145	LEU	N-CA-C	-7.87	105.65	114.62
1	v	154	TYR	N-CA-C	-7.83	103.33	113.12
1	b	156	SER	N-CA-C	-7.82	104.90	114.75
2	V	93	GLU	CA-C-N	7.80	136.44	121.54
2	V	93	GLU	C-N-CA	7.80	136.44	121.54
2	Q	119	TYR	N-CA-C	-7.76	96.60	109.24
1	s	155	LYS	N-CA-C	-7.74	100.73	113.50
2	T	113	ILE	CA-C-N	7.74	128.45	119.47
2	T	113	ILE	C-N-CA	7.74	128.45	119.47
1	g	119	ALA	CA-C-N	7.74	131.28	120.29
1	g	119	ALA	C-N-CA	7.74	131.28	120.29
1	e	36	HIS	CA-C-N	7.68	127.22	118.85
1	e	36	HIS	C-N-CA	7.68	127.22	118.85
2	A	75	GLU	CA-C-N	7.64	135.46	121.70
2	A	75	GLU	C-N-CA	7.64	135.46	121.70
1	o	155	LYS	N-CA-C	-7.62	102.88	114.16
2	Q	116	PHE	CA-CB-CG	7.61	121.41	113.80
1	v	153	ASP	N-CA-C	-7.60	103.08	112.88
2	D	81	LEU	N-CA-C	-7.58	103.63	113.17
1	f	72	VAL	N-CA-C	-7.55	98.38	108.35
1	q	135	VAL	CA-C-N	7.53	132.12	120.75
1	q	135	VAL	C-N-CA	7.53	132.12	120.75
1	a	83	THR	N-CA-C	-7.53	106.04	114.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	27	MET	CA-C-N	7.51	135.22	121.70
1	e	27	MET	C-N-CA	7.51	135.22	121.70
1	k	131	SER	CA-C-N	7.48	135.16	121.70
1	k	131	SER	C-N-CA	7.48	135.16	121.70
2	I	113	ILE	CA-C-O	-7.47	116.06	119.94
2	B	113	ILE	N-CA-C	-7.46	103.07	109.19
1	b	131	SER	CA-C-N	7.46	135.12	121.70
1	b	131	SER	C-N-CA	7.46	135.12	121.70
2	P	74	HIS	CA-CB-CG	7.45	121.25	113.80
1	u	100	ILE	CA-C-N	7.40	130.19	120.28
1	u	100	ILE	C-N-CA	7.40	130.19	120.28
1	r	71	ASP	CA-CB-CG	7.39	119.99	112.60
2	Q	81	LEU	N-CA-C	-7.38	103.84	112.92
1	i	158	ARG	N-CA-C	-7.35	104.46	113.50
2	W	55	SER	N-CA-CB	7.32	122.86	110.49
1	l	158	ARG	N-CA-C	-7.29	104.53	113.50
2	L	88	LEU	N-CA-C	-7.28	104.91	114.31
2	V	57	ASP	N-CA-C	-7.28	95.30	110.80
2	I	153	ARG	N-CA-C	-7.27	106.33	114.62
2	F	170	ILE	N-CA-C	-7.26	106.41	113.53
2	M	81	LEU	N-CA-C	-7.26	104.02	113.17
2	W	57	ASP	N-CA-C	-7.26	105.60	114.75
1	r	155	LYS	N-CA-C	-7.22	101.59	113.50
1	d	157	LYS	N-CA-C	-7.20	105.67	114.75
1	f	153	ASP	N-CA-C	-7.19	103.81	112.59
1	p	27	MET	CA-C-N	7.19	134.65	121.70
1	p	27	MET	C-N-CA	7.19	134.65	121.70
1	g	83	THR	N-CA-C	-7.18	105.70	114.75
2	T	148	GLU	N-CA-C	-7.18	98.23	109.72
1	s	156	SER	N-CA-C	-7.17	106.45	114.62
2	N	79	ASP	N-CA-C	7.15	119.08	111.28
2	I	64	GLU	N-CA-C	-7.15	103.01	114.09
2	N	84	LEU	N-CA-C	-7.14	104.17	113.17
2	E	85	LEU	N-CA-C	-7.13	105.11	113.88
1	l	106	MET	N-CA-C	-7.08	103.20	112.41
1	n	131	SER	CA-C-N	7.08	134.44	121.70
1	n	131	SER	C-N-CA	7.08	134.44	121.70
1	o	149	ALA	N-CA-C	-7.04	103.87	113.30
1	s	133	PRO	N-CA-C	7.01	119.25	110.70
1	p	154	TYR	N-CA-C	-7.01	103.61	112.93
1	n	30	ILE	N-CA-C	-7.00	105.52	112.17
2	R	66	LEU	N-CA-C	-6.99	104.64	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	p	157	LYS	CA-C-N	6.98	130.34	120.28
1	p	157	LYS	C-N-CA	6.98	130.34	120.28
1	b	83	THR	N-CA-C	-6.97	105.71	114.56
2	L	77	ALA	N-CA-C	6.97	118.95	111.36
1	t	155	LYS	N-CA-C	-6.96	101.78	112.99
1	c	83	THR	N-CA-C	-6.95	106.70	114.62
2	T	84	LEU	N-CA-C	-6.95	106.70	114.62
1	x	131	SER	CA-C-N	6.95	134.20	121.70
1	x	131	SER	C-N-CA	6.95	134.20	121.70
1	s	72	VAL	N-CA-C	-6.94	99.19	108.35
1	s	130	LEU	CA-C-N	6.94	131.02	120.82
1	s	130	LEU	C-N-CA	6.94	131.02	120.82
1	x	100	ILE	N-CA-C	-6.93	104.10	110.82
1	g	157	LYS	N-CA-C	-6.92	104.99	113.50
1	b	46	PRO	CA-C-N	6.91	134.14	121.70
1	b	46	PRO	C-N-CA	6.91	134.14	121.70
2	G	67	ASN	N-CA-C	-6.90	103.95	114.16
1	e	135	VAL	N-CA-C	-6.89	106.58	113.20
1	x	124	THR	N-CA-C	-6.89	104.18	112.59
1	s	83	THR	N-CA-C	-6.87	106.10	114.75
1	r	69	CYS	N-CA-C	-6.86	104.94	113.38
2	S	86	ASP	CA-CB-CG	6.86	119.46	112.60
1	t	131	SER	O-C-N	-6.86	115.30	122.84
1	r	154	TYR	CA-C-N	6.85	130.72	120.17
1	r	154	TYR	C-N-CA	6.85	130.72	120.17
1	g	106	MET	N-CA-C	-6.83	104.26	112.59
1	w	99	ALA	N-CA-C	-6.83	104.57	113.17
1	j	132	LEU	CA-C-N	6.82	127.40	120.38
1	j	132	LEU	C-N-CA	6.82	127.40	120.38
2	J	79	ASP	N-CA-CB	6.81	122.07	110.50
2	E	101	ASP	CA-C-N	6.80	134.21	121.97
2	E	101	ASP	C-N-CA	6.80	134.21	121.97
1	k	130	LEU	N-CA-C	-6.79	104.11	114.16
1	l	155	LYS	N-CA-C	-6.78	102.31	113.50
2	M	75	GLU	CA-C-N	6.78	133.91	121.70
2	M	75	GLU	C-N-CA	6.78	133.91	121.70
2	L	85	LEU	CA-C-N	6.78	129.67	120.38
2	L	85	LEU	C-N-CA	6.78	129.67	120.38
2	N	61	VAL	N-CA-CB	6.77	120.69	111.21
2	V	91	LEU	N-CA-C	-6.76	103.75	113.21
2	X	170	ILE	CA-C-N	6.76	129.22	120.44
2	X	170	ILE	C-N-CA	6.76	129.22	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	j	83	THR	N-CA-C	-6.75	106.24	114.75
2	B	61	VAL	CA-C-O	-6.72	110.94	119.95
1	r	107	THR	N-CA-C	-6.72	105.15	113.15
2	D	88	LEU	N-CA-C	-6.71	105.07	112.72
1	j	42	HIS	CA-C-N	6.71	129.27	120.28
1	j	42	HIS	C-N-CA	6.71	129.27	120.28
2	X	102	VAL	N-CA-C	-6.71	98.83	108.42
1	x	27	MET	CA-C-N	6.70	133.76	121.70
1	x	27	MET	C-N-CA	6.70	133.76	121.70
2	V	95	HIS	N-CA-C	-6.70	102.10	108.13
1	m	147	ILE	N-CA-C	-6.69	106.48	112.90
1	h	155	LYS	N-CA-C	-6.68	102.47	113.50
2	C	75	GLU	CA-C-N	6.68	133.72	121.70
2	C	75	GLU	C-N-CA	6.68	133.72	121.70
2	K	111	LEU	N-CA-C	-6.67	97.19	108.26
1	r	158	ARG	N-CA-C	-6.67	105.05	113.72
2	U	78	ASP	N-CA-C	6.67	118.55	111.28
1	x	100	ILE	CA-C-N	6.67	129.22	120.28
1	x	100	ILE	C-N-CA	6.67	129.22	120.28
1	d	152	LYS	N-CA-C	-6.66	104.97	113.23
2	E	65	VAL	N-CA-C	-6.66	106.80	113.20
2	H	62	PRO	N-CA-C	-6.66	105.26	114.98
1	c	94	PHE	CA-CB-CG	-6.65	107.15	113.80
1	q	153	ASP	N-CA-C	-6.65	106.11	114.56
2	V	135	PRO	N-CA-C	-6.65	106.17	114.68
2	R	60	VAL	N-CA-C	-6.64	98.73	108.23
1	j	133	PRO	N-CA-C	6.64	118.80	110.70
1	b	132	LEU	N-CA-CB	6.62	121.75	110.50
1	o	106	MET	N-CA-C	-6.61	103.82	112.41
1	i	157	LYS	N-CA-C	-6.60	105.26	113.38
1	q	36	HIS	CA-C-N	6.59	126.17	119.19
1	q	36	HIS	C-N-CA	6.59	126.17	119.19
1	r	133	PRO	N-CA-C	6.59	118.74	110.70
1	n	69	CYS	N-CA-C	-6.58	106.45	114.75
2	W	75	GLU	CA-C-N	6.58	133.54	121.70
2	W	75	GLU	C-N-CA	6.58	133.54	121.70
1	a	72	VAL	N-CA-C	-6.58	99.26	108.27
2	A	125	PRO	CA-C-O	-6.58	116.17	120.90
1	i	108	GLU	N-CA-C	-6.56	105.84	114.31
2	K	125	PRO	CA-C-N	6.54	128.01	119.84
2	K	125	PRO	C-N-CA	6.54	128.01	119.84
2	J	145	LEU	N-CA-C	-6.54	107.17	114.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	155	LYS	N-CA-C	-6.53	102.48	112.99
1	f	155	LYS	N-CA-C	-6.52	102.74	113.50
2	Q	170	ILE	N-CA-C	-6.52	105.80	113.42
2	H	124	GLN	CA-C-N	6.51	127.08	120.38
2	H	124	GLN	C-N-CA	6.51	127.08	120.38
1	f	26	HIS	ND1-CE1-NE2	6.49	114.89	108.40
1	o	153	ASP	N-CA-C	-6.49	104.51	112.88
1	f	132	LEU	CA-C-N	6.49	127.06	120.38
1	f	132	LEU	C-N-CA	6.49	127.06	120.38
1	b	155	LYS	N-CA-C	-6.48	102.80	113.50
1	b	131	SER	O-C-N	-6.47	116.50	123.42
1	b	32	LYS	N-CA-C	-6.46	104.54	112.88
1	b	160	THR	CA-C-N	6.46	126.23	119.05
1	b	160	THR	C-N-CA	6.46	126.23	119.05
1	n	153	ASP	N-CA-C	-6.46	105.43	113.38
2	R	81	LEU	N-CA-C	-6.46	104.54	112.88
1	b	91	PHE	CA-CB-CG	6.46	120.26	113.80
2	C	146	ASN	N-CA-C	-6.45	106.62	114.75
2	W	77	ALA	N-CA-C	-6.45	104.03	112.41
2	U	77	ALA	N-CA-C	6.44	118.38	111.36
1	p	31	THR	CA-C-N	6.43	128.90	120.28
1	p	31	THR	C-N-CA	6.43	128.90	120.28
2	R	76	GLU	CA-C-N	6.42	133.81	121.54
2	R	76	GLU	C-N-CA	6.42	133.81	121.54
2	C	92	SER	N-CA-C	-6.42	105.48	113.38
1	n	37	PRO	CA-C-N	6.41	128.87	120.28
1	n	37	PRO	C-N-CA	6.41	128.87	120.28
2	E	81	LEU	N-CA-C	-6.40	102.94	113.50
2	Q	131	TRP	N-CA-C	-6.40	98.96	109.40
1	u	156	SER	N-CA-C	-6.40	107.32	114.62
1	j	106	MET	N-CA-C	-6.40	105.11	113.17
1	k	149	ALA	N-CA-C	-6.39	105.52	113.38
1	s	27	MET	CA-C-N	6.39	133.20	121.70
1	s	27	MET	C-N-CA	6.39	133.20	121.70
1	w	149	ALA	N-CA-C	-6.38	105.53	113.38
1	n	149	ALA	N-CA-C	-6.38	103.94	112.94
1	d	158	ARG	N-CA-C	-6.37	104.99	112.89
2	W	120	VAL	N-CA-C	-6.37	98.94	108.12
1	c	72	VAL	N-CA-C	-6.37	99.02	108.45
1	m	148	LYS	N-CA-C	-6.37	104.67	112.88
2	K	142	PHE	CA-CB-CG	-6.36	107.44	113.80
1	r	157	LYS	N-CA-C	-6.36	104.78	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	p	131	SER	CA-C-N	6.36	133.14	121.70
1	p	131	SER	C-N-CA	6.36	133.14	121.70
1	q	149	ALA	N-CA-C	-6.35	105.47	113.72
1	d	131	SER	CA-C-N	6.34	133.12	121.70
1	d	131	SER	C-N-CA	6.34	133.12	121.70
2	R	169	ALA	N-CA-C	-6.34	105.03	112.89
1	u	158	ARG	N-CA-C	-6.33	105.71	113.50
2	N	111	LEU	N-CA-C	-6.33	99.09	109.40
2	H	84	LEU	N-CA-C	-6.33	105.39	113.23
1	o	157	LYS	N-CA-C	-6.32	105.69	113.41
2	X	80	TYR	CA-CB-CG	-6.32	102.52	113.90
1	r	37	PRO	CA-C-N	6.32	128.75	120.28
1	r	37	PRO	C-N-CA	6.32	128.75	120.28
1	n	137	LEU	N-CA-C	-6.32	99.07	108.99
1	b	30	ILE	N-CA-C	-6.31	106.62	112.43
2	J	81	LEU	N-CA-C	-6.30	104.83	114.16
1	j	139	CYS	CA-C-N	6.30	128.72	120.28
1	j	139	CYS	C-N-CA	6.30	128.72	120.28
2	U	100	PRO	CA-C-N	6.29	133.55	121.54
2	U	100	PRO	C-N-CA	6.29	133.55	121.54
2	S	102	VAL	N-CA-C	-6.29	98.83	107.75
1	u	131	SER	CA-C-N	6.28	133.00	121.70
1	u	131	SER	C-N-CA	6.28	133.00	121.70
2	K	75	GLU	CA-C-N	6.28	133.00	121.70
2	K	75	GLU	C-N-CA	6.28	133.00	121.70
2	V	84	LEU	N-CA-C	-6.27	104.34	112.68
1	q	129	GLU	N-CA-C	-6.26	106.28	114.04
2	V	147	GLY	N-CA-C	-6.26	107.03	115.36
2	A	92	SER	CA-C-N	6.26	133.49	121.54
2	A	92	SER	C-N-CA	6.26	133.49	121.54
1	g	119	ALA	N-CA-C	-6.26	105.29	113.17
2	N	124	GLN	CA-C-N	6.26	126.82	120.38
2	N	124	GLN	C-N-CA	6.26	126.82	120.38
1	v	107	THR	N-CA-C	-6.26	107.49	114.62
1	o	129	GLU	N-CA-C	6.25	117.76	111.07
1	r	27	MET	CA-C-N	6.25	132.95	121.70
1	r	27	MET	C-N-CA	6.25	132.95	121.70
1	r	131	SER	CA-C-N	6.25	132.95	121.70
1	r	131	SER	C-N-CA	6.25	132.95	121.70
2	V	124	GLN	CA-C-N	6.25	126.82	120.38
2	V	124	GLN	C-N-CA	6.25	126.82	120.38
2	W	64	GLU	N-CA-C	-6.24	103.21	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	o	131	SER	N-CA-C	-6.23	102.31	110.53
1	s	106	MET	N-CA-C	-6.23	105.32	113.17
1	r	156	SER	N-CA-C	-6.22	106.91	114.75
2	W	68	LEU	N-CA-C	-6.22	102.31	110.39
1	s	79	VAL	CA-C-N	6.22	129.54	120.71
1	s	79	VAL	C-N-CA	6.22	129.54	120.71
2	B	75	GLU	CA-C-N	6.21	132.88	121.70
2	B	75	GLU	C-N-CA	6.21	132.88	121.70
1	j	55	LYS	N-CA-C	-6.21	101.35	108.49
2	L	82	ASP	CA-C-N	6.21	128.60	120.28
2	L	82	ASP	C-N-CA	6.21	128.60	120.28
1	i	92	LYS	N-CA-C	-6.21	99.25	108.99
2	P	75	GLU	CA-C-N	6.19	132.84	121.70
2	P	75	GLU	C-N-CA	6.19	132.84	121.70
1	a	131	SER	CA-C-N	6.18	132.83	121.70
1	a	131	SER	C-N-CA	6.18	132.83	121.70
2	D	80	TYR	N-CA-C	-6.18	105.05	112.59
1	b	106	MET	N-CA-C	-6.18	105.05	112.59
1	a	46	PRO	CA-C-N	6.17	132.81	121.70
1	a	46	PRO	C-N-CA	6.17	132.81	121.70
1	f	83	THR	N-CA-C	-6.17	107.59	114.62
1	f	99	ALA	CA-C-N	6.17	128.45	120.56
1	f	99	ALA	C-N-CA	6.17	128.45	120.56
1	o	130	LEU	N-CA-C	-6.16	104.57	111.28
