



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2021 – 05:39 AM EDT

PDB ID : 3IA0  
Title : Ethanolamine Utilization Microcompartment Shell Subunit, EutS-G39V mutant  
Authors : Tanaka, S.; Sawaya, M.R.; Yeates, T.O.  
Deposited on : 2009-07-13  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

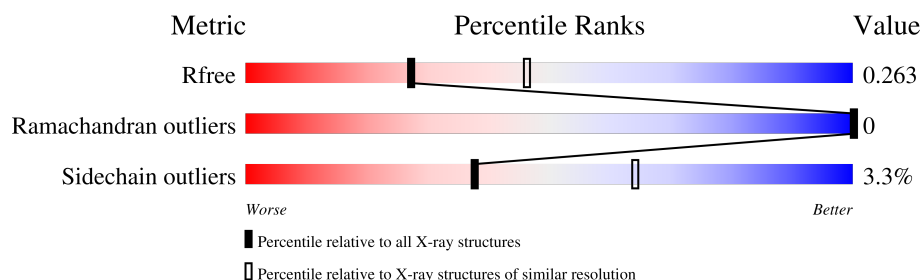
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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.
















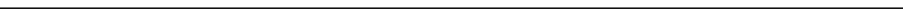











Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	119	91% 7%
1	B	119	91% 7%
1	C	119	91% 7%
1	D	119	91% 7%
1	E	119	91% 7%
1	F	119	91% 7%
1	G	119	91% 7%
1	H	119	91% 7%




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Mol	Chain	Length	Quality of chain
1	I	119	 91% • 7%
1	J	119	 91% • 7%
1	K	119	 92% • 7%
1	L	119	 91% • 7%
1	M	119	 91% • 7%
1	N	119	 91% • 7%
1	O	119	 91% • 7%
1	P	119	 91% • 7%
1	Q	119	 91% • 7%
1	R	119	 91% • 7%
1	S	119	 91% • 7%
1	T	119	 91% • 7%
1	U	119	 91% • 7%
1	V	119	 91% • 7%
1	W	119	 91% • 7%
1	X	119	 91% • 7%
1	Y	119	 91% • 7%
1	Z	119	 91% • 7%
1	a	119	 91% • 7%
1	b	119	 91% • 7%
1	c	119	 91% • 7%
1	d	119	 91% • 7%
1	e	119	 91% • 7%
1	f	119	 91% • 7%
1	g	119	 91% • 7%

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Mol	Chain	Length	Quality of chain
1	h	119	 91% • 7%
1	i	119	 92% • 7%
1	j	119	 92% • 7%
1	k	119	 91% • 7%
1	l	119	 91% • 7%
1	m	119	 92% • 7%
1	n	119	 91% • 7%
1	o	119	 91% • 7%
1	p	119	 91% • 7%
1	q	119	 91% • 7%
1	r	119	 92% • 7%
1	s	119	 91% • 7%
1	t	119	 91% • 7%
1	u	119	 91% • 7%
1	v	119	 92% • 7%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 39312 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Ethanolamine utilization protein eutS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	B	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	C	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	D	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	E	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	F	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	G	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	H	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	I	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	J	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	K	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	L	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	M	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	N	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	O	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	P	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	111	Total 819	C 524	N 136	O 155	S 4	0	0	0
1	R	111	Total 819	C 524	N 136	O 155	S 4	0	0	0
1	S	111	Total 819	C 524	N 136	O 155	S 4	0	0	0
1	T	111	Total 819	C 524	N 136	O 155	S 4	0	0	0
1	U	111	Total 819	C 524	N 136	O 155	S 4	0	0	0
1	V	111	Total 819	C 524	N 136	O 155	S 4	0	0	0
1	W	111	Total 819	C 524	N 136	O 155	S 4	0	0	0
1	X	111	Total 819	C 524	N 136	O 155	S 4	0	0	0
1	Y	111	Total 819	C 524	N 136	O 155	S 4	0	0	0
1	Z	111	Total 819	C 524	N 136	O 155	S 4	0	0	0
1	a	111	Total 819	C 524	N 136	O 155	S 4	0	0	0
1	b	111	Total 819	C 524	N 136	O 155	S 4	0	0	0
1	c	111	Total 819	C 524	N 136	O 155	S 4	0	0	0
1	d	111	Total 819	C 524	N 136	O 155	S 4	0	0	0
1	e	111	Total 819	C 524	N 136	O 155	S 4	0	0	0
1	f	111	Total 819	C 524	N 136	O 155	S 4	0	0	0
1	g	111	Total 819	C 524	N 136	O 155	S 4	0	0	0
1	h	111	Total 819	C 524	N 136	O 155	S 4	0	0	0
1	i	111	Total 819	C 524	N 136	O 155	S 4	0	0	0
1	j	111	Total 819	C 524	N 136	O 155	S 4	0	0	0
1	k	111	Total 819	C 524	N 136	O 155	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	l	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	m	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	n	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	o	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	p	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	q	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	r	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	s	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	t	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	u	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	v	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			

