



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 3, 2017 – 06:57 AM EDT

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

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

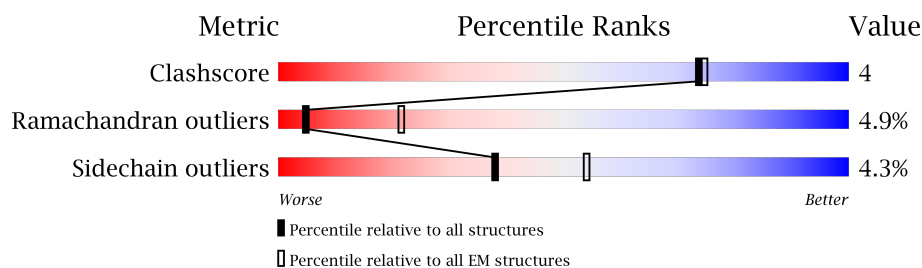
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 15.60 Å.

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







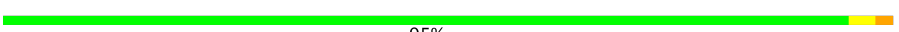







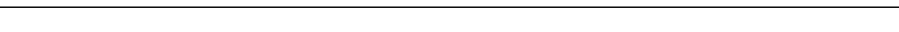

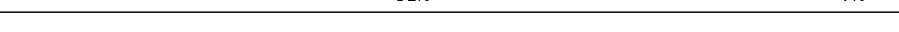

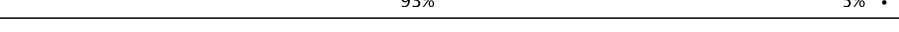








Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	a	142	92% 8%
1	b	142	92% 8%
1	c	142	91% 9%
1	d	142	89% 9% .
1	e	142	90% 8% .
1	f	142	93% 6% .
1	g	142	92% 7% .
1	h	142	85% 13% .
1	i	142	89% 10% .

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

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

2 Entry composition

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

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

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

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

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

There are 96 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

There are 24 discrepancies between the modelled and reference sequences:

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

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

3 Residue-property plots

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

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

Chain a: 



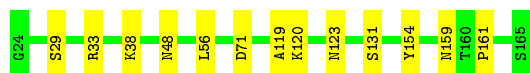
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain b: 



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

Chain c: 




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

Chain d: 



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

Chain e: 



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

Chain f: 



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

Chain g: 92% 7%



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

Chain h: 85% 13%



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

Chain i: 89% 10%



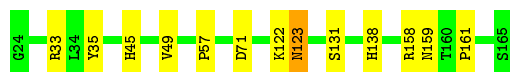
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain j: 87% 12%



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

Chain k: 91% 8%



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

Chain l: 89% 11%



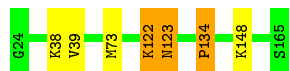
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain m: 89% 11%



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

Chain n:  95%




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

Chain o:  92%




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

Chain p:  87%




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

Chain q:  90%




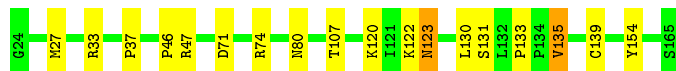
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain r:  89%



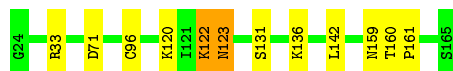
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain s:  87%




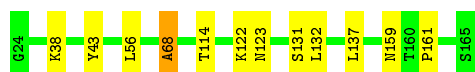
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain t:  92%



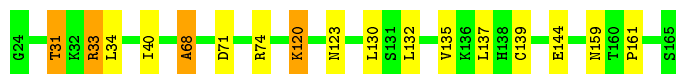
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain u:  92% 8% .



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

Chain v:  88% 9% .




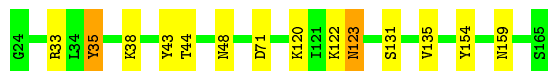
- Molecule 1: Iron sulfur cluster assembly protein 1, mitochondrial

Chain w:  92% 7% .



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

Chain x:  90% 8% .




- Molecule 2: Frataxin homolog, mitochondrial

Chain A:  93% 5% .




- Molecule 2: Frataxin homolog, mitochondrial

Chain B:  83% 16% .