1	d	30	ILE	N-CA-C	-6.15	106.99	112.90
1	p	140	SER	N-CA-C	-6.15	105.81	113.38
1	j	140	SER	CA-C-N	6.14	129.12	120.28
1	j	140	SER	C-N-CA	6.14	129.12	120.28
1	s	30	ILE	N-CA-C	-6.14	107.14	113.10
2	W	84	LEU	N-CA-C	-6.13	105.75	113.72
2	J	74	HIS	CA-CB-CG	-6.13	107.67	113.80
1	w	27	MET	CA-C-N	6.13	132.74	121.70
1	w	27	MET	C-N-CA	6.13	132.74	121.70
2	A	63	GLN	N-CA-C	6.13	119.56	111.28
2	B	125	PRO	CA-C-N	6.13	127.50	119.84
2	B	125	PRO	C-N-CA	6.13	127.50	119.84
2	D	75	GLU	CA-C-N	6.12	132.72	121.70
2	D	75	GLU	C-N-CA	6.12	132.72	121.70
1	j	31	THR	N-CA-C	-6.12	104.98	112.88
1	i	124	THR	N-CA-C	-6.12	105.68	113.02
2	I	129	GLN	CA-C-N	6.12	132.98	121.97
2	I	129	GLN	C-N-CA	6.12	132.98	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	133	PRO	CA-C-O	-6.11	111.69	120.56
1	e	163	MET	CA-C-N	6.11	128.39	120.44
1	e	163	MET	C-N-CA	6.11	128.39	120.44
1	r	83	THR	N-CA-C	-6.11	107.05	114.75
1	s	153	ASP	N-CA-C	-6.10	105.02	112.88
2	A	77	ALA	N-CA-C	6.09	117.59	111.07
1	h	27	MET	CA-C-N	6.09	132.67	121.70
1	h	27	MET	C-N-CA	6.09	132.67	121.70
2	O	83	HIS	CE1-NE2-CD2	-6.09	102.91	109.00
2	H	113	ILE	N-CA-C	-6.09	104.20	109.19
1	k	89	VAL	N-CA-C	-6.09	99.93	108.27
1	v	144	GLU	N-CA-C	-6.09	105.89	113.38
1	c	149	ALA	N-CA-C	-6.09	105.81	113.72
2	R	113	ILE	CA-C-N	6.08	126.53	119.47
2	R	113	ILE	C-N-CA	6.08	126.53	119.47
1	x	66	ALA	CA-C-N	6.08	125.57	119.24
1	x	66	ALA	C-N-CA	6.08	125.57	119.24
2	N	97	ASP	CA-CB-CG	-6.08	106.52	112.60
1	d	83	THR	N-CA-C	-6.07	107.70	114.62
1	t	153	ASP	N-CA-C	-6.07	105.46	112.92
1	u	27	MET	CA-C-N	6.06	132.61	121.70
1	u	27	MET	C-N-CA	6.06	132.61	121.70
2	O	82	ASP	N-CA-C	-6.05	106.44	113.88
2	E	58	GLY	N-CA-C	-6.04	101.56	110.87
1	d	31	THR	N-CA-C	-6.04	105.83	112.72
2	P	161	ILE	CA-C-N	6.03	128.96	120.28
2	P	161	ILE	C-N-CA	6.03	128.96	120.28
2	C	83	HIS	N-CA-C	6.02	117.92	111.36
2	S	127	ASN	N-CA-CB	6.02	120.66	110.49
2	Q	158	LEU	CA-C-N	6.02	128.34	120.28
2	Q	158	LEU	C-N-CA	6.02	128.34	120.28
1	m	130	LEU	N-CA-C	-6.01	105.26	112.59
1	f	26	HIS	CE1-NE2-CD2	-5.99	103.01	109.00
1	u	154	TYR	CA-C-N	5.99	129.40	120.17
1	u	154	TYR	C-N-CA	5.99	129.40	120.17
2	K	78	ASP	CA-C-N	5.99	128.90	120.28
2	K	78	ASP	C-N-CA	5.99	128.90	120.28
2	L	147	GLY	N-CA-C	-5.99	107.14	114.92
2	K	85	LEU	N-CA-C	-5.99	104.63	112.41
1	x	131	SER	O-C-N	-5.98	115.68	122.68
1	a	155	LYS	N-CA-C	-5.98	103.64	113.50
1	e	162	THR	N-CA-C	-5.97	105.96	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	h	158	ARG	N-CA-C	-5.97	105.83	113.23
2	J	156	THR	N-CA-C	-5.97	99.98	109.23
1	f	27	MET	CA-C-N	5.96	132.43	121.70
1	f	27	MET	C-N-CA	5.96	132.43	121.70
2	Q	148	GLU	N-CA-C	-5.96	99.57	109.46
1	i	27	MET	CA-C-N	5.95	132.41	121.70
1	i	27	MET	C-N-CA	5.95	132.41	121.70
1	m	45	HIS	O-C-N	-5.95	116.85	121.19
1	a	149	ALA	N-CA-C	-5.94	105.34	113.30
2	H	93	GLU	CA-C-N	5.94	132.89	121.54
2	H	93	GLU	C-N-CA	5.94	132.89	121.54
1	r	131	SER	O-C-N	-5.94	114.69	122.59
1	x	114	THR	CA-C-N	5.94	130.10	120.60
1	x	114	THR	C-N-CA	5.94	130.10	120.60
1	t	71	ASP	CA-CB-CG	5.93	118.53	112.60
1	e	59	VAL	CA-C-N	5.93	126.91	120.44
1	e	59	VAL	C-N-CA	5.93	126.91	120.44
1	k	34	LEU	N-CA-CB	5.93	120.52	110.49
2	D	170	ILE	N-CA-C	-5.93	107.48	113.47
1	r	129	GLU	CA-C-N	5.93	128.54	120.54
1	r	129	GLU	C-N-CA	5.93	128.54	120.54
1	b	94	PHE	CA-CB-CG	-5.92	107.88	113.80
1	d	161	PRO	N-CA-C	-5.92	107.87	114.92
1	x	134	PRO	N-CA-C	-5.92	100.27	112.47
1	w	83	THR	N-CA-C	-5.92	107.30	114.75
2	L	148	GLU	N-CA-C	-5.92	100.50	109.85
1	b	120	LYS	CA-C-N	5.91	128.56	120.35
1	b	120	LYS	C-N-CA	5.91	128.56	120.35
2	E	97	ASP	CA-C-N	5.91	132.83	121.54
2	E	97	ASP	C-N-CA	5.91	132.83	121.54
1	k	35	TYR	N-CA-C	-5.91	98.21	110.80
1	a	153	ASP	N-CA-C	-5.91	105.39	112.59
2	U	57	ASP	N-CA-C	-5.89	100.19	109.50
2	D	74	HIS	CE1-NE2-CD2	-5.89	103.11	109.00
2	H	98	CYS	N-CA-CB	5.88	120.44	110.49
1	e	30	ILE	N-CA-C	-5.88	105.64	111.88
1	a	37	PRO	CA-C-N	5.88	128.16	120.28
1	a	37	PRO	C-N-CA	5.88	128.16	120.28
2	P	80	TYR	N-CA-C	-5.88	101.65	110.06
1	h	153	ASP	N-CA-C	-5.88	104.65	112.94
1	e	131	SER	O-C-N	-5.88	114.78	122.59
2	L	75	GLU	CA-C-N	5.87	132.27	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	75	GLU	C-N-CA	5.87	132.27	121.70
2	V	59	GLN	N-CA-C	-5.87	105.48	114.16
1	n	89	VAL	N-CA-C	-5.86	100.61	108.35
2	M	158	LEU	CA-C-N	5.86	128.45	120.54
2	M	158	LEU	C-N-CA	5.86	128.45	120.54
2	J	102	VAL	CA-C-N	5.86	130.70	121.56
2	J	102	VAL	C-N-CA	5.86	130.70	121.56
1	b	122	LYS	N-CA-C	-5.86	100.59	109.85
1	m	42	HIS	CA-C-N	5.86	128.13	120.28
1	m	42	HIS	C-N-CA	5.86	128.13	120.28
2	T	98	CYS	N-CA-CB	5.85	120.38	110.49
2	D	154	ASN	CA-C-N	5.85	128.95	120.11
2	D	154	ASN	C-N-CA	5.85	128.95	120.11
2	C	90	GLU	N-CA-C	-5.85	105.80	113.17
2	G	68	LEU	N-CA-C	-5.84	97.17	108.45
1	t	143	ALA	CA-C-N	5.84	128.10	120.28
1	t	143	ALA	C-N-CA	5.84	128.10	120.28
1	l	27	MET	CA-C-N	5.83	132.20	121.70
1	l	27	MET	C-N-CA	5.83	132.20	121.70
1	c	153	ASP	N-CA-C	-5.83	105.82	113.17
1	i	156	SER	N-CA-C	-5.83	107.41	114.75
2	B	150	VAL	N-CA-C	-5.82	100.67	108.35
1	b	149	ALA	N-CA-C	-5.82	105.50	113.30
2	G	98	CYS	CA-C-N	5.82	132.89	122.13
2	G	98	CYS	C-N-CA	5.82	132.89	122.13
1	i	132	LEU	CA-C-N	5.81	126.37	120.38
1	i	132	LEU	C-N-CA	5.81	126.37	120.38
2	V	170	ILE	N-CA-C	-5.81	106.05	111.45
1	h	163	MET	N-CA-C	-5.81	106.17	113.72
2	U	103	GLU	CA-C-N	5.80	132.63	121.54
2	U	103	GLU	C-N-CA	5.80	132.63	121.54
1	b	158	ARG	NE-CZ-NH2	5.80	124.42	119.20
2	Q	84	LEU	CA-C-N	5.80	128.53	120.29
2	Q	84	LEU	C-N-CA	5.80	128.53	120.29
2	X	94	ALA	N-CA-CB	5.80	120.29	110.49
1	t	149	ALA	N-CA-C	-5.79	105.53	113.30
1	s	31	THR	CA-C-N	5.79	128.04	120.28
1	s	31	THR	C-N-CA	5.79	128.04	120.28
1	w	134	PRO	CA-C-N	5.79	132.12	121.70
1	w	134	PRO	C-N-CA	5.79	132.12	121.70
1	n	150	ALA	N-CA-C	-5.78	108.03	114.62
1	f	154	TYR	CA-C-N	5.78	129.06	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	154	TYR	C-N-CA	5.78	129.06	120.17
1	q	131	SER	CA-C-N	5.78	132.10	121.70
1	q	131	SER	C-N-CA	5.78	132.10	121.70
1	k	69	CYS	N-CA-C	-5.77	106.10	114.12
2	L	125	PRO	N-CA-C	5.76	117.73	110.70
2	V	114	PRO	N-CA-C	-5.76	100.60	112.47
2	E	83	HIS	CE1-NE2-CD2	-5.75	103.25	109.00
1	r	89	VAL	N-CA-C	-5.75	100.76	108.35
1	u	138	HIS	CE1-NE2-CD2	-5.75	103.25	109.00
1	v	31	THR	N-CA-C	-5.75	104.83	112.94
1	j	37	PRO	CA-C-N	5.75	127.98	120.28
1	j	37	PRO	C-N-CA	5.75	127.98	120.28
1	v	27	MET	CA-C-N	5.74	132.04	121.70
1	v	27	MET	C-N-CA	5.74	132.04	121.70
1	p	94	PHE	CA-CB-CG	-5.74	108.06	113.80
2	C	70	LEU	N-CA-C	-5.74	100.77	108.86
2	X	74	HIS	N-CA-C	-5.74	103.88	112.54
1	h	69	CYS	N-CA-C	-5.73	108.08	114.62
2	W	142	PHE	CA-CB-CG	-5.73	108.07	113.80
2	W	152	LEU	N-CA-C	-5.73	105.60	112.59
2	Q	59	GLN	CA-C-N	5.73	128.56	120.42
2	Q	59	GLN	C-N-CA	5.73	128.56	120.42
2	U	152	LEU	N-CA-C	5.73	119.25	112.72
1	p	45	HIS	CE1-NE2-CD2	-5.72	103.28	109.00
1	t	119	ALA	CA-C-N	5.72	127.95	120.28
1	t	119	ALA	C-N-CA	5.72	127.95	120.28
2	Q	125	PRO	CA-C-N	5.72	126.99	119.84
2	Q	125	PRO	C-N-CA	5.72	126.99	119.84
2	D	123	LYS	CA-C-N	5.72	128.61	120.49
2	D	123	LYS	C-N-CA	5.72	128.61	120.49
1	x	143	ALA	CA-C-N	5.71	127.94	120.28
1	x	143	ALA	C-N-CA	5.71	127.94	120.28
2	R	88	LEU	N-CA-C	-5.70	106.13	112.57
2	D	57	ASP	N-CA-CB	5.70	120.12	110.49
2	S	154	ASN	N-CA-C	-5.70	107.33	114.56
2	V	58	GLY	CA-C-N	5.70	129.98	120.70
2	V	58	GLY	C-N-CA	5.70	129.98	120.70
2	C	147	GLY	N-CA-C	-5.69	107.24	115.27
1	n	94	PHE	CA-CB-CG	-5.69	108.11	113.80
2	P	100	PRO	CA-C-N	5.69	132.41	121.54
2	P	100	PRO	C-N-CA	5.69	132.41	121.54
1	x	58	ASN	CA-C-N	5.68	128.25	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	x	58	ASN	C-N-CA	5.68	128.25	120.35
1	c	36	HIS	CA-C-N	5.68	125.04	118.85
1	c	36	HIS	C-N-CA	5.68	125.04	118.85
2	J	126	PRO	CA-C-N	5.67	132.38	121.54
2	J	126	PRO	C-N-CA	5.67	132.38	121.54
1	k	131	SER	O-C-N	-5.67	115.81	122.96
1	l	69	CYS	N-CA-C	-5.67	106.36	113.28
1	v	149	ALA	N-CA-C	-5.67	105.56	112.88
1	h	138	HIS	CE1-NE2-CD2	-5.67	103.33	109.00
2	J	95	HIS	CE1-NE2-CD2	-5.66	103.34	109.00
2	E	71	GLU	CA-C-N	5.66	132.34	121.54
2	E	71	GLU	C-N-CA	5.66	132.34	121.54
2	D	74	HIS	CG-CD2-NE2	5.65	112.85	107.20
2	A	105	SER	N-CA-C	5.64	117.43	111.28
1	c	42	HIS	O-C-N	5.64	128.10	122.12
2	O	71	GLU	CA-C-N	5.64	128.85	120.90
2	O	71	GLU	C-N-CA	5.64	128.85	120.90
1	a	58	ASN	CA-C-N	5.63	128.18	120.35
1	a	58	ASN	C-N-CA	5.63	128.18	120.35
2	N	141	ARG	N-CA-C	-5.63	100.92	108.86
1	i	130	LEU	CA-C-N	5.63	132.29	121.54
1	i	130	LEU	C-N-CA	5.63	132.29	121.54
2	P	124	GLN	CA-C-O	-5.62	115.47	120.19
2	G	80	TYR	CA-C-N	5.61	128.26	120.29
2	G	80	TYR	C-N-CA	5.61	128.26	120.29
2	B	100	PRO	CA-C-N	5.61	132.26	121.54
2	B	100	PRO	C-N-CA	5.61	132.26	121.54
2	A	138	GLY	CA-C-N	5.61	125.58	120.03
2	A	138	GLY	C-N-CA	5.61	125.58	120.03
2	H	119	TYR	N-CA-C	-5.61	99.76	108.90
1	f	158	ARG	N-CA-C	-5.61	106.48	113.38
2	M	95	HIS	N-CA-C	-5.61	103.06	110.40
1	j	149	ALA	N-CA-C	-5.60	106.49	113.38
2	N	61	VAL	O-C-N	-5.60	114.71	121.10
2	F	75	GLU	O-C-N	-5.60	115.14	122.59
2	O	81	LEU	N-CA-C	-5.60	105.80	113.30
1	t	154	TYR	N-CA-C	-5.60	103.61	110.61
1	u	148	LYS	N-CA-C	-5.59	106.12	113.17
1	m	151	ILE	N-CA-C	-5.59	107.34	113.43
2	R	106	HIS	CE1-NE2-CD2	-5.59	103.41	109.00
2	F	119	TYR	N-CA-C	-5.59	102.25	110.52
1	g	131	SER	CA-C-O	-5.59	115.47	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	j	61	THR	N-CA-C	-5.59	99.56	109.06
2	P	86	ASP	CA-C-N	5.58	127.76	120.28
2	P	86	ASP	C-N-CA	5.58	127.76	120.28
1	l	131	SER	O-C-N	-5.58	115.16	122.59
1	q	77	ILE	N-CA-CB	5.58	116.61	110.53
2	U	153	ARG	CA-C-N	5.58	132.19	121.54
2	U	153	ARG	C-N-CA	5.58	132.19	121.54
1	g	47	ARG	CA-C-N	5.57	132.18	121.54
1	g	47	ARG	C-N-CA	5.57	132.18	121.54
1	q	146	ALA	N-CA-C	-5.57	106.84	113.97
1	m	131	SER	CA-C-N	5.57	131.72	121.70
1	m	131	SER	C-N-CA	5.57	131.72	121.70
1	r	145	ASP	CA-CB-CG	-5.57	107.03	112.60
2	R	158	LEU	CA-C-N	5.57	128.01	120.38
2	R	158	LEU	C-N-CA	5.57	128.01	120.38
1	x	45	HIS	CE1-NE2-CD2	-5.57	103.43	109.00
1	i	31	THR	N-CA-C	-5.56	105.80	112.59
1	j	31	THR	CA-C-N	5.56	127.73	120.28
1	j	31	THR	C-N-CA	5.56	127.73	120.28
1	c	45	HIS	CE1-NE2-CD2	-5.56	103.44	109.00
1	h	25	SER	N-CA-C	-5.56	98.96	110.80
2	C	65	VAL	CA-C-N	5.55	128.27	120.28
2	C	65	VAL	C-N-CA	5.55	128.27	120.28
2	U	122	ASN	CA-CB-CG	-5.55	107.05	112.60
2	B	66	LEU	N-CA-C	-5.55	106.56	113.38
1	i	99	ALA	N-CA-C	-5.55	106.51	113.28
1	n	27	MET	CA-C-N	5.55	131.69	121.70
1	n	27	MET	C-N-CA	5.55	131.69	121.70
2	E	95	HIS	ND1-CE1-NE2	5.55	113.95	108.40