There are 432 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	VAL	GLY	engineered mutation	UNP P63746
A	112	LEU	-	expression tag	UNP P63746
A	113	GLU	-	expression tag	UNP P63746
A	114	HIS	-	expression tag	UNP P63746
A	115	HIS	-	expression tag	UNP P63746
A	116	HIS	-	expression tag	UNP P63746
A	117	HIS	-	expression tag	UNP P63746
A	118	HIS	-	expression tag	UNP P63746
A	119	HIS	-	expression tag	UNP P63746
B	39	VAL	GLY	engineered mutation	UNP P63746
B	112	LEU	-	expression tag	UNP P63746
B	113	GLU	-	expression tag	UNP P63746
B	114	HIS	-	expression tag	UNP P63746
B	115	HIS	-	expression tag	UNP P63746
B	116	HIS	-	expression tag	UNP P63746
B	117	HIS	-	expression tag	UNP P63746
B	118	HIS	-	expression tag	UNP P63746

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Chain	Residue	Modelled	Actual	Comment	Reference
B	119	HIS	-	expression tag	UNP P63746
C	39	VAL	GLY	engineered mutation	UNP P63746
C	112	LEU	-	expression tag	UNP P63746
C	113	GLU	-	expression tag	UNP P63746
C	114	HIS	-	expression tag	UNP P63746
C	115	HIS	-	expression tag	UNP P63746
C	116	HIS	-	expression tag	UNP P63746
C	117	HIS	-	expression tag	UNP P63746
C	118	HIS	-	expression tag	UNP P63746
C	119	HIS	-	expression tag	UNP P63746
D	39	VAL	GLY	engineered mutation	UNP P63746
D	112	LEU	-	expression tag	UNP P63746
D	113	GLU	-	expression tag	UNP P63746
D	114	HIS	-	expression tag	UNP P63746
D	115	HIS	-	expression tag	UNP P63746
D	116	HIS	-	expression tag	UNP P63746
D	117	HIS	-	expression tag	UNP P63746
D	118	HIS	-	expression tag	UNP P63746
D	119	HIS	-	expression tag	UNP P63746
E	39	VAL	GLY	engineered mutation	UNP P63746
E	112	LEU	-	expression tag	UNP P63746
E	113	GLU	-	expression tag	UNP P63746
E	114	HIS	-	expression tag	UNP P63746
E	115	HIS	-	expression tag	UNP P63746
E	116	HIS	-	expression tag	UNP P63746
E	117	HIS	-	expression tag	UNP P63746
E	118	HIS	-	expression tag	UNP P63746
E	119	HIS	-	expression tag	UNP P63746
F	39	VAL	GLY	engineered mutation	UNP P63746
F	112	LEU	-	expression tag	UNP P63746
F	113	GLU	-	expression tag	UNP P63746
F	114	HIS	-	expression tag	UNP P63746
F	115	HIS	-	expression tag	UNP P63746
F	116	HIS	-	expression tag	UNP P63746
F	117	HIS	-	expression tag	UNP P63746
F	118	HIS	-	expression tag	UNP P63746
F	119	HIS	-	expression tag	UNP P63746
G	39	VAL	GLY	engineered mutation	UNP P63746
G	112	LEU	-	expression tag	UNP P63746
G	113	GLU	-	expression tag	UNP P63746
G	114	HIS	-	expression tag	UNP P63746
G	115	HIS	-	expression tag	UNP P63746