- Molecule 2: Frataxin homolog, mitochondrial

Chain C:  80% 16% .



- Molecule 2: Frataxin homolog, mitochondrial

Chain D:  91% 8% .



- Molecule 2: Frataxin homolog, mitochondrial

Chain E: 90% 10%



- Molecule 2: Frataxin homolog, mitochondrial

Chain F: 85% 13%



- Molecule 2: Frataxin homolog, mitochondrial

Chain G: 89% 10%



- Molecule 2: Frataxin homolog, mitochondrial

Chain H: 88% 11%



- Molecule 2: Frataxin homolog, mitochondrial

Chain I: 83% 12%



- Molecule 2: Frataxin homolog, mitochondrial

Chain J: 88% 12%




- Molecule 2: Frataxin homolog, mitochondrial

Chain K: 88% 11%



- Molecule 2: Frataxin homolog, mitochondrial

Chain L:  83% 16% .



- Molecule 2: Frataxin homolog, mitochondrial

Chain M:  86% 13% .



- Molecule 2: Frataxin homolog, mitochondrial

Chain N:  93% 7% .




- Molecule 2: Frataxin homolog, mitochondrial

Chain O:  92% 8% .




- Molecule 2: Frataxin homolog, mitochondrial

Chain P:  86% 12% .



- Molecule 2: Frataxin homolog, mitochondrial

Chain Q:  89% 10% .




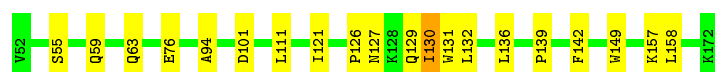
- Molecule 2: Frataxin homolog, mitochondrial

Chain R:  88% 11% .




- Molecule 2: Frataxin homolog, mitochondrial

Chain S:  83% 16%



- Molecule 2: Frataxin homolog, mitochondrial

Chain T:  84% 12%




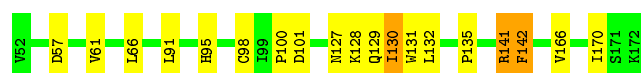
- Molecule 2: Frataxin homolog, mitochondrial

Chain U:  93% 7%




- Molecule 2: Frataxin homolog, mitochondrial

Chain V:  84% 13%



- Molecule 2: Frataxin homolog, mitochondrial

Chain W:  85% 12%



- Molecule 2: Frataxin homolog, mitochondrial

Chain X:  86% 11%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, O	Depositor
Number of particles used	4218	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; The ctf.auto function from EMAN2 was applied.	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	210	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	115000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	a	1.06	0/1089	1.32	3/1466 (0.2%)
1	b	1.04	0/1089	1.26	4/1466 (0.3%)
1	c	1.06	0/1089	1.27	0/1466
1	d	1.04	0/1089	1.29	5/1466 (0.3%)
1	e	1.04	0/1089	1.30	5/1466 (0.3%)
1	f	1.04	0/1089	1.28	4/1466 (0.3%)
1	g	1.03	0/1089	1.30	3/1466 (0.2%)
1	h	1.04	0/1089	1.30	6/1466 (0.4%)
1	i	1.03	0/1089	1.30	3/1466 (0.2%)
1	j	1.00	1/1089 (0.1%)	1.27	1/1466 (0.1%)
1	k	1.05	0/1089	1.30	6/1466 (0.4%)
1	l	1.05	0/1089	1.26	2/1466 (0.1%)
1	m	1.03	0/1089	1.32	4/1466 (0.3%)
1	n	1.01	0/1089	1.32	3/1466 (0.2%)
1	o	1.05	0/1089	1.25	4/1466 (0.3%)
1	p	1.04	0/1089	1.30	5/1466 (0.3%)
1	q	1.02	0/1089	1.35	11/1466 (0.8%)
1	r	1.03	0/1089	1.33	7/1466 (0.5%)
1	s	1.05	0/1089	1.28	4/1466 (0.3%)
1	t	1.03	0/1089	1.26	2/1466 (0.1%)
1	u	1.00	0/1089	1.29	4/1466 (0.3%)
1	v	1.05	0/1089	1.34	3/1466 (0.2%)
1	w	1.04	0/1089	1.32	5/1466 (0.3%)
1	x	1.06	0/1089	1.32	8/1466 (0.5%)
2	A	0.99	0/967	1.28	5/1319 (0.4%)
2	B	1.01	0/967	1.26	2/1319 (0.2%)
2	C	1.01	1/967 (0.1%)	1.17	1/1319 (0.1%)
2	D	0.99	0/967	1.21	0/1319
2	E	1.01	0/967	1.21	0/1319
2	F	1.02	0/967	1.21	3/1319 (0.2%)
2	G	1.02	0/967	1.19	0/1319
2	H	1.00	0/967	1.22	1/1319 (0.1%)
2	I	1.04	1/967 (0.1%)	1.28	4/1319 (0.3%)
2	J	1.03	0/967	1.20	0/1319