1	v	43	TYR	CA-C-N	5.55	127.71	120.28
1	v	43	TYR	C-N-CA	5.55	127.71	120.28
2	G	161	ILE	CA-C-N	5.54	128.26	120.28
2	G	161	ILE	C-N-CA	5.54	128.26	120.28
1	v	42	HIS	CE1-NE2-CD2	-5.54	103.46	109.00
2	X	95	HIS	CE1-NE2-CD2	-5.54	103.46	109.00
2	L	108	VAL	N-CA-C	-5.54	100.14	108.12
2	B	53	GLU	N-CA-C	-5.54	103.69	110.61
2	S	87	SER	CA-C-N	5.54	127.70	120.28
2	S	87	SER	C-N-CA	5.54	127.70	120.28
1	e	128	LYS	N-CA-C	-5.54	104.95	112.26
1	h	131	SER	N-CA-C	-5.53	99.02	110.80
1	g	149	ALA	N-CA-C	-5.53	105.89	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	78	ASP	CA-C-N	5.53	129.53	120.63
2	R	78	ASP	C-N-CA	5.53	129.53	120.63
2	S	59	GLN	CA-C-N	5.53	128.19	122.27
2	S	59	GLN	C-N-CA	5.53	128.19	122.27
2	C	62	PRO	N-CA-C	-5.53	108.34	114.92
1	m	106	MET	N-CA-C	-5.52	106.21	113.17
1	l	157	LYS	N-CA-C	-5.52	106.59	113.38
1	m	83	THR	N-CA-C	-5.52	107.55	114.56
1	v	123	ASN	CA-C-N	5.52	128.23	120.28
1	v	123	ASN	C-N-CA	5.52	128.23	120.28
1	d	122	LYS	CA-C-N	5.52	127.67	120.28
1	d	122	LYS	C-N-CA	5.52	127.67	120.28
1	a	135	VAL	N-CA-C	-5.51	107.37	112.83
2	V	59	GLN	CA-C-N	5.51	129.10	122.26
2	V	59	GLN	C-N-CA	5.51	129.10	122.26
1	l	123	ASN	N-CA-C	-5.51	106.23	113.17
1	h	154	TYR	CA-C-N	5.51	128.65	120.17
1	h	154	TYR	C-N-CA	5.51	128.65	120.17
1	k	119	ALA	CA-C-N	5.51	128.11	120.29
1	k	119	ALA	C-N-CA	5.51	128.11	120.29
1	d	69	CYS	N-CA-C	-5.50	106.73	113.50
1	f	42	HIS	CE1-NE2-CD2	-5.50	103.50	109.00
1	f	92	LYS	N-CA-C	-5.50	100.43	109.40
2	P	58	GLY	CA-C-N	5.50	132.05	121.54
2	P	58	GLY	C-N-CA	5.50	132.05	121.54
2	S	75	GLU	CA-C-N	5.50	131.60	121.70
2	S	75	GLU	C-N-CA	5.50	131.60	121.70
1	h	158	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	p	119	ALA	CA-C-N	5.49	132.03	121.54
1	p	119	ALA	C-N-CA	5.49	132.03	121.54
2	E	95	HIS	CA-C-N	5.49	125.19	119.64
2	E	95	HIS	C-N-CA	5.49	125.19	119.64
1	i	89	VAL	N-CA-C	-5.49	101.10	108.35
1	l	116	ASP	CA-C-N	5.49	127.64	120.28
1	l	116	ASP	C-N-CA	5.49	127.64	120.28
2	L	124	GLN	CA-C-N	5.49	126.04	120.38
2	L	124	GLN	C-N-CA	5.49	126.04	120.38
1	p	94	PHE	N-CA-C	-5.49	101.02	109.52
2	O	111	LEU	N-CA-C	-5.48	99.50	108.76
2	S	62	PRO	CA-C-N	5.48	130.35	122.35
2	S	62	PRO	C-N-CA	5.48	130.35	122.35
1	e	67	PRO	N-CA-C	-5.48	106.88	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	k	47	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	k	104	SER	CA-C-N	5.47	127.62	120.28
1	k	104	SER	C-N-CA	5.47	127.62	120.28
2	N	89	GLU	N-CA-C	-5.47	104.86	112.03
1	m	132	LEU	CA-C-N	5.47	126.02	120.38
1	m	132	LEU	C-N-CA	5.47	126.02	120.38
2	U	61	VAL	N-CA-C	5.47	120.70	108.88
1	u	59	VAL	CA-C-N	5.47	126.40	120.44
1	u	59	VAL	C-N-CA	5.47	126.40	120.44
2	F	148	GLU	N-CA-C	-5.47	100.40	108.99
1	o	42	HIS	CA-C-N	5.47	127.61	120.28
1	o	42	HIS	C-N-CA	5.47	127.61	120.28
2	J	73	ALA	CA-C-N	5.47	128.47	120.71
2	J	73	ALA	C-N-CA	5.47	128.47	120.71
1	o	152	LYS	N-CA-C	-5.46	105.98	113.30
2	N	127	ASN	N-CA-CB	5.46	119.72	110.49
1	j	116	ASP	N-CA-C	-5.46	106.39	113.16
2	J	78	ASP	O-C-N	-5.46	116.45	122.07
2	C	148	GLU	N-CA-C	-5.46	100.99	109.72
1	q	71	ASP	CA-CB-CG	5.45	118.05	112.60
2	H	90	GLU	N-CA-C	-5.45	106.80	113.50
1	u	149	ALA	N-CA-C	-5.44	106.31	113.17
1	c	33	ARG	CA-C-N	5.44	127.57	120.28
1	c	33	ARG	C-N-CA	5.44	127.57	120.28
1	s	58	ASN	CA-C-N	5.44	127.91	120.35
1	s	58	ASN	C-N-CA	5.44	127.91	120.35
1	v	154	TYR	N-CA-CB	5.44	118.74	110.42
2	O	85	LEU	CA-C-N	5.44	127.56	120.28
2	O	85	LEU	C-N-CA	5.44	127.56	120.28
1	s	94	PHE	CA-CB-CG	-5.44	108.36	113.80
2	G	88	LEU	CA-C-N	5.43	127.56	120.28
2	G	88	LEU	C-N-CA	5.43	127.56	120.28
2	O	75	GLU	CA-C-N	5.43	131.48	121.70
2	O	75	GLU	C-N-CA	5.43	131.48	121.70
2	H	68	LEU	CA-C-N	5.43	125.73	119.92
2	H	68	LEU	C-N-CA	5.43	125.73	119.92
2	K	57	ASP	CA-CB-CG	5.43	118.03	112.60
1	d	147	ILE	N-CA-C	-5.43	107.45	112.83
1	i	138	HIS	CE1-NE2-CD2	-5.43	103.57	109.00
1	a	38	LYS	CA-C-N	5.43	127.40	120.56
1	a	38	LYS	C-N-CA	5.43	127.40	120.56
1	b	45	HIS	ND1-CE1-NE2	5.42	113.82	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	74	HIS	ND1-CE1-NE2	5.42	113.82	108.40
1	i	36	HIS	CA-C-N	5.42	124.76	118.85
1	i	36	HIS	C-N-CA	5.42	124.76	118.85
1	t	136	LYS	CA-C-N	5.42	131.89	121.54
1	t	136	LYS	C-N-CA	5.42	131.89	121.54
2	T	114	PRO	N-CA-C	5.42	121.67	113.81
2	U	158	LEU	CA-C-N	5.42	127.54	120.28
2	U	158	LEU	C-N-CA	5.42	127.54	120.28
2	X	113	ILE	CA-C-N	5.42	126.61	119.84
2	X	113	ILE	C-N-CA	5.42	126.61	119.84
1	e	36	HIS	CE1-NE2-CD2	-5.42	103.58	109.00
2	A	171	SER	N-CA-C	-5.41	106.72	113.38
1	h	58	ASN	CA-C-N	5.41	127.88	120.35
1	h	58	ASN	C-N-CA	5.41	127.88	120.35
2	Q	124	GLN	CA-C-N	5.41	125.96	120.38
2	Q	124	GLN	C-N-CA	5.41	125.96	120.38
2	V	106	HIS	CE1-NE2-CD2	-5.41	103.59	109.00
1	w	131	SER	CA-C-N	5.41	131.45	121.70
1	w	131	SER	C-N-CA	5.41	131.45	121.70
1	c	123	ASN	CA-CB-CG	5.41	118.01	112.60
2	E	54	SER	CA-C-N	5.41	129.81	122.07
2	E	54	SER	C-N-CA	5.41	129.81	122.07
1	d	27	MET	N-CA-C	5.41	116.98	111.14
1	f	164	LEU	N-CA-C	-5.41	105.46	111.36
2	F	90	GLU	N-CA-C	-5.41	106.36	113.17
2	C	68	LEU	CA-C-N	5.40	125.31	119.85
2	C	68	LEU	C-N-CA	5.40	125.31	119.85
1	p	144	GLU	CA-C-N	5.40	127.78	120.38
1	p	144	GLU	C-N-CA	5.40	127.78	120.38
2	O	85	LEU	N-CA-C	5.40	117.87	111.33
1	b	46	PRO	CA-C-O	-5.40	115.27	121.86
2	G	103	GLU	CA-C-N	5.39	128.43	120.82
2	G	103	GLU	C-N-CA	5.39	128.43	120.82
2	V	140	ASN	N-CA-C	5.39	117.24	111.36
1	o	94	PHE	CA-CB-CG	-5.39	108.41	113.80
2	F	163	THR	CA-C-N	5.39	127.94	120.29
2	F	163	THR	C-N-CA	5.39	127.94	120.29
2	R	154	ASN	N-CA-C	-5.39	106.19	114.16
1	b	26	HIS	CE1-NE2-CD2	-5.39	103.61	109.00
2	D	133	ALA	N-CA-C	-5.39	98.78	108.48
2	L	157	LYS	N-CA-C	-5.38	100.62	109.40
2	M	158	LEU	N-CA-C	-5.38	106.08	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	x	42	HIS	CE1-NE2-CD2	-5.38	103.61	109.00
2	H	75	GLU	N-CA-C	5.38	117.15	111.28
1	g	55	LYS	N-CA-C	-5.38	101.12	108.38
1	h	26	HIS	CE1-NE2-CD2	-5.38	103.62	109.00
2	U	83	HIS	CE1-NE2-CD2	-5.37	103.63	109.00
2	V	67	ASN	CA-CB-CG	5.37	117.97	112.60
2	H	88	LEU	N-CA-C	-5.37	105.43	112.41
2	N	137	SER	N-CA-CB	5.37	118.53	110.53
1	u	26	HIS	ND1-CE1-NE2	5.37	113.77	108.40
1	v	47	ARG	NE-CZ-NH2	5.36	124.03	119.20
2	M	138	GLY	CA-C-N	5.36	125.30	119.78
2	M	138	GLY	C-N-CA	5.36	125.30	119.78
2	U	95	HIS	CE1-NE2-CD2	-5.36	103.64	109.00
2	D	142	PHE	CB-CA-C	-5.36	99.90	109.71
2	V	162	LEU	CA-C-N	5.36	127.46	120.28
2	V	162	LEU	C-N-CA	5.36	127.46	120.28
2	B	126	PRO	CA-C-N	5.35	131.76	121.54
2	B	126	PRO	C-N-CA	5.35	131.76	121.54
1	a	161	PRO	N-CA-C	-5.35	108.56	114.92
2	N	95	HIS	N-CA-C	-5.35	101.21	108.11
2	R	138	GLY	CA-C-N	5.35	125.35	119.90
2	R	138	GLY	C-N-CA	5.35	125.35	119.90
2	N	75	GLU	CA-C-N	5.34	131.32	121.70
2	N	75	GLU	C-N-CA	5.34	131.32	121.70
2	P	80	TYR	CA-C-N	5.34	131.75	121.54
2	P	80	TYR	C-N-CA	5.34	131.75	121.54
1	b	75	LEU	N-CA-C	-5.34	99.81	108.52
1	l	72	VAL	N-CA-C	-5.34	100.54	108.45
2	B	158	LEU	CA-C-N	5.34	127.43	120.28
2	B	158	LEU	C-N-CA	5.34	127.43	120.28
1	x	138	HIS	CE1-NE2-CD2	-5.34	103.66	109.00
1	b	105	TYR	CA-CB-CG	-5.34	104.29	113.90
2	E	120	VAL	N-CA-C	-5.34	100.43	108.12
1	a	133	PRO	N-CA-C	5.33	117.21	110.70
1	e	148	LYS	N-CA-C	-5.33	106.82	113.38
2	S	157	LYS	N-CA-C	-5.33	103.35	110.55
1	d	117	ASP	CA-CB-CG	-5.33	107.27	112.60
2	C	59	GLN	N-CA-CB	5.33	119.50	110.49
1	r	132	LEU	CA-C-N	5.33	125.87	120.38
1	r	132	LEU	C-N-CA	5.33	125.87	120.38
2	R	93	GLU	CA-C-N	5.33	131.72	121.54
2	R	93	GLU	C-N-CA	5.33	131.72	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	l	154	TYR	CA-C-N	5.33	128.37	120.17
1	l	154	TYR	C-N-CA	5.33	128.37	120.17
2	M	57	ASP	CA-C-N	5.33	125.40	120.34
2	M	57	ASP	C-N-CA	5.33	125.40	120.34
2	E	125	PRO	N-CA-C	5.32	117.19	110.70
1	n	36	HIS	ND1-CE1-NE2	5.32	113.72	108.40
1	d	118	ALA	N-CA-C	-5.32	106.81	113.72
2	H	113	ILE	CB-CA-C	5.32	114.54	109.33
2	J	63	GLN	N-CA-CB	5.32	119.48	110.49
1	d	144	GLU	N-CA-C	-5.32	107.17	113.97
1	c	26	HIS	ND1-CE1-NE2	5.31	113.71	108.40
2	M	125	PRO	CA-C-N	5.31	126.14	119.98
2	M	125	PRO	C-N-CA	5.31	126.14	119.98
1	u	83	THR	N-CA-C	-5.31	108.06	114.75
2	U	95	HIS	ND1-CE1-NE2	5.31	113.71	108.40
2	W	113	ILE	N-CA-C	-5.31	104.06	108.63
2	I	74	HIS	ND1-CE1-NE2	5.31	113.71	108.40
1	r	128	LYS	CA-C-N	5.31	127.39	120.28
1	r	128	LYS	C-N-CA	5.31	127.39	120.28
2	R	68	LEU	N-CA-C	-5.30	102.31	110.32
2	R	95	HIS	O-C-N	-5.30	115.22	121.32
1	e	36	HIS	ND1-CE1-NE2	5.30	113.70	108.40
1	x	123	ASN	N-CA-C	-5.30	106.49	113.17
2	K	152	LEU	CA-C-N	5.30	127.65	120.44
2	K	152	LEU	C-N-CA	5.30	127.65	120.44
2	J	142	PHE	N-CA-C	-5.30	100.67	108.99
1	e	46	PRO	CA-C-N	5.29	131.23	121.70
1	e	46	PRO	C-N-CA	5.29	131.23	121.70
1	n	72	VAL	N-CA-C	-5.29	100.70	108.11
1	o	58	ASN	CA-C-N	5.29	127.71	120.35
1	o	58	ASN	C-N-CA	5.29	127.71	120.35
2	S	143	ASP	CA-C-N	5.29	131.65	121.54
2	S	143	ASP	C-N-CA	5.29	131.65	121.54
1	o	61	THR	N-CA-C	-5.29	101.03	109.23
2	V	97	ASP	N-CA-C	-5.29	107.84	114.56
1	e	45	HIS	CE1-NE2-CD2	-5.29	103.72	109.00
1	o	133	PRO	CA-C-O	-5.29	112.90	120.56
2	F	53	GLU	CA-C-N	5.28	127.36	120.28
2	F	53	GLU	C-N-CA	5.28	127.36	120.28
2	H	95	HIS	ND1-CE1-NE2	5.28	113.68	108.40
2	W	153	ARG	N-CA-C	-5.28	107.21	113.97
2	X	90	GLU	N-CA-C	-5.28	106.78	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	65	VAL	N-CA-C	-5.28	100.64	108.45
2	V	131	TRP	N-CA-C	-5.28	101.05	109.07
2	V	148	GLU	N-CA-C	-5.28	102.39	110.14
2	W	161	ILE	N-CA-C	-5.28	105.39	110.72
2	E	113	ILE	CA-C-N	5.27	126.43	119.84
2	E	113	ILE	C-N-CA	5.27	126.43	119.84
2	D	54	SER	N-CA-C	-5.27	106.53	113.17
2	H	66	LEU	N-CA-C	-5.27	106.69	113.23
2	R	55	SER	N-CA-C	-5.27	105.12	112.03
1	m	116	ASP	N-CA-C	-5.27	106.85	113.28
2	C	74	HIS	CE1-NE2-CD2	-5.27	103.73	109.00
1	f	89	VAL	N-CA-C	-5.27	101.40	108.35
1	j	27	MET	CA-C-N	5.26	131.18	121.70
1	j	27	MET	C-N-CA	5.26	131.18	121.70
1	o	37	PRO	CA-C-N	5.26	127.33	120.28
1	o	37	PRO	C-N-CA	5.26	127.33	120.28
2	B	68	LEU	CA-C-N	5.26	125.72	120.14
2	B	68	LEU	C-N-CA	5.26	125.72	120.14
1	e	142	LEU	CA-C-N	5.26	131.59	121.54
1	e	142	LEU	C-N-CA	5.26	131.59	121.54
1	n	100	ILE	CA-C-N	5.26	127.76	120.29
1	n	100	ILE	C-N-CA	5.26	127.76	120.29
2	G	168	LYS	N-CA-C	-5.26	106.54	113.17
1	o	154	TYR	CA-C-N	5.26	129.27	120.70
1	o	154	TYR	C-N-CA	5.26	129.27	120.70
2	R	106	HIS	ND1-CE1-NE2	5.26	113.66	108.40
2	U	83	HIS	ND1-CE1-NE2	5.26	113.66	108.40
1	h	154	TYR	N-CA-C	-5.25	104.21	110.41
2	S	134	SER	N-CA-C	-5.25	101.33	108.11
1	v	162	THR	N-CA-CB	5.25	119.37	110.49
1	v	42	HIS	CG-CD2-NE2	5.25	112.45	107.20