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Chain	Residue	Modelled	Actual	Comment	Reference
G	116	HIS	-	expression tag	UNP P63746
G	117	HIS	-	expression tag	UNP P63746
G	118	HIS	-	expression tag	UNP P63746
G	119	HIS	-	expression tag	UNP P63746
H	39	VAL	GLY	engineered mutation	UNP P63746
H	112	LEU	-	expression tag	UNP P63746
H	113	GLU	-	expression tag	UNP P63746
H	114	HIS	-	expression tag	UNP P63746
H	115	HIS	-	expression tag	UNP P63746
H	116	HIS	-	expression tag	UNP P63746
H	117	HIS	-	expression tag	UNP P63746
H	118	HIS	-	expression tag	UNP P63746
H	119	HIS	-	expression tag	UNP P63746
I	39	VAL	GLY	engineered mutation	UNP P63746
I	112	LEU	-	expression tag	UNP P63746
I	113	GLU	-	expression tag	UNP P63746
I	114	HIS	-	expression tag	UNP P63746
I	115	HIS	-	expression tag	UNP P63746
I	116	HIS	-	expression tag	UNP P63746
I	117	HIS	-	expression tag	UNP P63746
I	118	HIS	-	expression tag	UNP P63746
I	119	HIS	-	expression tag	UNP P63746
J	39	VAL	GLY	engineered mutation	UNP P63746
J	112	LEU	-	expression tag	UNP P63746
J	113	GLU	-	expression tag	UNP P63746
J	114	HIS	-	expression tag	UNP P63746
J	115	HIS	-	expression tag	UNP P63746
J	116	HIS	-	expression tag	UNP P63746
J	117	HIS	-	expression tag	UNP P63746
J	118	HIS	-	expression tag	UNP P63746
J	119	HIS	-	expression tag	UNP P63746
K	39	VAL	GLY	engineered mutation	UNP P63746
K	112	LEU	-	expression tag	UNP P63746
K	113	GLU	-	expression tag	UNP P63746
K	114	HIS	-	expression tag	UNP P63746
K	115	HIS	-	expression tag	UNP P63746
K	116	HIS	-	expression tag	UNP P63746
K	117	HIS	-	expression tag	UNP P63746
K	118	HIS	-	expression tag	UNP P63746
K	119	HIS	-	expression tag	UNP P63746
L	39	VAL	GLY	engineered mutation	UNP P63746
L	112	LEU	-	expression tag	UNP P63746

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Chain	Residue	Modelled	Actual	Comment	Reference
L	113	GLU	-	expression tag	UNP P63746
L	114	HIS	-	expression tag	UNP P63746
L	115	HIS	-	expression tag	UNP P63746
L	116	HIS	-	expression tag	UNP P63746
L	117	HIS	-	expression tag	UNP P63746
L	118	HIS	-	expression tag	UNP P63746
L	119	HIS	-	expression tag	UNP P63746
M	39	VAL	GLY	engineered mutation	UNP P63746
M	112	LEU	-	expression tag	UNP P63746
M	113	GLU	-	expression tag	UNP P63746
M	114	HIS	-	expression tag	UNP P63746
M	115	HIS	-	expression tag	UNP P63746
M	116	HIS	-	expression tag	UNP P63746
M	117	HIS	-	expression tag	UNP P63746
M	118	HIS	-	expression tag	UNP P63746
M	119	HIS	-	expression tag	UNP P63746
N	39	VAL	GLY	engineered mutation	UNP P63746
N	112	LEU	-	expression tag	UNP P63746
N	113	GLU	-	expression tag	UNP P63746
N	114	HIS	-	expression tag	UNP P63746
N	115	HIS	-	expression tag	UNP P63746
N	116	HIS	-	expression tag	UNP P63746
N	117	HIS	-	expression tag	UNP P63746
N	118	HIS	-	expression tag	UNP P63746
N	119	HIS	-	expression tag	UNP P63746
O	39	VAL	GLY	engineered mutation	UNP P63746
O	112	LEU	-	expression tag	UNP P63746
O	113	GLU	-	expression tag	UNP P63746
O	114	HIS	-	expression tag	UNP P63746
O	115	HIS	-	expression tag	UNP P63746
O	116	HIS	-	expression tag	UNP P63746
O	117	HIS	-	expression tag	UNP P63746
O	118	HIS	-	expression tag	UNP P63746
O	119	HIS	-	expression tag	UNP P63746
P	39	VAL	GLY	engineered mutation	UNP P63746
P	112	LEU	-	expression tag	UNP P63746
P	113	GLU	-	expression tag	UNP P63746
P	114	HIS	-	expression tag	UNP P63746
P	115	HIS	-	expression tag	UNP P63746
P	116	HIS	-	expression tag	UNP P63746
P	117	HIS	-	expression tag	UNP P63746
P	118	HIS	-	expression tag	UNP P63746