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	h	0	1
1	i	0	1
1	l	0	1
1	s	0	1
1	t	0	1
1	v	0	1
1	x	0	1
2	A	0	1
2	B	0	1
2	C	0	1
2	F	0	1
2	K	0	1
All	All	0	12

All (3) bond length outliers are listed below:

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

The worst 5 of 143 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	m	43	TYR	CB-CG-CD2	-10.44	114.73	121.00
2	V	142	PHE	CB-CG-CD1	9.62	127.53	120.80
1	g	35	TYR	CB-CG-CD1	9.20	126.52	121.00
1	m	43	TYR	CB-CG-CD1	8.99	126.39	121.00
1	q	35	TYR	CB-CG-CD1	8.93	126.36	121.00

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	80	TYR	Sidechain
2	B	119	TYR	Sidechain
2	C	75	GLU	Peptide
2	F	128	LYS	Peptide
1	h	74	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	1072	0	1106	0	0
1	b	1072	0	1106	0	0
1	c	1072	0	1106	0	0
1	d	1072	0	1106	0	0
1	e	1072	0	1108	0	0
1	f	1072	0	1106	0	0
1	g	1072	0	1108	0	0
1	h	1072	0	1106	0	0
1	i	1072	0	1108	0	0
1	j	1072	0	1106	0	0
1	k	1072	0	1108	0	0
1	l	1072	0	1108	0	0
1	m	1072	0	1108	0	0
1	n	1072	0	1106	0	0
1	o	1072	0	1106	0	0
1	p	1072	0	1108	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	q	1072	0	1108	0	0
1	r	1072	0	1106	0	0
1	s	1072	0	1108	0	0
1	t	1072	0	1108	0	0
1	u	1072	0	1108	0	0
1	v	1072	0	1106	0	0
1	w	1072	0	1108	0	0
1	x	1072	0	1108	0	0
2	A	947	0	921	6	0
2	B	947	0	921	3	0
2	C	947	0	921	17	0
2	D	947	0	921	0	0
2	E	947	0	921	0	0
2	F	947	0	921	16	0
2	G	947	0	921	2	0
2	H	947	0	921	7	0
2	I	947	0	921	16	0
2	J	947	0	921	19	0
2	K	947	0	921	0	0
2	L	947	0	921	35	0
2	M	947	0	921	24	0
2	N	947	0	921	0	0
2	O	947	0	921	3	0
2	P	947	0	921	28	0
2	Q	947	0	921	3	0
2	R	947	0	921	6	0
2	S	947	0	921	28	0
2	T	947	0	921	1	0
2	U	947	0	921	0	0
2	V	947	0	921	45	0
2	W	947	0	921	37	0
2	X	947	0	921	0	0
All	All	48456	0	48674	284	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 284 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:131:TRP:CZ2	2:S:139:PRO:CB	1.75	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:131:TRP:CZ2	2:S:139:PRO:HB3	1.11	1.58
2:L:121:ILE:HG12	2:L:132:LEU:CD2	1.33	1.57
2:P:130:ILE:CD1	2:P:149:TRP:NE1	1.72	1.52
2:M:121:ILE:HG22	2:M:132:LEU:CD2	1.36	1.51