2	H	87	SER	N-CA-C	-5.25	104.54	112.99
1	g	70	GLY	N-CA-C	-5.25	107.56	115.32
2	N	106	HIS	CE1-NE2-CD2	-5.25	103.75	109.00
1	i	122	LYS	N-CA-C	-5.24	101.10	109.23
1	h	40	ILE	CA-C-N	5.24	127.30	120.28
1	h	40	ILE	C-N-CA	5.24	127.30	120.28
2	R	148	GLU	N-CA-C	-5.24	101.34	109.72
1	s	31	THR	N-CA-C	-5.24	106.75	112.72
2	U	65	VAL	N-CA-C	-5.24	100.52	108.17
2	H	156	THR	N-CA-C	-5.24	100.77	108.99
1	f	130	LEU	N-CA-C	-5.23	106.13	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	47	ARG	CA-C-N	5.23	131.11	121.70
1	a	47	ARG	C-N-CA	5.23	131.11	121.70
2	V	95	HIS	ND1-CE1-NE2	5.23	113.63	108.40
1	t	157	LYS	N-CA-C	-5.23	106.21	112.59
1	b	27	MET	CA-C-N	5.22	131.10	121.70
1	b	27	MET	C-N-CA	5.22	131.10	121.70
1	l	119	ALA	CA-C-N	5.22	127.80	120.28
1	l	119	ALA	C-N-CA	5.22	127.80	120.28
2	E	124	GLN	N-CA-C	-5.22	102.44	110.32
2	M	83	HIS	N-CA-C	-5.22	106.94	113.72
1	m	89	VAL	N-CA-C	-5.21	101.13	108.27
2	Q	99	ILE	CA-C-N	5.21	124.39	118.97
2	Q	99	ILE	C-N-CA	5.21	124.39	118.97
2	P	124	GLN	CA-C-N	5.21	125.75	120.38
2	P	124	GLN	C-N-CA	5.21	125.75	120.38
1	t	26	HIS	ND1-CE1-NE2	5.21	113.61	108.40
2	A	125	PRO	CA-C-N	5.21	126.35	119.84
2	A	125	PRO	C-N-CA	5.21	126.35	119.84
2	B	78	ASP	CA-CB-CG	-5.21	107.39	112.60
1	w	72	VAL	N-CA-C	-5.21	101.14	108.27
1	w	77	ILE	N-CA-CB	5.21	116.21	110.53
1	p	130	LEU	N-CA-C	-5.21	106.24	112.59
2	R	124	GLN	CA-C-N	5.21	125.74	120.38
2	R	124	GLN	C-N-CA	5.21	125.74	120.38
1	v	131	SER	CA-C-N	5.20	131.07	121.70
1	v	131	SER	C-N-CA	5.20	131.07	121.70
2	W	126	PRO	CA-C-N	5.20	131.48	121.54
2	W	126	PRO	C-N-CA	5.20	131.48	121.54
1	c	131	SER	N-CA-C	-5.20	99.72	110.80
1	i	100	ILE	CA-C-N	5.20	127.25	120.28
1	i	100	ILE	C-N-CA	5.20	127.25	120.28
2	L	125	PRO	CB-CA-C	5.20	117.27	110.92
1	p	72	VAL	N-CA-C	-5.20	100.03	107.78
2	J	113	ILE	N-CA-C	-5.20	97.65	108.88
2	J	83	HIS	CE1-NE2-CD2	-5.20	103.80	109.00
2	C	83	HIS	CA-CB-CG	5.19	118.99	113.80
2	F	53	GLU	N-CA-C	-5.19	105.23	112.03
2	S	74	HIS	CA-C-N	5.19	127.24	120.28
2	S	74	HIS	C-N-CA	5.19	127.24	120.28
2	E	83	HIS	CG-CD2-NE2	5.19	112.39	107.20
1	i	108	GLU	CA-C-N	5.19	127.50	120.44
1	i	108	GLU	C-N-CA	5.19	127.50	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	q	37	PRO	CA-C-N	5.19	127.23	120.28
1	q	37	PRO	C-N-CA	5.19	127.23	120.28
1	h	37	PRO	N-CA-C	-5.19	108.04	114.68
1	u	153	ASP	N-CA-C	-5.19	106.54	112.92
2	A	61	VAL	N-CA-C	5.18	120.08	108.88
1	w	124	THR	CA-C-N	5.18	127.22	120.28
1	w	124	THR	C-N-CA	5.18	127.22	120.28
2	I	168	LYS	N-CA-C	-5.18	107.01	113.38
1	k	151	ILE	N-CA-CB	5.18	119.21	110.56
2	P	89	GLU	CA-C-N	5.18	127.47	120.38
2	P	89	GLU	C-N-CA	5.18	127.47	120.38
1	l	153	ASP	N-CA-C	-5.18	106.27	112.59
1	a	46	PRO	CA-C-O	-5.17	115.55	121.86
2	Q	75	GLU	CA-C-N	5.17	131.01	121.70
2	Q	75	GLU	C-N-CA	5.17	131.01	121.70
2	P	114	PRO	CA-C-N	5.17	127.21	120.28
2	P	114	PRO	C-N-CA	5.17	127.21	120.28
1	r	117	ASP	CA-C-N	5.17	127.21	120.28
1	r	117	ASP	C-N-CA	5.17	127.21	120.28
1	r	107	THR	N-CA-CB	5.17	118.42	110.46
2	Q	83	HIS	CE1-NE2-CD2	-5.17	103.83	109.00
2	I	74	HIS	CE1-NE2-CD2	-5.17	103.83	109.00
1	a	47	ARG	N-CA-CB	5.17	119.28	110.50
1	f	42	HIS	CA-CB-CG	5.16	118.96	113.80
1	l	114	THR	CA-C-N	5.16	128.86	120.60
1	l	114	THR	C-N-CA	5.16	128.86	120.60
1	a	157	LYS	N-CA-C	-5.16	107.03	113.38
2	N	138	GLY	CA-C-N	5.16	125.56	119.99
2	N	138	GLY	C-N-CA	5.16	125.56	119.99
1	j	119	ALA	N-CA-C	-5.16	107.04	113.38
1	o	123	ASN	N-CA-C	-5.16	106.99	113.28
1	d	161	PRO	CA-C-N	5.15	127.19	120.28
1	d	161	PRO	C-N-CA	5.15	127.19	120.28
2	X	75	GLU	CA-C-N	5.15	130.97	121.70
2	X	75	GLU	C-N-CA	5.15	130.97	121.70
2	R	137	SER	N-CA-CB	5.15	118.47	110.80
1	u	36	HIS	CA-C-N	5.15	124.94	119.28
1	u	36	HIS	C-N-CA	5.15	124.94	119.28
1	k	131	SER	N-CA-C	-5.14	101.48	109.14
1	l	55	LYS	N-CA-CB	5.14	119.18	110.49
1	u	129	GLU	N-CA-C	-5.14	107.03	113.72
2	L	128	LYS	CA-C-N	5.14	128.07	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	128	LYS	C-N-CA	5.14	128.07	120.82
2	B	82	ASP	N-CA-C	-5.14	107.68	114.31
1	t	27	MET	CA-C-N	5.14	130.95	121.70
1	t	27	MET	C-N-CA	5.14	130.95	121.70
2	H	98	CYS	N-CA-C	-5.14	99.86	110.80
2	X	146	ASN	N-CA-C	-5.13	103.82	108.75
2	C	98	CYS	N-CA-C	5.13	118.83	112.47
1	q	27	MET	CA-C-N	5.13	130.94	121.70
1	q	27	MET	C-N-CA	5.13	130.94	121.70
1	a	116	ASP	CB-CA-C	-5.13	102.83	110.88
2	A	86	ASP	CA-CB-CG	5.13	117.73	112.60
1	s	36	HIS	CE1-NE2-CD2	-5.13	103.87	109.00
1	i	37	PRO	CA-C-N	5.13	127.15	120.28
1	i	37	PRO	C-N-CA	5.13	127.15	120.28
1	o	36	HIS	CA-C-N	5.13	124.74	119.05
1	o	36	HIS	C-N-CA	5.13	124.74	119.05
1	v	30	ILE	N-CA-C	-5.13	107.98	112.90
2	M	95	HIS	CE1-NE2-CD2	-5.12	103.88	109.00
1	t	142	LEU	CA-C-N	5.12	131.33	121.54
1	t	142	LEU	C-N-CA	5.12	131.33	121.54
2	V	62	PRO	N-CA-C	-5.12	107.53	114.80
1	n	133	PRO	N-CA-C	-5.12	104.45	110.70
1	v	148	LYS	N-CA-C	-5.12	106.62	112.92
2	P	81	LEU	N-CA-C	-5.12	99.90	110.80
1	x	36	HIS	CA-C-N	5.12	124.91	119.28
1	x	36	HIS	C-N-CA	5.12	124.91	119.28
2	Q	54	SER	CA-C-N	5.12	129.82	122.40
2	Q	54	SER	C-N-CA	5.12	129.82	122.40
2	U	106	HIS	ND1-CE1-NE2	5.12	113.52	108.40
2	G	87	SER	CA-C-N	5.11	127.13	120.28
2	G	87	SER	C-N-CA	5.11	127.13	120.28
1	l	118	ALA	CA-C-N	5.11	128.08	120.31
1	l	118	ALA	C-N-CA	5.11	128.08	120.31
1	u	125	GLU	N-CA-C	-5.11	105.73	112.94
2	L	138	GLY	CA-C-N	5.11	124.87	119.76
2	L	138	GLY	C-N-CA	5.11	124.87	119.76
2	L	165	GLU	N-CA-C	-5.11	107.10	113.38
2	W	68	LEU	CA-C-O	-5.11	115.37	120.63
2	G	147	GLY	N-CA-C	-5.11	108.61	114.69
2	N	170	ILE	N-CA-C	-5.11	107.44	113.42
2	Q	95	HIS	CE1-NE2-CD2	-5.11	103.89	109.00
1	g	50	GLY	CA-C-N	5.11	131.29	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	50	GLY	C-N-CA	5.11	131.29	121.54
1	p	141	MET	N-CA-C	-5.10	106.46	113.30
2	V	142	PHE	CA-CB-CG	5.10	118.90	113.80
1	x	42	HIS	CG-CD2-NE2	5.10	112.30	107.20
1	j	36	HIS	CA-C-N	5.10	124.41	118.85
1	j	36	HIS	C-N-CA	5.10	124.41	118.85
1	n	142	LEU	N-CA-C	-5.10	104.84	112.54
1	d	27	MET	CA-C-N	5.10	130.87	121.70
1	d	27	MET	C-N-CA	5.10	130.87	121.70
2	L	67	ASN	N-CA-C	-5.10	106.07	113.21
2	O	117	GLY	N-CA-C	-5.10	106.93	112.08
2	P	97	ASP	CA-C-N	5.10	127.95	120.71
2	P	97	ASP	C-N-CA	5.10	127.95	120.71
1	f	139	CYS	CA-C-N	5.10	127.53	120.29
1	f	139	CYS	C-N-CA	5.10	127.53	120.29
1	h	45	HIS	CE1-NE2-CD2	-5.09	103.91	109.00
2	L	90	GLU	N-CA-C	-5.09	106.92	113.23
1	m	105	TYR	N-CA-C	-5.09	105.97	113.61
1	k	73	MET	CG-SD-CE	-5.09	89.70	100.90
1	w	45	HIS	ND1-CE1-NE2	5.09	113.49	108.40
1	f	131	SER	CA-C-N	5.09	130.86	121.70
1	f	131	SER	C-N-CA	5.09	130.86	121.70
2	B	83	HIS	CE1-NE2-CD2	-5.09	103.91	109.00
2	D	124	GLN	CA-C-N	5.09	125.62	120.38
2	D	124	GLN	C-N-CA	5.09	125.62	120.38
2	H	106	HIS	CE1-NE2-CD2	-5.09	103.91	109.00
2	E	75	GLU	N-CA-C	5.08	116.82	111.28
2	M	106	HIS	ND1-CE1-NE2	5.08	113.48	108.40
2	W	70	LEU	CA-C-N	5.08	128.43	120.75
2	W	70	LEU	C-N-CA	5.08	128.43	120.75
1	c	39	VAL	CA-C-N	5.08	127.42	120.46
1	c	39	VAL	C-N-CA	5.08	127.42	120.46
1	t	26	HIS	CE1-NE2-CD2	-5.08	103.92	109.00
2	Q	53	GLU	N-CA-C	-5.08	104.81	112.99
2	F	88	LEU	N-CA-C	-5.07	106.34	112.88
2	T	102	VAL	N-CA-C	-5.07	101.01	108.11
2	G	124	GLN	CA-C-O	-5.07	114.96	120.69
2	X	68	LEU	CA-C-N	5.07	124.83	119.76
2	X	68	LEU	C-N-CA	5.07	124.83	119.76
2	C	111	LEU	N-CA-C	-5.07	100.26	108.52
1	e	36	HIS	CA-CB-CG	-5.07	108.73	113.80
2	H	53	GLU	N-CA-C	-5.07	104.26	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	154	TYR	CA-C-N	5.07	127.38	120.54
1	e	154	TYR	C-N-CA	5.07	127.38	120.54
1	l	148	LYS	N-CA-C	-5.07	106.69	112.92
1	m	99	ALA	N-CA-C	-5.07	106.78	113.17
1	n	138	HIS	CE1-NE2-CD2	-5.07	103.93	109.00
1	u	31	THR	CA-C-N	5.07	127.07	120.28
1	u	31	THR	C-N-CA	5.07	127.07	120.28
2	W	163	THR	N-CA-C	-5.07	107.05	113.43
2	A	158	LEU	CA-C-N	5.07	127.07	120.28
2	A	158	LEU	C-N-CA	5.07	127.07	120.28
2	Q	70	LEU	N-CA-C	-5.07	99.72	108.69
1	b	157	LYS	N-CA-C	-5.06	107.49	113.97
1	n	163	MET	N-CA-C	-5.06	107.49	113.97
2	S	113	ILE	N-CA-C	-5.06	97.94	108.88
2	U	154	ASN	N-CA-CB	5.06	119.05	110.49
2	T	89	GLU	CA-C-N	5.06	127.06	120.28
2	T	89	GLU	C-N-CA	5.06	127.06	120.28
2	N	65	VAL	N-CA-C	-5.06	108.19	113.10
2	P	55	SER	CB-CA-C	5.06	118.51	111.63
1	b	154	TYR	CA-C-N	5.05	127.95	120.17
1	b	154	TYR	C-N-CA	5.05	127.95	120.17
2	M	82	ASP	N-CA-C	-5.05	106.53	113.30
2	N	106	HIS	ND1-CE1-NE2	5.05	113.45	108.40
1	w	163	MET	CA-C-N	5.05	127.05	120.28
1	w	163	MET	C-N-CA	5.05	127.05	120.28
1	f	157	LYS	N-CA-C	-5.05	107.17	113.38
2	H	83	HIS	CE1-NE2-CD2	-5.05	103.95	109.00
2	R	88	LEU	CA-C-N	5.05	127.00	120.44
2	R	88	LEU	C-N-CA	5.05	127.00	120.44
1	p	31	THR	N-CA-C	-5.04	106.72	112.92
1	x	115	LEU	CA-C-N	5.04	127.04	120.28
1	x	115	LEU	C-N-CA	5.04	127.04	120.28
1	r	36	HIS	CA-C-N	5.04	124.83	119.28
1	r	36	HIS	C-N-CA	5.04	124.83	119.28
2	B	113	ILE	O-C-N	-5.04	118.51	121.69
2	O	75	GLU	CB-CA-C	-5.04	102.02	110.29
1	u	157	LYS	N-CA-C	-5.04	107.18	113.38
1	l	116	ASP	CA-CB-CG	-5.04	107.56	112.60
2	F	96	PRO	CA-C-N	5.04	131.16	121.54
2	F	96	PRO	C-N-CA	5.04	131.16	121.54
1	a	26	HIS	CE1-NE2-CD2	-5.03	103.97	109.00
1	l	33	ARG	N-CA-C	-5.03	107.53	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	u	36	HIS	CE1-NE2-CD2	-5.03	103.97	109.00
2	D	141	ARG	N-CA-C	-5.03	100.97	109.07
1	m	152	LYS	N-CA-C	-5.03	106.73	112.92
2	R	94	ALA	N-CA-CB	5.03	118.99	110.49
2	V	61	VAL	N-CA-C	-5.03	103.33	109.01
2	A	58	GLY	CA-C-N	5.03	131.14	121.54
2	A	58	GLY	C-N-CA	5.03	131.14	121.54
1	s	38	LYS	CA-C-N	5.03	127.35	120.46
1	s	38	LYS	C-N-CA	5.03	127.35	120.46
1	m	135	VAL	N-CA-C	-5.03	107.94	112.96
1	b	133	PRO	CA-C-N	5.02	126.12	119.84
1	b	133	PRO	C-N-CA	5.02	126.12	119.84
1	p	99	ALA	N-CA-C	-5.02	107.19	113.72
1	h	37	PRO	N-CA-CB	5.02	106.05	101.83
1	h	38	LYS	CA-C-N	5.02	127.34	120.46
1	h	38	LYS	C-N-CA	5.02	127.34	120.46
2	N	169	ALA	N-CA-C	-5.02	106.57	113.30
1	g	126	ILE	N-CA-C	-5.02	108.08	112.90
1	h	83	THR	N-CA-C	-5.02	108.43	114.75
2	X	98	CYS	N-CA-C	-5.02	100.12	110.80
1	r	149	ALA	N-CA-C	-5.01	107.22	113.38
2	O	83	HIS	ND1-CE1-NE2	5.01	113.41	108.40
2	I	80	TYR	CB-CA-C	-5.01	102.48	110.79
1	e	58	ASN	CA-C-N	5.01	127.31	120.35
1	e	58	ASN	C-N-CA	5.01	127.31	120.35
2	T	122	ASN	N-CA-C	-5.01	101.80	108.86
1	v	163	MET	N-CA-C	-5.01	106.68	112.89
1	m	36	HIS	CA-C-N	5.00	124.78	119.28
1	m	36	HIS	C-N-CA	5.00	124.78	119.28
1	p	56	LEU	N-CA-C	-5.00	106.06	113.16
1	d	36	HIS	CA-C-N	5.00	124.60	119.05
1	d	36	HIS	C-N-CA	5.00	124.60	119.05
1	u	130	LEU	CA-C-N	5.00	131.09	121.54
1	u	130	LEU	C-N-CA	5.00	131.09	121.54