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Chain	Residue	Modelled	Actual	Comment	Reference
P	119	HIS	-	expression tag	UNP P63746
Q	39	VAL	GLY	engineered mutation	UNP P63746
Q	112	LEU	-	expression tag	UNP P63746
Q	113	GLU	-	expression tag	UNP P63746
Q	114	HIS	-	expression tag	UNP P63746
Q	115	HIS	-	expression tag	UNP P63746
Q	116	HIS	-	expression tag	UNP P63746
Q	117	HIS	-	expression tag	UNP P63746
Q	118	HIS	-	expression tag	UNP P63746
Q	119	HIS	-	expression tag	UNP P63746
R	39	VAL	GLY	engineered mutation	UNP P63746
R	112	LEU	-	expression tag	UNP P63746
R	113	GLU	-	expression tag	UNP P63746
R	114	HIS	-	expression tag	UNP P63746
R	115	HIS	-	expression tag	UNP P63746
R	116	HIS	-	expression tag	UNP P63746
R	117	HIS	-	expression tag	UNP P63746
R	118	HIS	-	expression tag	UNP P63746
R	119	HIS	-	expression tag	UNP P63746
S	39	VAL	GLY	engineered mutation	UNP P63746
S	112	LEU	-	expression tag	UNP P63746
S	113	GLU	-	expression tag	UNP P63746
S	114	HIS	-	expression tag	UNP P63746
S	115	HIS	-	expression tag	UNP P63746
S	116	HIS	-	expression tag	UNP P63746
S	117	HIS	-	expression tag	UNP P63746
S	118	HIS	-	expression tag	UNP P63746
S	119	HIS	-	expression tag	UNP P63746
T	39	VAL	GLY	engineered mutation	UNP P63746
T	112	LEU	-	expression tag	UNP P63746
T	113	GLU	-	expression tag	UNP P63746
T	114	HIS	-	expression tag	UNP P63746
T	115	HIS	-	expression tag	UNP P63746
T	116	HIS	-	expression tag	UNP P63746
T	117	HIS	-	expression tag	UNP P63746
T	118	HIS	-	expression tag	UNP P63746
T	119	HIS	-	expression tag	UNP P63746
U	39	VAL	GLY	engineered mutation	UNP P63746
U	112	LEU	-	expression tag	UNP P63746
U	113	GLU	-	expression tag	UNP P63746
U	114	HIS	-	expression tag	UNP P63746
U	115	HIS	-	expression tag	UNP P63746

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Chain	Residue	Modelled	Actual	Comment	Reference
U	116	HIS	-	expression tag	UNP P63746
U	117	HIS	-	expression tag	UNP P63746
U	118	HIS	-	expression tag	UNP P63746
U	119	HIS	-	expression tag	UNP P63746
V	39	VAL	GLY	engineered mutation	UNP P63746
V	112	LEU	-	expression tag	UNP P63746
V	113	GLU	-	expression tag	UNP P63746
V	114	HIS	-	expression tag	UNP P63746
V	115	HIS	-	expression tag	UNP P63746
V	116	HIS	-	expression tag	UNP P63746
V	117	HIS	-	expression tag	UNP P63746
V	118	HIS	-	expression tag	UNP P63746
V	119	HIS	-	expression tag	UNP P63746
W	39	VAL	GLY	engineered mutation	UNP P63746
W	112	LEU	-	expression tag	UNP P63746
W	113	GLU	-	expression tag	UNP P63746
W	114	HIS	-	expression tag	UNP P63746
W	115	HIS	-	expression tag	UNP P63746
W	116	HIS	-	expression tag	UNP P63746
W	117	HIS	-	expression tag	UNP P63746
W	118	HIS	-	expression tag	UNP P63746
W	119	HIS	-	expression tag	UNP P63746
X	39	VAL	GLY	engineered mutation	UNP P63746
X	112	LEU	-	expression tag	UNP P63746
X	113	GLU	-	expression tag	UNP P63746
X	114	HIS	-	expression tag	UNP P63746
X	115	HIS	-	expression tag	UNP P63746
X	116	HIS	-	expression tag	UNP P63746
X	117	HIS	-	expression tag	UNP P63746
X	118	HIS	-	expression tag	UNP P63746
X	119	HIS	-	expression tag	UNP P63746
Y	39	VAL	GLY	engineered mutation	UNP P63746
Y	112	LEU	-	expression tag	UNP P63746
Y	113	GLU	-	expression tag	UNP P63746
Y	114	HIS	-	expression tag	UNP P63746
Y	115	HIS	-	expression tag	UNP P63746
Y	116	HIS	-	expression tag	UNP P63746
Y	117	HIS	-	expression tag	UNP P63746
Y	118	HIS	-	expression tag	UNP P63746
Y	119	HIS	-	expression tag	UNP P63746
Z	39	VAL	GLY	engineered mutation	UNP P63746
Z	112	LEU	-	expression tag	UNP P63746