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%)	121 (86%)	12 (9%)	7 (5%)	2	27
1	b	140/142 (99%)	124 (89%)	11 (8%)	5 (4%)	4	33
1	c	140/142 (99%)	122 (87%)	10 (7%)	8 (6%)	2	24
1	d	140/142 (99%)	123 (88%)	9 (6%)	8 (6%)	2	24
1	e	140/142 (99%)	123 (88%)	11 (8%)	6 (4%)	3	29
1	f	140/142 (99%)	120 (86%)	14 (10%)	6 (4%)	3	29
1	g	140/142 (99%)	118 (84%)	20 (14%)	2 (1%)	13	54
1	h	140/142 (99%)	118 (84%)	15 (11%)	7 (5%)	2	27
1	i	140/142 (99%)	124 (89%)	10 (7%)	6 (4%)	3	29
1	j	140/142 (99%)	118 (84%)	12 (9%)	10 (7%)	1	19
1	k	140/142 (99%)	120 (86%)	13 (9%)	7 (5%)	2	27
1	l	140/142 (99%)	122 (87%)	12 (9%)	6 (4%)	3	29
1	m	140/142 (99%)	118 (84%)	17 (12%)	5 (4%)	4	33
1	n	140/142 (99%)	118 (84%)	19 (14%)	3 (2%)	8	45
1	o	140/142 (99%)	121 (86%)	14 (10%)	5 (4%)	4	33
1	p	140/142 (99%)	123 (88%)	11 (8%)	6 (4%)	3	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	q	140/142 (99%)	122 (87%)	12 (9%)	6 (4%)	3	29
1	r	140/142 (99%)	118 (84%)	14 (10%)	8 (6%)	2	24
1	s	140/142 (99%)	125 (89%)	7 (5%)	8 (6%)	2	24
1	t	140/142 (99%)	120 (86%)	13 (9%)	7 (5%)	2	27
1	u	140/142 (99%)	122 (87%)	11 (8%)	7 (5%)	2	27
1	v	140/142 (99%)	119 (85%)	12 (9%)	9 (6%)	1	22
1	w	140/142 (99%)	118 (84%)	18 (13%)	4 (3%)	5	38
1	x	140/142 (99%)	124 (89%)	11 (8%)	5 (4%)	4	33
2	A	119/121 (98%)	93 (78%)	24 (20%)	2 (2%)	11	50
2	B	119/121 (98%)	95 (80%)	14 (12%)	10 (8%)	1	15
2	C	119/121 (98%)	96 (81%)	18 (15%)	5 (4%)	3	30
2	D	119/121 (98%)	102 (86%)	11 (9%)	6 (5%)	2	27
2	E	119/121 (98%)	92 (77%)	20 (17%)	7 (6%)	2	23
2	F	119/121 (98%)	92 (77%)	20 (17%)	7 (6%)	2	23
2	G	119/121 (98%)	99 (83%)	14 (12%)	6 (5%)	2	27
2	H	119/121 (98%)	98 (82%)	18 (15%)	3 (2%)	6	41
2	I	119/121 (98%)	101 (85%)	11 (9%)	7 (6%)	2	23
2	J	119/121 (98%)	94 (79%)	20 (17%)	5 (4%)	3	30
2	K	119/121 (98%)	97 (82%)	15 (13%)	7 (6%)	2	23
2	L	119/121 (98%)	95 (80%)	15 (13%)	9 (8%)	1	18
2	M	119/121 (98%)	97 (82%)	14 (12%)	8 (7%)	1	21
2	N	119/121 (98%)	98 (82%)	16 (13%)	5 (4%)	3	30
2	O	119/121 (98%)	94 (79%)	21 (18%)	4 (3%)	4	35
2	P	119/121 (98%)	99 (83%)	13 (11%)	7 (6%)	2	23
2	Q	119/121 (98%)	90 (76%)	22 (18%)	7 (6%)	2	23
2	R	119/121 (98%)	97 (82%)	18 (15%)	4 (3%)	4	35
2	S	119/121 (98%)	95 (80%)	19 (16%)	5 (4%)	3	30
2	T	119/121 (98%)	100 (84%)	8 (7%)	11 (9%)	1	15
2	U	119/121 (98%)	97 (82%)	16 (13%)	6 (5%)	2	27
2	V	119/121 (98%)	100 (84%)	13 (11%)	6 (5%)	2	27
2	W	119/121 (98%)	93 (78%)	21 (18%)	5 (4%)	3	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	X	119/121 (98%)	98 (82%)	12 (10%)	9 (8%)	1	18
All	All	6216/6312 (98%)	5213 (84%)	701 (11%)	302 (5%)	5	27