There are no chirality outliers.

All (7) planarity outliers are listed below:

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

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Mol	Chain	Res	Type	Group
1	n	105	TYR	Sidechain
1	r	33	ARG	Sidechain
1	r	47	ARG	Sidechain
1	t	47	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	1072	0	1106	0	0
1	b	1072	0	1108	14	0
1	c	1072	0	1108	1	0
1	d	1072	0	1108	1	0
1	e	1072	0	1108	4	0
1	f	1072	0	1108	2	0
1	g	1072	0	1108	3	0
1	h	1072	0	1108	2	0
1	i	1072	0	1106	1	0
1	j	1072	0	1108	1	0
1	k	1072	0	1106	2	0
1	l	1072	0	1108	3	0
1	m	1072	0	1108	0	0
1	n	1072	0	1106	37	0
1	o	1072	0	1108	56	0
1	p	1072	0	1108	2	0
1	q	1072	0	1108	3	0
1	r	1072	0	1105	23	0
1	s	1072	0	1106	2	0
1	t	1072	0	1108	2	0
1	u	1072	0	1108	5	0
1	v	1072	0	1108	2	0
1	w	1072	0	1106	6	0
1	x	1072	0	1108	0	0
2	A	947	0	921	2	0
2	B	947	0	921	3	0
2	C	947	0	921	4	0
2	D	947	0	921	1	0
2	E	947	0	921	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	947	0	921	1	0
2	G	947	0	921	2	0
2	H	947	0	921	3	0
2	I	947	0	921	2	0
2	J	947	0	921	4	0
2	K	947	0	921	2	0
2	L	947	0	920	19	0
2	M	947	0	921	5	0
2	N	947	0	920	26	0
2	O	947	0	920	68	0
2	P	947	0	921	2	0
2	Q	947	0	921	4	0
2	R	947	0	921	7	0
2	S	947	0	921	8	0
2	T	947	0	921	2	0
2	U	947	0	921	6	0
2	V	947	0	921	3	0
2	W	947	0	920	13	0
2	X	947	0	921	2	0
All	All	48456	0	48677	281	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (281) 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)
1:r:38:LYS:HE3	1:r:104:SER:CB	1.22	1.60
1:n:42:HIS:CE1	1:n:91:PHE:HE2	1.31	1.47
1:r:38:LYS:CE	1:r:104:SER:HB2	1.44	1.45
1:n:42:HIS:CE1	1:n:91:PHE:CE2	2.04	1.42
1:b:26:HIS:CD2	2:O:116:PHE:CE2	2.08	1.40
1:b:26:HIS:NE2	2:O:116:PHE:HE2	1.13	1.40
1:n:47:ARG:NH1	1:n:91:PHE:CZ	1.84	1.39
1:o:33:ARG:HH21	2:O:95:HIS:N	1.17	1.39
1:o:33:ARG:HH22	2:O:94:ALA:CA	1.36	1.36
1:o:129:GLU:OE1	2:O:168:LYS:NZ	1.58	1.35
1:r:38:LYS:CE	1:r:104:SER:CB	2.00	1.32
1:o:33:ARG:NH2	2:O:94:ALA:C	1.84	1.32
2:O:113:ILE:CG2	2:O:116:PHE:CD2	2.12	1.31
1:o:33:ARG:NH1	2:O:93:GLU:O	1.63	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:76:GLU:O	2:L:80:TYR:CD1	1.86	1.29
1:o:33:ARG:NH2	2:O:95:HIS:N	1.76	1.29
1:b:26:HIS:CD2	2:O:116:PHE:HE2	1.43	1.27
2:O:113:ILE:HG22	2:O:116:PHE:CD2	1.68	1.27
1:o:33:ARG:HH22	2:O:94:ALA:C	1.42	1.25
1:b:26:HIS:NE2	2:O:116:PHE:CE2	2.05	1.23
2:N:75:GLU:CD	2:N:80:TYR:CD2	2.17	1.23
1:n:42:HIS:ND1	1:n:91:PHE:CE2	2.09	1.19
1:n:47:ARG:NH2	1:n:91:PHE:CE1	2.12	1.17
2:N:75:GLU:CD	2:N:80:TYR:HD2	1.48	1.15
2:O:113:ILE:HG21	2:O:116:PHE:CD2	1.82	1.15
1:r:38:LYS:CD	1:r:104:SER:HB2	1.77	1.15
1:o:33:ARG:HE	2:O:95:HIS:CD2	1.64	1.14
1:r:38:LYS:HE3	1:r:104:SER:OG	1.46	1.13
1:o:33:ARG:NH2	2:O:94:ALA:N	1.95	1.13
1:n:47:ARG:NH1	1:n:91:PHE:CE2	2.15	1.13
1:o:33:ARG:HH22	2:O:94:ALA:N	1.46	1.13
2:N:80:TYR:HE1	2:N:148:GLU:CG	1.61	1.11
1:r:38:LYS:CE	1:r:104:SER:OG	1.96	1.11
1:n:47:ARG:HD3	1:n:91:PHE:O	1.47	1.11
1:r:38:LYS:HG3	1:r:104:SER:CB	1.79	1.11
1:o:128:LYS:NZ	2:O:116:PHE:HB3	1.65	1.10
2:W:80:TYR:CE1	2:W:148:GLU:HA	1.81	1.09
2:N:75:GLU:OE1	2:N:80:TYR:CD2	2.06	1.08
1:o:33:ARG:HE	2:O:95:HIS:CG	1.74	1.06
1:o:129:GLU:OE1	2:O:168:LYS:HG2	1.56	1.06
2:L:76:GLU:O	2:L:80:TYR:CE1	2.10	1.05
2:N:80:TYR:HE1	2:N:148:GLU:HG3	1.21	1.04
1:r:38:LYS:CG	1:r:104:SER:HB3	1.88	1.03
2:O:113:ILE:HG22	2:O:116:PHE:HD2	0.99	1.02
2:W:80:TYR:HE1	2:W:148:GLU:HA	1.18	1.02
1:r:38:LYS:HG3	1:r:104:SER:HB3	1.02	1.00
1:o:128:LYS:HZ3	2:O:116:PHE:HB3	1.26	1.00
1:r:38:LYS:CG	1:r:104:SER:CB	2.38	1.00
1:n:38:LYS:O	1:n:42:HIS:CD2	2.16	0.99
1:n:42:HIS:ND1	1:n:91:PHE:HE2	1.50	0.98
1:n:42:HIS:CE1	1:n:104:SER:HA	1.99	0.97
2:N:80:TYR:CE1	2:N:148:GLU:HG3	1.99	0.97
1:n:38:LYS:O	1:n:42:HIS:HD2	1.47	0.97
1:n:42:HIS:CE1	1:n:91:PHE:CD2	2.52	0.97
2:N:80:TYR:CE1	2:N:148:GLU:HA	1.99	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:76:GLU:HA	2:W:80:TYR:HE2	1.26	0.96
2:W:76:GLU:HA	2:W:80:TYR:CE2	2.01	0.95
1:b:26:HIS:CE1	2:O:116:PHE:CE2	2.54	0.95
1:o:129:GLU:OE2	2:O:168:LYS:HD3	1.66	0.95
2:L:76:GLU:O	2:L:80:TYR:HD1	1.30	0.95
1:o:33:ARG:CZ	2:O:93:GLU:C	2.40	0.94
1:o:33:ARG:NE	2:O:95:HIS:CD2	2.34	0.94
1:o:128:LYS:HD2	2:O:116:PHE:O	1.67	0.93
1:o:33:ARG:NH1	2:O:93:GLU:C	2.27	0.93
2:L:80:TYR:HE2	2:L:148:GLU:HG3	1.35	0.90
1:b:26:HIS:CE1	2:O:116:PHE:HE2	1.88	0.90
1:r:38:LYS:CD	1:r:104:SER:CB	2.42	0.89
1:o:33:ARG:NH2	2:O:94:ALA:CA	2.19	0.88
1:n:47:ARG:HH12	1:n:91:PHE:HZ	1.18	0.87
2:N:75:GLU:OE1	2:N:80:TYR:CE2	2.27	0.87
1:r:38:LYS:HE3	1:r:104:SER:HB2	0.90	0.87
1:b:26:HIS:CG	2:O:116:PHE:CE2	2.63	0.86
2:N:80:TYR:CE1	2:N:148:GLU:CG	2.54	0.86
1:o:129:GLU:OE1	2:O:168:LYS:CG	2.22	0.86
1:n:47:ARG:CZ	1:n:91:PHE:CE1	2.59	0.85
1:r:38:LYS:HE2	1:r:104:SER:OG	1.76	0.85
2:N:75:GLU:CD	2:N:80:TYR:CE2	2.55	0.84
1:o:129:GLU:CD	2:O:168:LYS:NZ	2.35	0.84
1:o:33:ARG:NH2	2:O:93:GLU:C	2.35	0.84
1:n:47:ARG:CZ	1:n:91:PHE:CZ	2.60	0.83
1:o:33:ARG:HH21	2:O:95:HIS:H	1.24	0.83
1:n:47:ARG:NH2	1:n:91:PHE:CD1	2.47	0.83
1:o:129:GLU:CD	2:O:168:LYS:HD3	2.03	0.83
1:o:129:GLU:OE1	2:O:168:LYS:CE	2.27	0.82
1:o:129:GLU:CD	2:O:168:LYS:CD	2.53	0.81
2:N:75:GLU:OE2	2:N:80:TYR:HD2	1.65	0.80
1:o:129:GLU:OE1	2:O:168:LYS:CD	2.29	0.79
1:n:47:ARG:NH1	1:n:91:PHE:CE1	2.51	0.78
1:n:42:HIS:ND1	1:n:91:PHE:CD2	2.50	0.78
1:n:47:ARG:HG2	1:n:90:LYS:HB3	1.66	0.77
2:L:80:TYR:CE2	2:L:148:GLU:HG3	2.18	0.76
1:n:42:HIS:HE1	1:n:104:SER:HA	1.51	0.76
1:b:26:HIS:CD2	2:O:116:PHE:CD2	2.73	0.75
1:b:26:HIS:CE1	2:O:116:PHE:CZ	2.75	0.75
1:o:128:LYS:HZ2	2:O:116:PHE:HB3	1.50	0.74
2:L:75:GLU:H	2:L:76:GLU:HA	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:129:GLU:OE2	2:O:168:LYS:CD	2.36	0.72
2:C:75:GLU:H	2:C:76:GLU:HA	1.53	0.72
2:L:80:TYR:OH	2:L:147:GLY:HA3	1.90	0.72
2:N:75:GLU:OE1	2:N:80:TYR:HD2	1.53	0.71
2:L:80:TYR:OH	2:L:147:GLY:CA	2.16	0.71
1:o:129:GLU:OE2	2:O:168:LYS:HB3	1.92	0.70
1:o:33:ARG:NH2	2:O:95:HIS:H	1.81	0.70
1:o:33:ARG:HD2	2:O:170:ILE:HD13	1.73	0.70
1:o:33:ARG:HH21	2:O:95:HIS:CA	2.04	0.69
2:N:80:TYR:CE1	2:N:148:GLU:CA	2.75	0.69
2:O:116:PHE:CZ	2:O:169:ALA:HA	2.30	0.67
2:N:80:TYR:CZ	2:N:148:GLU:HA	2.29	0.67
2:O:113:ILE:CG2	2:O:116:PHE:CE2	2.76	0.67
1:o:129:GLU:CD	2:O:168:LYS:CG	2.67	0.67
1:r:105:TYR:CE2	2:R:168:LYS:HD2	2.30	0.67
2:L:80:TYR:CE2	2:L:148:GLU:HA	2.30	0.67
1:v:159:ASN:HD22	1:w:158:ARG:HE	1.43	0.67
2:L:80:TYR:HE2	2:L:148:GLU:CG	2.07	0.67
1:n:47:ARG:HH22	1:n:91:PHE:HE1	1.35	0.66
2:O:113:ILE:CG2	2:O:116:PHE:HD2	1.71	0.66
1:o:130:LEU:N	1:o:130:LEU:HD22	2.11	0.65
1:o:129:GLU:CD	2:O:168:LYS:HG2	2.21	0.65
1:o:129:GLU:HG2	2:O:116:PHE:CD1	2.33	0.64
1:o:129:GLU:HG2	2:O:116:PHE:CE1	2.32	0.64
1:n:48:ASN:HD21	1:n:76:GLN:H	1.46	0.64
2:W:80:TYR:O	2:W:84:LEU:HB3	1.99	0.62
1:o:130:LEU:HD22	1:o:130:LEU:H	1.63	0.62
2:N:80:TYR:HE1	2:N:148:GLU:CB	2.12	0.61
1:q:33:ARG:HH12	2:Q:95:HIS:CD2	2.18	0.61
1:o:33:ARG:HD2	2:O:170:ILE:CD1	2.30	0.61
1:h:27:MET:H	1:h:28:SER:HA	1.66	0.61
1:o:129:GLU:OE2	2:O:168:LYS:CG	2.48	0.60
2:O:113:ILE:HG21	2:O:116:PHE:CG	2.36	0.60
2:M:75:GLU:H	2:M:76:GLU:HA	1.66	0.60
1:r:38:LYS:HD2	1:r:104:SER:HB2	1.80	0.60
2:C:144:LEU:HD12	2:C:144:LEU:H	1.67	0.59
2:N:80:TYR:CE1	2:N:148:GLU:CB	2.85	0.59
1:o:33:ARG:NE	2:O:95:HIS:CG	2.58	0.59
1:n:43:TYR:O	1:n:45:HIS:N	2.37	0.58
1:n:42:HIS:CG	1:n:47:ARG:HH11	2.21	0.58
2:O:116:PHE:HZ	2:O:169:ALA:HA	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:r:106:MET:SD	1:r:106:MET:N	2.78	0.57
2:L:76:GLU:CD	2:L:76:GLU:H	2.12	0.57
1:b:27:MET:H	1:b:28:SER:HA	1.70	0.57
1:c:106:MET:HE3	1:c:121:ILE:HG21	1.87	0.57
2:L:74:HIS:HD2	2:L:80:TYR:OH	1.89	0.56
1:o:130:LEU:H	1:o:130:LEU:CD2	2.18	0.56
2:O:113:ILE:HB	2:O:116:PHE:HB2	1.87	0.56
1:n:42:HIS:CG	1:n:91:PHE:HE2	2.22	0.56
1:o:129:GLU:OE2	2:O:168:LYS:CB	2.54	0.56
1:n:42:HIS:NE2	1:n:104:SER:HA	2.20	0.55
1:r:105:TYR:OH	2:R:168:LYS:HB2	2.06	0.55
1:r:38:LYS:HE3	1:r:104:SER:CA	2.26	0.55
1:n:43:TYR:O	1:n:44:THR:C	2.48	0.55
2:N:75:GLU:CG	2:N:80:TYR:CE2	2.90	0.55
2:N:75:GLU:OE2	2:N:80:TYR:CD2	2.49	0.55
1:o:129:GLU:HB2	2:O:168:LYS:NZ	2.23	0.54
2:U:92:SER:HB3	2:U:102:VAL:HG12	1.90	0.54
2:W:76:GLU:CA	2:W:80:TYR:CE2	2.84	0.53
2:N:75:GLU:HB3	2:N:79:ASP:H	1.74	0.53
1:o:31:THR:HA	1:o:34:LEU:CD1	2.39	0.53
2:M:153:ARG:HD2	2:N:80:TYR:CE2	2.43	0.53
1:p:123:ASN:HD22	2:Q:54:SER:HA	1.74	0.53
1:o:136:LYS:H	1:o:136:LYS:HD3	1.74	0.52
1:n:42:HIS:CG	1:n:91:PHE:CE2	2.96	0.52
2:W:80:TYR:CE1	2:W:148:GLU:CA	2.75	0.52
1:h:77:ILE:HG22	1:h:89:VAL:CG2	2.40	0.51
2:J:158:LEU:HD23	2:J:158:LEU:H	1.75	0.51
1:w:27:MET:H	1:w:28:SER:HA	1.75	0.51
1:b:26:HIS:HB2	2:O:115:ALA:HB3	1.92	0.51
2:L:76:GLU:O	2:L:80:TYR:HE1	1.82	0.51
1:n:42:HIS:CE1	1:n:107:THR:OG1	2.64	0.51
1:s:45:HIS:CG	1:s:90:LYS:HE2	2.46	0.51
2:S:144:LEU:HD12	2:S:144:LEU:H	1.75	0.51
2:C:70:LEU:HG	2:C:71:GLU:H	1.75	0.50
2:N:141:ARG:HB2	2:N:152:LEU:HD12	1.93	0.50
2:W:104:LEU:H	2:W:104:LEU:HD23	1.77	0.50
1:o:128:LYS:HZ2	2:O:116:PHE:CB	2.20	0.49
2:W:61:VAL:H	2:W:62:PRO:HD3	1.76	0.49
2:M:63:GLN:HE22	2:M:66:LEU:HD22	1.78	0.49
2:M:143:ASP:HB3	2:M:152:LEU:HD11	1.95	0.48
2:S:59:GLN:HE22	1:u:123:ASN:HD21	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:80:TYR:CE2	2:W:147:GLY:O	2.38	0.48
1:e:27:MET:H	1:e:28:SER:CA	2.27	0.48
2:L:74:HIS:CD2	2:L:80:TYR:OH	2.67	0.48
2:J:93:GLU:HB3	2:V:94:ALA:HB3	1.96	0.47
1:n:42:HIS:HE1	1:n:91:PHE:CD2	2.22	0.47
1:s:158:ARG:HE	1:u:161:PRO:HD3	1.78	0.47
1:r:105:TYR:CZ	2:R:168:LYS:HB2	2.49	0.47
1:e:134:PRO:HG3	1:e:138:HIS:CE1	2.50	0.47
2:A:105:SER:HA	2:E:105:SER:HB3	1.97	0.47
2:B:95:HIS:CD2	2:B:98:CYS:HB2	2.49	0.47
1:u:137:LEU:HD22	1:u:137:LEU:H	1.79	0.47
2:L:80:TYR:CE2	2:L:148:GLU:CA	2.96	0.46
2:S:145:LEU:HD22	2:U:151:SER:HB3	1.95	0.46
1:o:31:THR:HA	1:o:34:LEU:HG	1.98	0.46
1:r:105:TYR:O	1:r:108:GLU:HB3	2.14	0.46
1:j:33:ARG:HH21	2:J:170:ILE:HG12	1.80	0.46
1:o:130:LEU:N	1:o:130:LEU:CD2	2.76	0.46
2:R:141:ARG:HE	2:R:152:LEU:HD12	1.81	0.45
1:n:42:HIS:NE2	1:n:104:SER:CB	2.79	0.45
1:o:33:ARG:HH22	2:O:94:ALA:CB	2.19	0.45
1:w:47:ARG:HE	1:w:47:ARG:HA	1.82	0.45
1:e:38:LYS:H	1:e:38:LYS:HD2	1.80	0.45
2:T:110:THR:HG22	2:T:121:ILE:H	1.80	0.45
1:b:26:HIS:CE1	2:O:116:PHE:HZ	2.33	0.45
1:o:33:ARG:CZ	2:O:95:HIS:CD2	2.98	0.45
2:W:76:GLU:O	2:W:80:TYR:CD2	2.70	0.45
2:G:113:ILE:H	2:G:114:PRO:HD3	1.82	0.45
1:r:141:MET:HE3	1:r:141:MET:H	1.82	0.45
2:R:96:PRO:HG2	2:R:99:ILE:H	1.82	0.45
2:U:102:VAL:HG23	2:U:112:GLU:H	1.82	0.45
2:W:80:TYR:O	2:W:84:LEU:CB	2.63	0.45
2:F:75:GLU:HB3	2:F:80:TYR:H	1.81	0.45
1:n:38:LYS:C	1:n:42:HIS:HD2	2.19	0.44
1:l:118:ALA:HB1	1:l:151:ILE:HG21	1.98	0.44
2:N:76:GLU:CD	2:N:76:GLU:H	2.24	0.44
1:i:38:LYS:H	1:i:38:LYS:HD3	1.82	0.44
2:S:99:ILE:H	2:X:89:GLU:HG2	1.82	0.44
2:V:74:HIS:CE1	2:V:83:HIS:CD2	3.06	0.44
2:K:88:LEU:HB2	2:K:166:VAL:HB	2.00	0.44
2:S:152:LEU:HD21	2:U:153:ARG:HH21	1.83	0.44
2:B:73:ALA:H	1:o:134:PRO:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:76:GLU:CD	2:I:76:GLU:H	2.25	0.43
2:W:61:VAL:H	2:W:62:PRO:CD	2.30	0.43
2:H:92:SER:HA	2:H:102:VAL:H	1.83	0.43
1:w:106:MET:HE2	1:w:121:ILE:HG21	2.00	0.43
1:n:47:ARG:CZ	1:n:91:PHE:CD1	2.98	0.43
1:n:47:ARG:CZ	1:n:91:PHE:CE2	2.94	0.43
1:r:105:TYR:OH	2:R:168:LYS:CB	2.67	0.43
2:D:158:LEU:H	2:D:158:LEU:HD23	1.84	0.43
2:J:92:SER:O	2:J:99:ILE:HD13	2.19	0.43
2:S:75:GLU:N	2:S:76:GLU:HA	2.34	0.43
1:b:43:TYR:HA	1:b:47:ARG:HH12	1.84	0.42
2:S:60:VAL:HG12	1:u:142:LEU:HB3	2.00	0.42
2:P:103:GLU:HG3	2:P:105:SER:H	1.85	0.42
2:K:113:ILE:HD12	2:K:116:PHE:HB2	2.01	0.42
2:L:80:TYR:CE2	2:L:148:GLU:CG	2.92	0.42
1:t:59:VAL:HG11	1:t:79:VAL:H	1.84	0.42
1:e:62:GLY:H	1:e:76:GLN:HG2	1.84	0.42
2:L:80:TYR:OH	2:L:148:GLU:OE1	2.37	0.42
2:E:75:GLU:N	2:E:76:GLU:HA	2.35	0.42
2:I:77:ALA:HA	2:I:80:TYR:CD2	2.54	0.42
1:q:33:ARG:HH12	2:Q:95:HIS:CG	2.37	0.42
1:l:138:HIS:CD2	1:l:139:CYS:H	2.37	0.42
2:G:99:ILE:HD12	2:G:99:ILE:HA	2.01	0.42
1:k:161:PRO:HD3	1:l:158:ARG:HE	1.84	0.42
2:T:75:GLU:N	2:T:76:GLU:HA	2.35	0.42
2:L:158:LEU:HD23	2:L:158:LEU:H	1.85	0.42
2:N:80:TYR:HE1	2:N:148:GLU:HG2	1.70	0.42
1:v:88:ASP:HB3	1:v:90:LYS:HZ2	1.85	0.42
2:R:116:PHE:CZ	1:u:26:HIS:CD2	3.08	0.42
1:n:42:HIS:NE2	1:n:104:SER:CA	2.83	0.41
2:H:75:GLU:H	2:H:79:ASP:HB2	1.85	0.41
1:g:27:MET:H	1:g:28:SER:HA	1.85	0.41
1:w:152:LYS:HD3	2:X:71:GLU:H	1.85	0.41
2:M:153:ARG:HD2	2:N:80:TYR:CZ	2.55	0.41
1:o:128:LYS:O	1:o:131:SER:O	2.38	0.41
2:Q:113:ILE:HB	2:Q:116:PHE:CD1	2.55	0.41
2:V:93:GLU:O	2:V:95:HIS:CE1	2.73	0.41
2:E:113:ILE:HD12	2:E:116:PHE:HB3	2.03	0.41
2:N:81:LEU:O	2:N:84:LEU:HB3	2.21	0.41
1:o:31:THR:CB	1:o:34:LEU:HD12	2.50	0.41
2:S:145:LEU:HD23	2:U:153:ARG:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:158:ARG:HE	1:f:161:PRO:HD3	1.85	0.41
2:L:75:GLU:H	2:L:76:GLU:CA	2.27	0.41
1:q:136:LYS:HD3	1:q:136:LYS:H	1.86	0.41
1:t:27:MET:H	1:t:28:SER:HA	1.86	0.41
2:N:95:HIS:CE1	2:P:98:CYS:HB3	2.56	0.41
1:p:56:LEU:HB2	1:p:57:PRO:HD3	2.03	0.41
2:H:109:MET:HB3	2:H:121:ILE:H	1.86	0.41
2:U:130:ILE:HD12	2:U:149:TRP:CE3	2.56	0.41
1:n:43:TYR:C	1:n:45:HIS:N	2.79	0.40
1:k:27:MET:H	1:k:28:SER:CA	2.34	0.40
2:O:113:ILE:HG22	2:O:116:PHE:CE2	2.38	0.40
1:b:64:VAL:HG12	1:b:146:ALA:HB2	2.02	0.40
2:B:144:LEU:HD12	2:B:144:LEU:H	1.86	0.40
1:f:27:MET:H	1:f:28:SER:HA	1.87	0.40
1:g:131:SER:HA	1:g:132:LEU:HB2	2.02	0.40
2:C:145:LEU:HD12	2:C:145:LEU:HA	1.99	0.40
1:r:64:VAL:HG12	1:r:146:ALA:HB2	2.02	0.40
2:A:75:GLU:H	2:A:76:GLU:HA	1.87	0.40
1:g:130:LEU:HB3	1:g:141:MET:HE2	2.04	0.40
1:n:47:ARG:HA	1:n:48:ASN:HA	1.77	0.40
1:w:84:GLY:HA2	1:w:158:ARG:HH22	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	140/142 (99%)	124 (89%)	11 (8%)	5 (4%)	2	20
1	b	140/142 (99%)	120 (86%)	17 (12%)	3 (2%)	5	30
1	c	140/142 (99%)	119 (85%)	15 (11%)	6 (4%)	2	17
1	d	140/142 (99%)	123 (88%)	16 (11%)	1 (1%)	18	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	e	140/142 (99%)	117 (84%)	18 (13%)	5 (4%)	2	20
1	f	140/142 (99%)	118 (84%)	18 (13%)	4 (3%)	3	23
1	g	140/142 (99%)	121 (86%)	13 (9%)	6 (4%)	2	17
1	h	140/142 (99%)	116 (83%)	19 (14%)	5 (4%)	2	20
1	i	140/142 (99%)	122 (87%)	12 (9%)	6 (4%)	2	17
1	j	140/142 (99%)	123 (88%)	12 (9%)	5 (4%)	2	20
1	k	140/142 (99%)	119 (85%)	14 (10%)	7 (5%)	1	16
1	l	140/142 (99%)	119 (85%)	13 (9%)	8 (6%)	1	14
1	m	140/142 (99%)	126 (90%)	10 (7%)	4 (3%)	3	23
1	n	140/142 (99%)	127 (91%)	9 (6%)	4 (3%)	3	23
1	o	140/142 (99%)	121 (86%)	16 (11%)	3 (2%)	5	30
1	p	140/142 (99%)	123 (88%)	10 (7%)	7 (5%)	1	16
1	q	140/142 (99%)	121 (86%)	12 (9%)	7 (5%)	1	16
1	r	140/142 (99%)	120 (86%)	15 (11%)	5 (4%)	2	20
1	s	140/142 (99%)	124 (89%)	13 (9%)	3 (2%)	5	30
1	t	140/142 (99%)	118 (84%)	16 (11%)	6 (4%)	2	17
1	u	140/142 (99%)	127 (91%)	10 (7%)	3 (2%)	5	30
1	v	140/142 (99%)	127 (91%)	8 (6%)	5 (4%)	2	20
1	w	140/142 (99%)	127 (91%)	11 (8%)	2 (1%)	9	40
1	x	140/142 (99%)	116 (83%)	19 (14%)	5 (4%)	2	20
2	A	119/121 (98%)	89 (75%)	15 (13%)	15 (13%)	0	4
2	B	119/121 (98%)	89 (75%)	21 (18%)	9 (8%)	1	10
2	C	119/121 (98%)	96 (81%)	12 (10%)	11 (9%)	0	8
2	D	119/121 (98%)	83 (70%)	21 (18%)	15 (13%)	0	4
2	E	119/121 (98%)	95 (80%)	14 (12%)	10 (8%)	0	9
2	F	119/121 (98%)	88 (74%)	23 (19%)	8 (7%)	1	12
2	G	119/121 (98%)	87 (73%)	15 (13%)	17 (14%)	0	3
2	H	119/121 (98%)	94 (79%)	13 (11%)	12 (10%)	0	7
2	I	119/121 (98%)	87 (73%)	24 (20%)	8 (7%)	1	12
2	J	119/121 (98%)	88 (74%)	18 (15%)	13 (11%)	0	6
2	K	119/121 (98%)	93 (78%)	13 (11%)	13 (11%)	0	6