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	113	GLU	-	expression tag	UNP P63746
Z	114	HIS	-	expression tag	UNP P63746
Z	115	HIS	-	expression tag	UNP P63746
Z	116	HIS	-	expression tag	UNP P63746
Z	117	HIS	-	expression tag	UNP P63746
Z	118	HIS	-	expression tag	UNP P63746
Z	119	HIS	-	expression tag	UNP P63746
a	39	VAL	GLY	engineered mutation	UNP P63746
a	112	LEU	-	expression tag	UNP P63746
a	113	GLU	-	expression tag	UNP P63746
a	114	HIS	-	expression tag	UNP P63746
a	115	HIS	-	expression tag	UNP P63746
a	116	HIS	-	expression tag	UNP P63746
a	117	HIS	-	expression tag	UNP P63746
a	118	HIS	-	expression tag	UNP P63746
a	119	HIS	-	expression tag	UNP P63746
b	39	VAL	GLY	engineered mutation	UNP P63746
b	112	LEU	-	expression tag	UNP P63746
b	113	GLU	-	expression tag	UNP P63746
b	114	HIS	-	expression tag	UNP P63746
b	115	HIS	-	expression tag	UNP P63746
b	116	HIS	-	expression tag	UNP P63746
b	117	HIS	-	expression tag	UNP P63746
b	118	HIS	-	expression tag	UNP P63746
b	119	HIS	-	expression tag	UNP P63746
c	39	VAL	GLY	engineered mutation	UNP P63746
c	112	LEU	-	expression tag	UNP P63746
c	113	GLU	-	expression tag	UNP P63746
c	114	HIS	-	expression tag	UNP P63746
c	115	HIS	-	expression tag	UNP P63746
c	116	HIS	-	expression tag	UNP P63746
c	117	HIS	-	expression tag	UNP P63746
c	118	HIS	-	expression tag	UNP P63746
c	119	HIS	-	expression tag	UNP P63746
d	39	VAL	GLY	engineered mutation	UNP P63746
d	112	LEU	-	expression tag	UNP P63746
d	113	GLU	-	expression tag	UNP P63746
d	114	HIS	-	expression tag	UNP P63746
d	115	HIS	-	expression tag	UNP P63746
d	116	HIS	-	expression tag	UNP P63746
d	117	HIS	-	expression tag	UNP P63746
d	118	HIS	-	expression tag	UNP P63746