5 of 302 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	39	VAL
1	b	68	ALA
2	B	127	ASN
2	B	136	LEU
1	c	123	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	121/121 (100%)	119 (98%)	2 (2%)	66	84
1	b	121/121 (100%)	117 (97%)	4 (3%)	43	70
1	c	121/121 (100%)	116 (96%)	5 (4%)	35	65
1	d	121/121 (100%)	116 (96%)	5 (4%)	35	65
1	e	121/121 (100%)	115 (95%)	6 (5%)	28	60
1	f	121/121 (100%)	118 (98%)	3 (2%)	53	77
1	g	121/121 (100%)	113 (93%)	8 (7%)	19	52
1	h	121/121 (100%)	111 (92%)	10 (8%)	13	43
1	i	121/121 (100%)	115 (95%)	6 (5%)	28	60
1	j	121/121 (100%)	114 (94%)	7 (6%)	23	56
1	k	121/121 (100%)	118 (98%)	3 (2%)	53	77
1	l	121/121 (100%)	113 (93%)	8 (7%)	19	52
1	m	121/121 (100%)	112 (93%)	9 (7%)	16	48
1	n	121/121 (100%)	117 (97%)	4 (3%)	43	70
1	o	121/121 (100%)	118 (98%)	3 (2%)	53	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	p	121/121 (100%)	111 (92%)	10 (8%)	13	43
1	q	121/121 (100%)	118 (98%)	3 (2%)	53	77
1	r	121/121 (100%)	116 (96%)	5 (4%)	35	65
1	s	121/121 (100%)	114 (94%)	7 (6%)	23	56
1	t	121/121 (100%)	117 (97%)	4 (3%)	43	70
1	u	121/121 (100%)	119 (98%)	2 (2%)	66	84
1	v	121/121 (100%)	113 (93%)	8 (7%)	19	52
1	w	121/121 (100%)	115 (95%)	6 (5%)	28	60
1	x	121/121 (100%)	117 (97%)	4 (3%)	43	70
2	A	109/109 (100%)	106 (97%)	3 (3%)	49	74
2	B	109/109 (100%)	105 (96%)	4 (4%)	39	68
2	C	109/109 (100%)	101 (93%)	8 (7%)	16	49
2	D	109/109 (100%)	103 (94%)	6 (6%)	25	58
2	E	109/109 (100%)	104 (95%)	5 (5%)	31	62
2	F	109/109 (100%)	103 (94%)	6 (6%)	25	58
2	G	109/109 (100%)	104 (95%)	5 (5%)	31	62
2	H	109/109 (100%)	105 (96%)	4 (4%)	39	68
2	I	109/109 (100%)	104 (95%)	5 (5%)	31	62
2	J	109/109 (100%)	105 (96%)	4 (4%)	39	68
2	K	109/109 (100%)	103 (94%)	6 (6%)	25	58
2	L	109/109 (100%)	107 (98%)	2 (2%)	64	84
2	M	109/109 (100%)	105 (96%)	4 (4%)	39	68
2	N	109/109 (100%)	107 (98%)	2 (2%)	64	84
2	O	109/109 (100%)	106 (97%)	3 (3%)	49	74
2	P	109/109 (100%)	105 (96%)	4 (4%)	39	68
2	Q	109/109 (100%)	104 (95%)	5 (5%)	31	62
2	R	109/109 (100%)	107 (98%)	2 (2%)	64	84
2	S	109/109 (100%)	104 (95%)	5 (5%)	31	62
2	T	109/109 (100%)	101 (93%)	8 (7%)	16	49
2	U	109/109 (100%)	106 (97%)	3 (3%)	49	74
2	V	109/109 (100%)	106 (97%)	3 (3%)	49	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	W	109/109 (100%)	105 (96%)	4 (4%)	39	68
2	X	109/109 (100%)	103 (94%)	6 (6%)	25	58
All	All	5520/5520 (100%)	5281 (96%)	239 (4%)	38	64

5 of 239 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	k	158	ARG
1	m	132	LEU
1	w	106	MET
2	K	119	TYR
1	l	109	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	127	ASN
2	L	122	ASN
2	V	124	GLN
2	J	106	HIS
2	K	95	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.