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

All (356) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	47	ARG
1	a	66	ALA
2	A	59	GLN
2	A	93	GLU
2	A	94	ALA
1	b	132	LEU
2	C	100	PRO
2	C	102	VAL
2	D	75	GLU
2	D	98	CYS
2	E	94	ALA
2	E	98	CYS
1	f	121	ILE
2	F	82	ASP
2	F	97	ASP
2	F	127	ASN
1	g	51	SER
2	G	99	ILE
2	G	100	PRO

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Mol	Chain	Res	Type
2	G	127	ASN
2	G	154	ASN
1	h	25	SER
1	h	68	ALA
2	H	92	SER
2	H	98	CYS
1	i	120	LYS
1	i	134	PRO
2	I	127	ASN
2	J	64	GLU
2	J	127	ASN
2	K	96	PRO
2	K	100	PRO
2	K	115	ALA
2	K	154	ASN
2	L	125	PRO
2	L	130	ILE
2	M	63	GLN
1	n	132	LEU
2	N	61	VAL
2	N	98	CYS
1	o	46	PRO
2	O	94	ALA
2	O	127	ASN
2	P	59	GLN
2	P	75	GLU
2	P	127	ASN
1	q	47	ARG
2	Q	72	LYS
1	r	46	PRO
2	R	77	ALA
2	R	94	ALA
2	S	127	ASN
1	t	137	LEU
1	t	143	ALA
2	T	98	CYS
2	T	127	ASN
2	U	102	VAL
2	U	154	ASN
1	v	162	THR
2	V	94	ALA
2	V	98	CYS

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Mol	Chain	Res	Type
2	V	127	ASN
2	V	130	ILE
1	w	140	SER
2	W	55	SER
2	W	127	ASN
2	X	94	ALA
2	X	100	PRO
2	X	127	ASN
2	A	62	PRO
2	A	92	SER
2	A	98	CYS
2	A	127	ASN
1	b	159	ASN
2	B	101	ASP
2	B	115	ALA
2	B	154	ASN
1	c	137	LEU
2	C	56	THR
2	C	130	ILE
2	D	57	ASP
2	D	101	ASP
2	D	127	ASN
2	D	130	ILE
1	e	143	ALA
2	E	62	PRO
2	E	92	SER
2	E	127	ASN
1	f	134	PRO
2	F	94	ALA
2	F	130	ILE
2	G	60	VAL
2	G	95	HIS
2	G	115	ALA
2	H	65	VAL
2	H	86	ASP
2	H	94	ALA
2	H	127	ASN
2	H	154	ASN
2	I	59	GLN
2	I	65	VAL
2	I	130	ILE
1	j	133	PRO

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Mol	Chain	Res	Type
1	j	142	LEU
2	J	65	VAL
2	J	73	ALA
2	J	77	ALA
2	J	79	ASP
2	J	80	TYR
2	J	94	ALA
1	k	34	LEU
1	k	35	TYR
1	k	134	PRO
1	k	137	LEU
1	k	159	ASN
2	K	130	ILE
1	l	47	ARG
2	L	98	CYS
2	L	145	LEU
1	m	134	PRO
2	M	73	ALA
2	M	127	ASN
2	M	130	ILE
1	n	44	THR
2	N	63	GLN
2	N	127	ASN
2	N	130	ILE
1	o	159	ASN
1	p	30	ILE
1	p	120	LYS
2	P	65	VAL
2	P	79	ASP
2	P	130	ILE
1	q	32	LYS
1	q	159	ASN
2	Q	127	ASN
2	Q	154	ASN
2	R	127	ASN
2	R	130	ILE
1	s	116	ASP
2	S	130	ILE
2	S	145	LEU
1	t	34	LEU
1	t	134	PRO
2	T	65	VAL

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Mol	Chain	Res	Type
2	T	154	ASN
1	u	134	PRO
1	u	143	ALA
2	U	104	LEU
2	U	127	ASN
1	v	159	ASN
2	W	63	GLN
2	W	65	VAL
2	W	76	GLU
2	W	130	ILE
1	x	68	ALA
1	x	159	ASN
2	X	98	CYS
2	X	130	ILE
1	a	134	PRO
2	A	64	GLU
2	A	100	PRO
2	A	158	LEU
1	b	135	VAL
2	B	127	ASN
2	B	143	ASP
1	c	159	ASN
2	C	64	GLU
2	D	90	GLU
1	e	46	PRO
1	e	159	ASN
1	e	161	PRO
1	f	46	PRO
1	g	48	ASN
1	g	134	PRO
2	G	57	ASP
2	G	63	GLN
2	G	96	PRO
2	G	107	GLY
2	G	130	ILE
2	H	63	GLN
2	H	115	ALA
1	i	131	SER
1	i	135	VAL
2	I	62	PRO
2	I	97	ASP
2	I	100	PRO

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Mol	Chain	Res	Type
2	I	154	ASN
1	j	114	THR
1	j	159	ASN
2	J	130	ILE
2	J	154	ASN
2	K	70	LEU
2	K	92	SER
2	K	94	ALA
2	K	147	GLY
2	K	169	ALA
1	l	46	PRO
1	l	55	LYS
1	l	137	LEU
2	L	73	ALA
1	m	159	ASN
1	n	161	PRO
2	N	115	ALA
2	N	145	LEU
2	O	130	ILE
1	p	121	ILE
1	p	134	PRO
1	p	159	ASN
2	P	81	LEU
1	q	114	THR
2	Q	92	SER
1	r	120	LYS
1	s	55	LYS
2	S	57	ASP
2	S	67	ASN
2	S	98	CYS
1	t	135	VAL
1	t	141	MET
2	T	130	ILE
2	U	98	CYS
2	U	101	ASP
2	U	107	GLY
2	U	130	ILE
2	V	90	GLU
2	V	114	PRO
2	W	61	VAL
2	W	75	GLU
1	x	134	PRO

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Mol	Chain	Res	Type
1	x	138	HIS
2	X	97	ASP
2	A	130	ILE
2	B	63	GLN
2	B	94	ALA
2	B	130	ILE
2	C	96	PRO
2	C	115	ALA
2	C	145	LEU
2	D	100	PRO
2	D	135	PRO
2	E	70	LEU
2	E	72	LYS
2	E	130	ILE
1	f	66	ALA
2	F	62	PRO
2	G	113	ILE
1	h	137	LEU
2	H	130	ILE
1	j	134	PRO
1	l	129	GLU
1	l	161	PRO
1	m	138	HIS
2	M	64	GLU
2	M	66	LEU
2	P	96	PRO
2	Q	90	GLU
1	r	161	PRO
2	S	99	ILE
2	S	144	LEU
2	U	66	LEU
2	U	75	GLU
2	U	97	ASP
2	U	144	LEU
1	v	134	PRO
2	V	99	ILE
2	V	100	PRO
2	W	54	SER
2	W	154	ASN
1	a	121	ILE
2	A	101	ASP
1	c	99	ALA

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Mol	Chain	Res	Type
1	c	134	PRO
2	C	99	ILE
2	C	154	ASN
2	D	61	VAL
2	D	99	ILE
2	D	136	LEU
2	E	154	ASN
2	F	101	ASP
1	g	161	PRO
1	h	134	PRO
1	h	161	PRO
2	H	89	GLU
2	H	137	SER
2	J	63	GLN
1	k	161	PRO
2	K	65	VAL
2	L	92	SER
2	L	95	HIS
1	n	25	SER
1	o	114	THR
2	O	100	PRO
2	P	99	ILE
2	Q	130	ILE
1	r	134	PRO
1	s	46	PRO
2	S	100	PRO
1	u	131	SER
2	U	61	VAL
2	U	85	LEU
2	U	87	SER
1	v	46	PRO
1	v	132	LEU
2	V	63	GLN
2	W	94	ALA
1	x	120	LYS
2	X	106	HIS
2	A	65	VAL
2	A	126	PRO
2	A	154	ASN
1	c	32	LYS
2	C	63	GLN
2	D	96	PRO

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Mol	Chain	Res	Type
2	D	137	SER
1	e	134	PRO
2	F	136	LEU
2	G	54	SER
2	G	158	LEU
1	l	138	HIS
1	l	139	CYS
1	q	30	ILE
1	q	59	VAL
2	S	61	VAL
2	S	62	PRO
2	S	96	PRO
2	W	53	GLU
2	X	89	GLU
1	d	46	PRO
1	g	46	PRO
2	K	61	VAL
1	r	133	PRO
2	U	134	SER
2	E	102	VAL
1	i	46	PRO
2	J	100	PRO
2	K	60	VAL
2	L	126	PRO
1	m	161	PRO
2	V	96	PRO
1	a	67	PRO
1	c	161	PRO
1	g	132	LEU
2	G	65	VAL
2	J	61	VAL
2	O	114	PRO
1	p	66	ALA
1	q	134	PRO
1	w	160	THR
2	D	139	PRO
1	p	132	LEU
2	R	100	PRO
2	B	61	VAL
2	G	61	VAL
1	i	133	PRO
1	k	135	VAL

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Mol	Chain	Res	Type
2	L	96	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	121/121 (100%)	116 (96%)	5 (4%)	27	49
1	b	121/121 (100%)	117 (97%)	4 (3%)	33	55
1	c	121/121 (100%)	113 (93%)	8 (7%)	15	37
1	d	121/121 (100%)	119 (98%)	2 (2%)	53	69
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%)	119 (98%)	2 (2%)	53	69
1	h	121/121 (100%)	115 (95%)	6 (5%)	22	43
1	i	121/121 (100%)	116 (96%)	5 (4%)	27	49
1	j	121/121 (100%)	116 (96%)	5 (4%)	27	49
1	k	121/121 (100%)	116 (96%)	5 (4%)	27	49
1	l	121/121 (100%)	117 (97%)	4 (3%)	33	55
1	m	121/121 (100%)	117 (97%)	4 (3%)	33	55
1	n	121/121 (100%)	117 (97%)	4 (3%)	33	55
1	o	121/121 (100%)	116 (96%)	5 (4%)	27	49
1	p	121/121 (100%)	113 (93%)	8 (7%)	15	37
1	q	121/121 (100%)	118 (98%)	3 (2%)	42	63
1	r	121/121 (100%)	115 (95%)	6 (5%)	22	43
1	s	121/121 (100%)	117 (97%)	4 (3%)	33	55
1	t	121/121 (100%)	112 (93%)	9 (7%)	13	33
1	u	121/121 (100%)	116 (96%)	5 (4%)	27	49
1	v	121/121 (100%)	118 (98%)	3 (2%)	42	63
1	w	121/121 (100%)	116 (96%)	5 (4%)	27	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	x	121/121 (100%)	114 (94%)	7 (6%)	18	40
2	A	109/109 (100%)	100 (92%)	9 (8%)	10	30
2	B	109/109 (100%)	106 (97%)	3 (3%)	38	60
2	C	109/109 (100%)	103 (94%)	6 (6%)	19	41
2	D	109/109 (100%)	104 (95%)	5 (5%)	24	45
2	E	109/109 (100%)	104 (95%)	5 (5%)	24	45
2	F	109/109 (100%)	103 (94%)	6 (6%)	19	41
2	G	109/109 (100%)	105 (96%)	4 (4%)	30	51
2	H	109/109 (100%)	104 (95%)	5 (5%)	24	45
2	I	109/109 (100%)	107 (98%)	2 (2%)	51	68
2	J	109/109 (100%)	106 (97%)	3 (3%)	38	60
2	K	109/109 (100%)	101 (93%)	8 (7%)	13	34
2	L	109/109 (100%)	105 (96%)	4 (4%)	30	51
2	M	109/109 (100%)	107 (98%)	2 (2%)	51	68
2	N	109/109 (100%)	99 (91%)	10 (9%)	8	27
2	O	109/109 (100%)	104 (95%)	5 (5%)	24	45
2	P	109/109 (100%)	105 (96%)	4 (4%)	30	51
2	Q	109/109 (100%)	103 (94%)	6 (6%)	19	41
2	R	109/109 (100%)	107 (98%)	2 (2%)	51	68
2	S	109/109 (100%)	105 (96%)	4 (4%)	30	51
2	T	109/109 (100%)	102 (94%)	7 (6%)	16	37
2	U	109/109 (100%)	103 (94%)	6 (6%)	19	41
2	V	109/109 (100%)	103 (94%)	6 (6%)	19	41
2	W	109/109 (100%)	105 (96%)	4 (4%)	30	51
2	X	109/109 (100%)	106 (97%)	3 (3%)	38	60
All	All	5520/5520 (100%)	5285 (96%)	235 (4%)	27	47