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Chain	Residue	Modelled	Actual	Comment	Reference
d	119	HIS	-	expression tag	UNP P63746
e	39	VAL	GLY	engineered mutation	UNP P63746
e	112	LEU	-	expression tag	UNP P63746
e	113	GLU	-	expression tag	UNP P63746
e	114	HIS	-	expression tag	UNP P63746
e	115	HIS	-	expression tag	UNP P63746
e	116	HIS	-	expression tag	UNP P63746
e	117	HIS	-	expression tag	UNP P63746
e	118	HIS	-	expression tag	UNP P63746
e	119	HIS	-	expression tag	UNP P63746
f	39	VAL	GLY	engineered mutation	UNP P63746
f	112	LEU	-	expression tag	UNP P63746
f	113	GLU	-	expression tag	UNP P63746
f	114	HIS	-	expression tag	UNP P63746
f	115	HIS	-	expression tag	UNP P63746
f	116	HIS	-	expression tag	UNP P63746
f	117	HIS	-	expression tag	UNP P63746
f	118	HIS	-	expression tag	UNP P63746
f	119	HIS	-	expression tag	UNP P63746
g	39	VAL	GLY	engineered mutation	UNP P63746
g	112	LEU	-	expression tag	UNP P63746
g	113	GLU	-	expression tag	UNP P63746
g	114	HIS	-	expression tag	UNP P63746
g	115	HIS	-	expression tag	UNP P63746
g	116	HIS	-	expression tag	UNP P63746
g	117	HIS	-	expression tag	UNP P63746
g	118	HIS	-	expression tag	UNP P63746
g	119	HIS	-	expression tag	UNP P63746
h	39	VAL	GLY	engineered mutation	UNP P63746
h	112	LEU	-	expression tag	UNP P63746
h	113	GLU	-	expression tag	UNP P63746
h	114	HIS	-	expression tag	UNP P63746
h	115	HIS	-	expression tag	UNP P63746
h	116	HIS	-	expression tag	UNP P63746
h	117	HIS	-	expression tag	UNP P63746
h	118	HIS	-	expression tag	UNP P63746
h	119	HIS	-	expression tag	UNP P63746
i	39	VAL	GLY	engineered mutation	UNP P63746
i	112	LEU	-	expression tag	UNP P63746
i	113	GLU	-	expression tag	UNP P63746
i	114	HIS	-	expression tag	UNP P63746
i	115	HIS	-	expression tag	UNP P63746

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Chain	Residue	Modelled	Actual	Comment	Reference
i	116	HIS	-	expression tag	UNP P63746
i	117	HIS	-	expression tag	UNP P63746
i	118	HIS	-	expression tag	UNP P63746
i	119	HIS	-	expression tag	UNP P63746
j	39	VAL	GLY	engineered mutation	UNP P63746
j	112	LEU	-	expression tag	UNP P63746
j	113	GLU	-	expression tag	UNP P63746
j	114	HIS	-	expression tag	UNP P63746
j	115	HIS	-	expression tag	UNP P63746
j	116	HIS	-	expression tag	UNP P63746
j	117	HIS	-	expression tag	UNP P63746
j	118	HIS	-	expression tag	UNP P63746
j	119	HIS	-	expression tag	UNP P63746
k	39	VAL	GLY	engineered mutation	UNP P63746
k	112	LEU	-	expression tag	UNP P63746
k	113	GLU	-	expression tag	UNP P63746
k	114	HIS	-	expression tag	UNP P63746
k	115	HIS	-	expression tag	UNP P63746
k	116	HIS	-	expression tag	UNP P63746
k	117	HIS	-	expression tag	UNP P63746
k	118	HIS	-	expression tag	UNP P63746
k	119	HIS	-	expression tag	UNP P63746
l	39	VAL	GLY	engineered mutation	UNP P63746
l	112	LEU	-	expression tag	UNP P63746
l	113	GLU	-	expression tag	UNP P63746
l	114	HIS	-	expression tag	UNP P63746
l	115	HIS	-	expression tag	UNP P63746
l	116	HIS	-	expression tag	UNP P63746
l	117	HIS	-	expression tag	UNP P63746
l	118	HIS	-	expression tag	UNP P63746
l	119	HIS	-	expression tag	UNP P63746
m	39	VAL	GLY	engineered mutation	UNP P63746
m	112	LEU	-	expression tag	UNP P63746
m	113	GLU	-	expression tag	UNP P63746
m	114	HIS	-	expression tag	UNP P63746
m	115	HIS	-	expression tag	UNP P63746
m	116	HIS	-	expression tag	UNP P63746
m	117	HIS	-	expression tag	UNP P63746
m	118	HIS	-	expression tag	UNP P63746
m	119	HIS	-	expression tag	UNP P63746
n	39	VAL	GLY	engineered mutation	UNP P63746
n	112	LEU	-	expression tag	UNP P63746