All (235) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	30	ILE
1	a	45	HIS
1	a	89	VAL

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Mol	Chain	Res	Type
1	a	90	LYS
1	a	144	GLU
2	A	64	GLU
2	A	76	GLU
2	A	89	GLU
2	A	99	ILE
2	A	113	ILE
2	A	126	PRO
2	A	128	LYS
2	A	157	LYS
2	A	158	LEU
1	b	30	ILE
1	b	57	PRO
1	b	90	LYS
1	b	141	MET
2	B	95	HIS
2	B	148	GLU
2	B	157	LYS
1	c	32	LYS
1	c	89	VAL
1	c	90	LYS
1	c	132	LEU
1	c	136	LYS
1	c	137	LEU
1	c	141	MET
1	c	144	GLU
2	C	61	VAL
2	C	93	GLU
2	C	128	LYS
2	C	136	LEU
2	C	144	LEU
2	C	170	ILE
1	d	52	LEU
1	d	89	VAL
2	D	53	GLU
2	D	75	GLU
2	D	76	GLU
2	D	93	GLU
2	D	95	HIS
1	e	81	ASP
1	e	129	GLU
1	e	164	LEU

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Mol	Chain	Res	Type
2	E	76	GLU
2	E	86	ASP
2	E	113	ILE
2	E	144	LEU
2	E	157	LYS
1	f	105	TYR
1	f	130	LEU
1	f	136	LYS
1	f	144	GLU
2	F	75	GLU
2	F	76	GLU
2	F	91	LEU
2	F	128	LYS
2	F	145	LEU
2	F	166	VAL
1	g	106	MET
1	g	144	GLU
2	G	99	ILE
2	G	131	TRP
2	G	152	LEU
2	G	157	LYS
1	h	30	ILE
1	h	77	ILE
1	h	89	VAL
1	h	90	LYS
1	h	132	LEU
1	h	141	MET
2	H	64	GLU
2	H	76	GLU
2	H	79	ASP
2	H	156	THR
2	H	157	LYS
1	i	89	VAL
1	i	123	ASN
1	i	126	ILE
1	i	135	VAL
1	i	141	MET
2	I	134	SER
2	I	144	LEU
1	j	45	HIS
1	j	57	PRO
1	j	89	VAL

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Mol	Chain	Res	Type
1	j	120	LYS
1	j	135	VAL
2	J	72	LYS
2	J	89	GLU
2	J	157	LYS
1	k	47	ARG
1	k	89	VAL
1	k	121	ILE
1	k	130	LEU
1	k	141	MET
2	K	84	LEU
2	K	88	LEU
2	K	90	GLU
2	K	113	ILE
2	K	128	LYS
2	K	144	LEU
2	K	156	THR
2	K	157	LYS
1	l	52	LEU
1	l	89	VAL
1	l	141	MET
1	l	144	GLU
2	L	68	LEU
2	L	93	GLU
2	L	125	PRO
2	L	157	LYS
1	m	47	ARG
1	m	89	VAL
1	m	135	VAL
1	m	136	LYS
2	M	85	LEU
2	M	154	ASN
1	n	56	LEU
1	n	106	MET
1	n	130	LEU
1	n	141	MET
2	N	75	GLU
2	N	76	GLU
2	N	85	LEU
2	N	88	LEU
2	N	93	GLU
2	N	125	PRO

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Mol	Chain	Res	Type
2	N	144	LEU
2	N	154	ASN
2	N	157	LYS
2	N	172	LYS
1	o	64	VAL
1	o	89	VAL
1	o	130	LEU
1	o	141	MET
1	o	144	GLU
2	O	80	TYR
2	O	104	LEU
2	O	137	SER
2	O	157	LYS
2	O	166	VAL
1	p	26	HIS
1	p	30	ILE
1	p	45	HIS
1	p	57	PRO
1	p	89	VAL
1	p	90	LYS
1	p	106	MET
1	p	148	LYS
2	P	76	GLU
2	P	102	VAL
2	P	128	LYS
2	P	172	LYS
1	q	89	VAL
1	q	125	GLU
1	q	141	MET
2	Q	60	VAL
2	Q	61	VAL
2	Q	116	PHE
2	Q	125	PRO
2	Q	144	LEU
2	Q	157	LYS
1	r	33	ARG
1	r	52	LEU
1	r	89	VAL
1	r	121	ILE
1	r	141	MET
1	r	144	GLU
2	R	67	ASN

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Mol	Chain	Res	Type
2	R	76	GLU
1	s	56	LEU
1	s	89	VAL
1	s	90	LYS
1	s	110	VAL
2	S	113	ILE
2	S	145	LEU
2	S	158	LEU
2	S	172	LYS
1	t	34	LEU
1	t	45	HIS
1	t	89	VAL
1	t	90	LYS
1	t	121	ILE
1	t	135	VAL
1	t	136	LYS
1	t	137	LEU
1	t	141	MET
2	T	61	VAL
2	T	64	GLU
2	T	76	GLU
2	T	113	ILE
2	T	142	PHE
2	T	153	ARG
2	T	157	LYS
1	u	47	ARG
1	u	89	VAL
1	u	135	VAL
1	u	141	MET
1	u	144	GLU
2	U	64	GLU
2	U	65	VAL
2	U	91	LEU
2	U	99	ILE
2	U	150	VAL
2	U	157	LYS
1	v	89	VAL
1	v	90	LYS
1	v	106	MET
2	V	59	GLN
2	V	95	HIS
2	V	130	ILE

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Mol	Chain	Res	Type
2	V	142	PHE
2	V	157	LYS
2	V	158	LEU
1	w	30	ILE
1	w	47	ARG
1	w	90	LYS
1	w	121	ILE
1	w	139	CYS
2	W	108	VAL
2	W	128	LYS
2	W	157	LYS
2	W	158	LEU
1	x	47	ARG
1	x	86	ILE
1	x	121	ILE
1	x	130	LEU
1	x	138	HIS
1	x	141	MET
1	x	144	GLU
2	X	114	PRO
2	X	144	LEU
2	X	152	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (180) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	26	HIS
1	a	42	HIS
1	a	123	ASN
2	A	59	GLN
2	A	74	HIS
2	A	122	ASN
1	b	26	HIS
1	b	42	HIS
1	b	80	ASN
2	B	124	GLN
2	B	127	ASN
1	c	26	HIS
1	c	36	HIS
1	c	138	HIS
1	c	159	ASN
2	C	83	HIS

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Mol	Chain	Res	Type
2	C	106	HIS
2	C	122	ASN
2	C	127	ASN
1	d	26	HIS
1	d	36	HIS
1	d	42	HIS
1	d	45	HIS
1	d	80	ASN
1	d	123	ASN
2	D	59	GLN
2	D	63	GLN
2	D	67	ASN
2	D	140	ASN
1	e	45	HIS
1	e	48	ASN
1	e	58	ASN
1	e	80	ASN
1	e	138	HIS
2	E	63	GLN
2	E	127	ASN
2	E	129	GLN
1	f	26	HIS
1	f	45	HIS
1	f	48	ASN
1	f	123	ASN
1	f	138	HIS
2	F	83	HIS
2	F	95	HIS
2	F	106	HIS
2	F	122	ASN
2	F	146	ASN
1	g	42	HIS
1	g	45	HIS
1	g	48	ASN
1	g	76	GLN
1	g	111	GLN
2	G	74	HIS
2	G	146	ASN
1	h	26	HIS
1	h	42	HIS
1	h	111	GLN
1	h	138	HIS

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Mol	Chain	Res	Type
2	H	95	HIS
1	i	26	HIS
1	i	48	ASN
1	i	76	GLN
1	i	159	ASN
2	I	95	HIS
2	I	129	GLN
2	I	140	ASN
2	I	154	ASN
1	j	26	HIS
1	j	76	GLN
1	j	111	GLN
2	J	67	ASN
2	J	74	HIS
2	J	146	ASN
1	k	48	ASN
1	k	58	ASN
1	l	45	HIS
1	l	48	ASN
1	l	80	ASN
1	l	111	GLN
1	l	138	HIS
2	L	74	HIS
2	L	83	HIS
2	L	106	HIS
2	L	122	ASN
2	L	127	ASN
2	L	140	ASN
2	L	154	ASN
1	m	45	HIS
1	m	58	ASN
1	m	111	GLN
2	M	63	GLN
2	M	67	ASN
2	M	95	HIS
2	M	106	HIS
2	M	124	GLN
1	n	42	HIS
1	n	111	GLN
2	N	59	GLN
2	N	67	ASN
2	N	95	HIS

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Mol	Chain	Res	Type
2	N	124	GLN
1	o	45	HIS
1	o	48	ASN
1	o	123	ASN
2	O	67	ASN
2	O	74	HIS
2	O	83	HIS
2	O	95	HIS
2	O	122	ASN
1	p	42	HIS
1	p	111	GLN
1	p	123	ASN
1	p	138	HIS
2	P	59	GLN
2	P	122	ASN
2	P	146	ASN
2	P	154	ASN
1	q	36	HIS
1	q	42	HIS
1	q	48	ASN
1	q	76	GLN
1	q	111	GLN
2	Q	74	HIS
2	Q	95	HIS
2	Q	124	GLN
1	r	26	HIS
1	r	45	HIS
1	r	48	ASN
1	r	76	GLN
1	r	111	GLN
1	r	123	ASN
1	r	138	HIS
2	R	59	GLN
2	R	106	HIS
2	R	154	ASN
1	s	42	HIS
1	s	45	HIS
1	s	111	GLN
2	S	83	HIS
2	S	122	ASN
2	S	129	GLN
2	S	140	ASN

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Mol	Chain	Res	Type
1	t	36	HIS
1	t	58	ASN
1	t	76	GLN
1	t	159	ASN
2	T	59	GLN
2	T	67	ASN
2	T	95	HIS
2	T	122	ASN
2	T	146	ASN
1	u	26	HIS
1	u	42	HIS
1	u	111	GLN
1	u	123	ASN
1	u	138	HIS
1	u	159	ASN
2	U	106	HIS
1	v	42	HIS
1	v	45	HIS
1	v	76	GLN
1	v	159	ASN
2	V	63	GLN
2	V	74	HIS
2	V	83	HIS
2	V	95	HIS
2	V	127	ASN
2	V	154	ASN
1	w	36	HIS
1	w	76	GLN
1	w	111	GLN
1	w	123	ASN
1	w	159	ASN
2	W	67	ASN
2	W	95	HIS
2	W	129	GLN
2	W	140	ASN
2	W	154	ASN
1	x	80	ASN
2	X	83	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8341. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 144



Y Index: 144



Z Index: 144

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 144



Y Index: 144

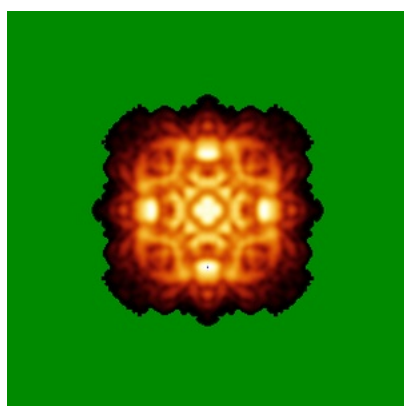


Z Index: 144

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

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

6.4.1 Primary map



X



Y

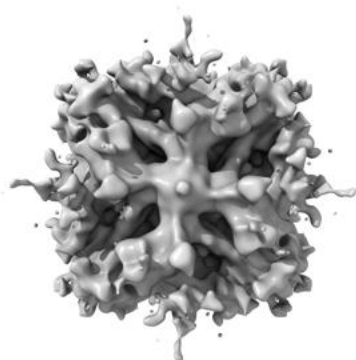


Z

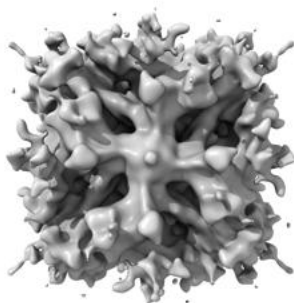
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

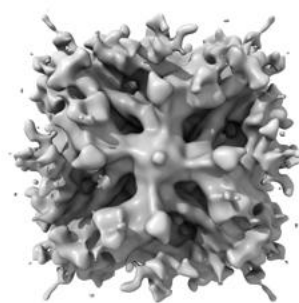
6.5.1 Primary map



X



Y



Z

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

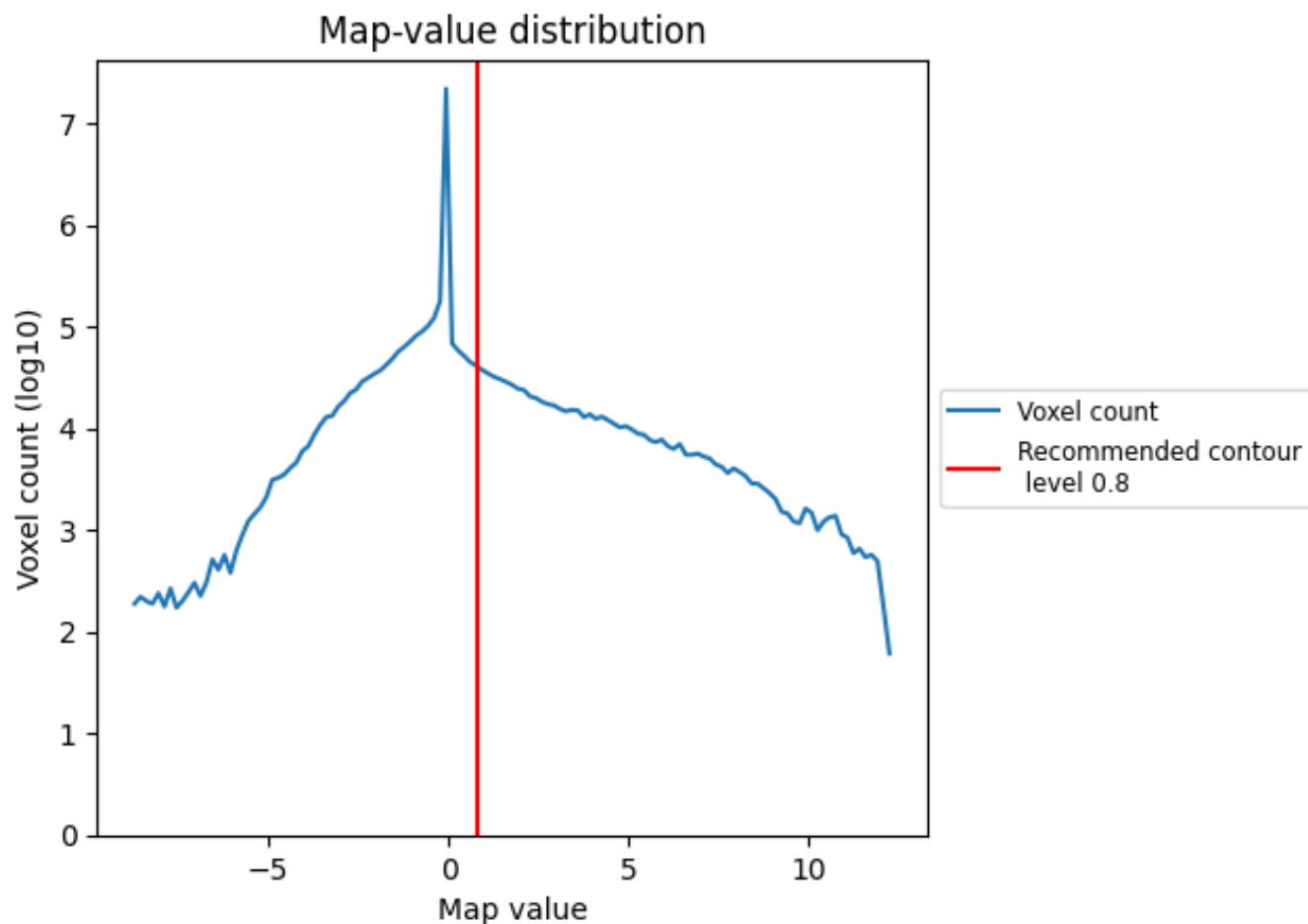
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

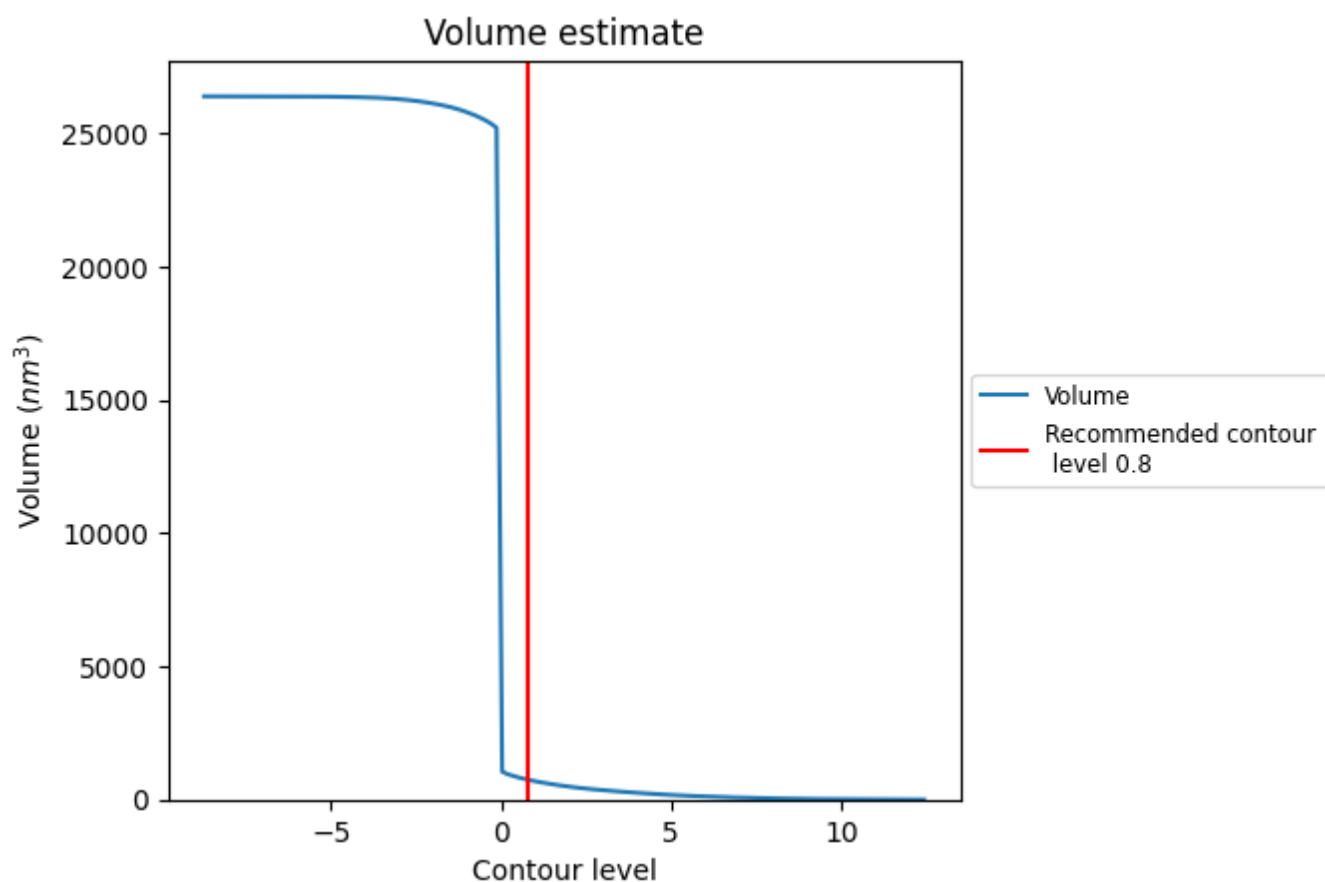
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

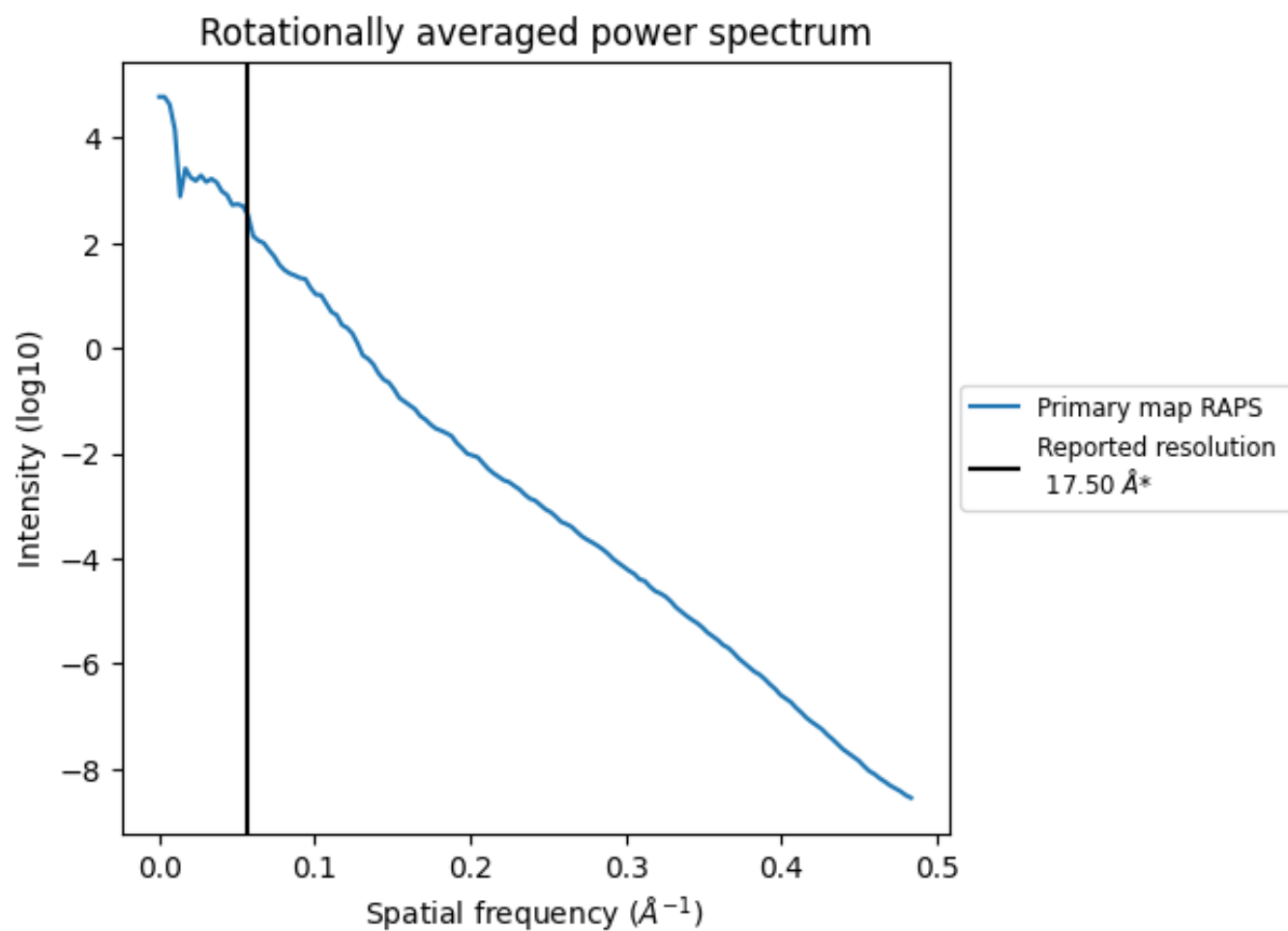
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 743 nm³; this corresponds to an approximate mass of 672 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

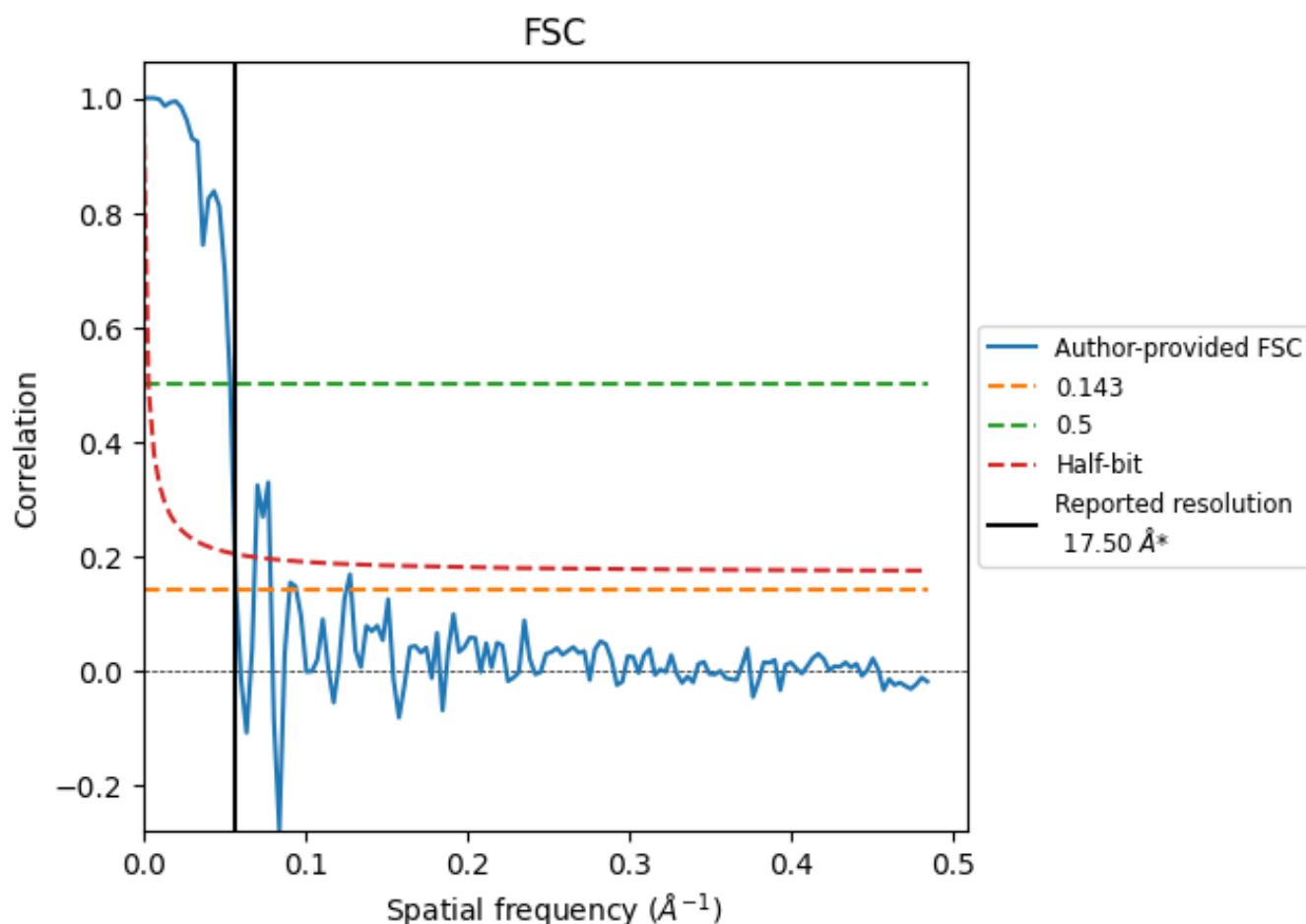


*Reported resolution corresponds to spatial frequency of 0.057 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.057 Å⁻¹

8.2 Resolution estimates [i](#)

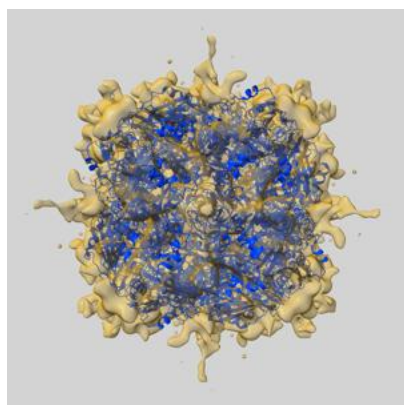
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	17.50	-	-
Author-provided FSC curve	17.45	18.59	17.67
Unmasked-calculated*	-	-	-

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

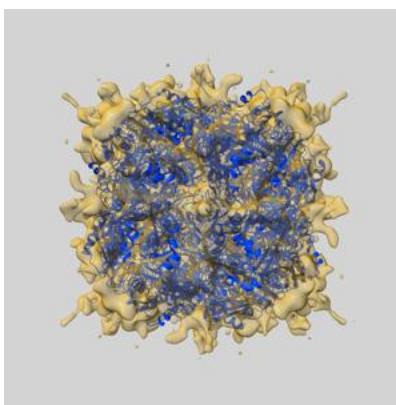
9 Map-model fit [i](#)

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

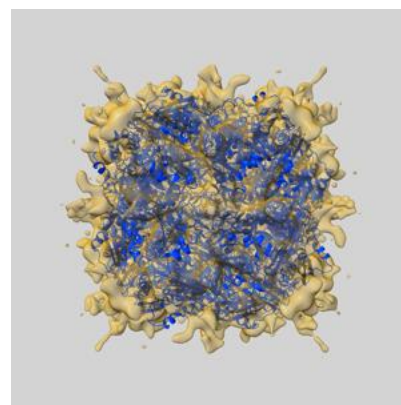
9.1 Map-model overlay [i](#)



X



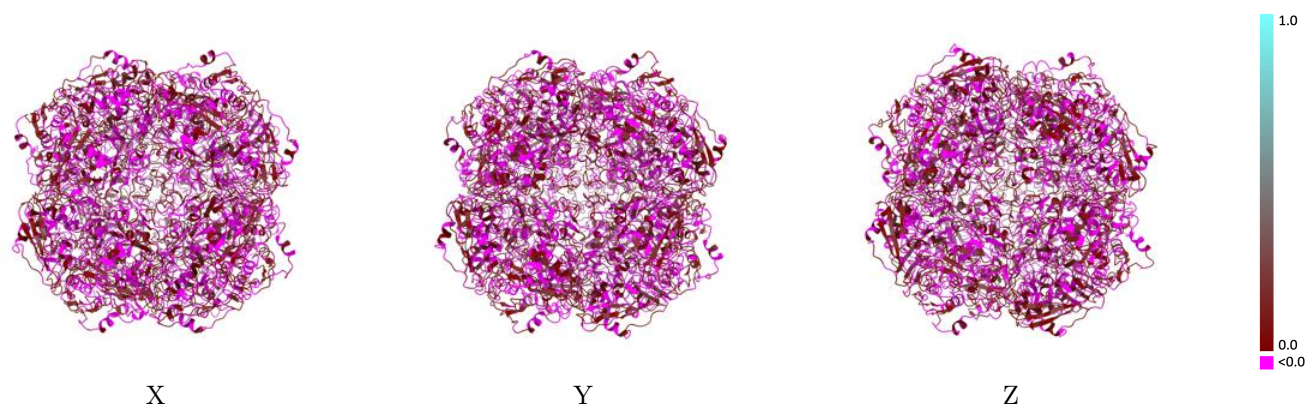
Y



Z

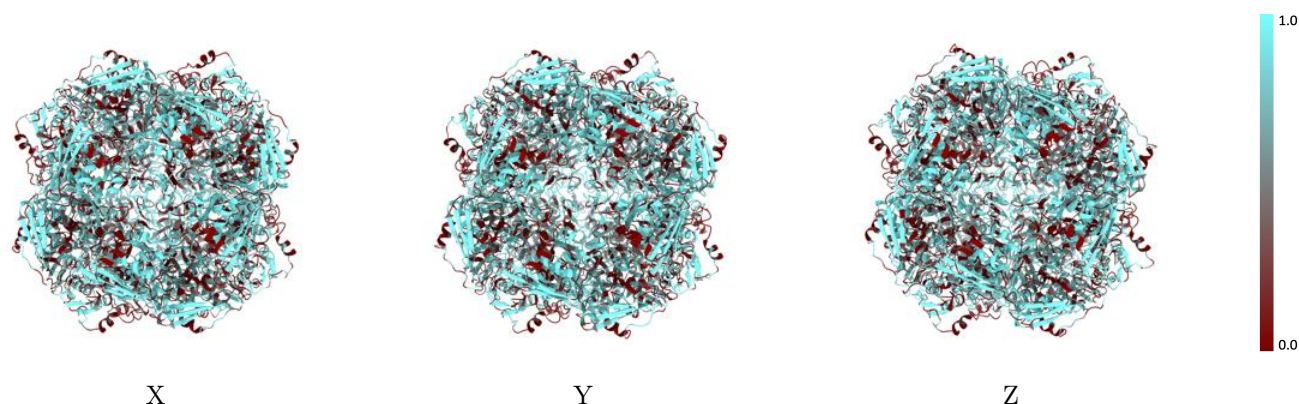
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



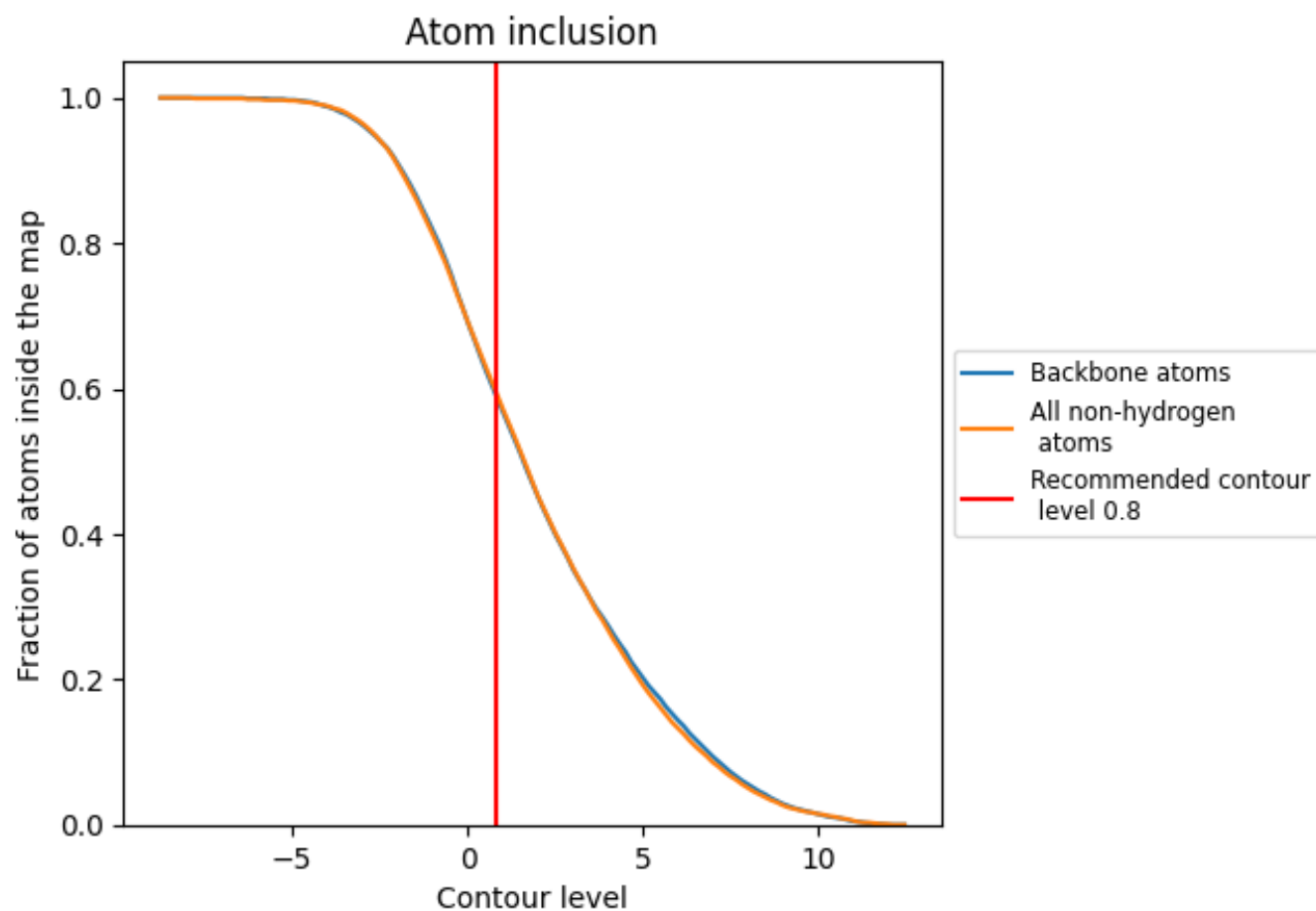
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.8).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

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

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



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