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Chain	Residue	Modelled	Actual	Comment	Reference
n	113	GLU	-	expression tag	UNP P63746
n	114	HIS	-	expression tag	UNP P63746
n	115	HIS	-	expression tag	UNP P63746
n	116	HIS	-	expression tag	UNP P63746
n	117	HIS	-	expression tag	UNP P63746
n	118	HIS	-	expression tag	UNP P63746
n	119	HIS	-	expression tag	UNP P63746
o	39	VAL	GLY	engineered mutation	UNP P63746
o	112	LEU	-	expression tag	UNP P63746
o	113	GLU	-	expression tag	UNP P63746
o	114	HIS	-	expression tag	UNP P63746
o	115	HIS	-	expression tag	UNP P63746
o	116	HIS	-	expression tag	UNP P63746
o	117	HIS	-	expression tag	UNP P63746
o	118	HIS	-	expression tag	UNP P63746
o	119	HIS	-	expression tag	UNP P63746
p	39	VAL	GLY	engineered mutation	UNP P63746
p	112	LEU	-	expression tag	UNP P63746
p	113	GLU	-	expression tag	UNP P63746
p	114	HIS	-	expression tag	UNP P63746
p	115	HIS	-	expression tag	UNP P63746
p	116	HIS	-	expression tag	UNP P63746
p	117	HIS	-	expression tag	UNP P63746
p	118	HIS	-	expression tag	UNP P63746
p	119	HIS	-	expression tag	UNP P63746
q	39	VAL	GLY	engineered mutation	UNP P63746
q	112	LEU	-	expression tag	UNP P63746
q	113	GLU	-	expression tag	UNP P63746
q	114	HIS	-	expression tag	UNP P63746
q	115	HIS	-	expression tag	UNP P63746
q	116	HIS	-	expression tag	UNP P63746
q	117	HIS	-	expression tag	UNP P63746
q	118	HIS	-	expression tag	UNP P63746
q	119	HIS	-	expression tag	UNP P63746
r	39	VAL	GLY	engineered mutation	UNP P63746
r	112	LEU	-	expression tag	UNP P63746
r	113	GLU	-	expression tag	UNP P63746
r	114	HIS	-	expression tag	UNP P63746
r	115	HIS	-	expression tag	UNP P63746
r	116	HIS	-	expression tag	UNP P63746
r	117	HIS	-	expression tag	UNP P63746
r	118	HIS	-	expression tag	UNP P63746

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Chain	Residue	Modelled	Actual	Comment	Reference
r	119	HIS	-	expression tag	UNP P63746
s	39	VAL	GLY	engineered mutation	UNP P63746
s	112	LEU	-	expression tag	UNP P63746
s	113	GLU	-	expression tag	UNP P63746
s	114	HIS	-	expression tag	UNP P63746
s	115	HIS	-	expression tag	UNP P63746
s	116	HIS	-	expression tag	UNP P63746
s	117	HIS	-	expression tag	UNP P63746
s	118	HIS	-	expression tag	UNP P63746
s	119	HIS	-	expression tag	UNP P63746
t	39	VAL	GLY	engineered mutation	UNP P63746
t	112	LEU	-	expression tag	UNP P63746
t	113	GLU	-	expression tag	UNP P63746
t	114	HIS	-	expression tag	UNP P63746
t	115	HIS	-	expression tag	UNP P63746
t	116	HIS	-	expression tag	UNP P63746
t	117	HIS	-	expression tag	UNP P63746
t	118	HIS	-	expression tag	UNP P63746
t	119	HIS	-	expression tag	UNP P63746
u	39	VAL	GLY	engineered mutation	UNP P63746
u	112	LEU	-	expression tag	UNP P63746
u	113	GLU	-	expression tag	UNP P63746
u	114	HIS	-	expression tag	UNP P63746
u	115	HIS	-	expression tag	UNP P63746
u	116	HIS	-	expression tag	UNP P63746
u	117	HIS	-	expression tag	UNP P63746
u	118	HIS	-	expression tag	UNP P63746
u	119	HIS	-	expression tag	UNP P63746
v	39	VAL	GLY	engineered mutation	UNP P63746
v	112	LEU	-	expression tag	UNP P63746
v	113	GLU	-	expression tag	UNP P63746
v	114	HIS	-	expression tag	UNP P63746
v	115	HIS	-	expression tag	UNP P63746
v	116	HIS	-	expression tag	UNP P63746
v	117	HIS	-	expression tag	UNP P63746
v	118	HIS	-	expression tag	UNP P63746
v	119	HIS	-	expression tag	UNP P63746

### 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. 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: Ethanolamine utilization protein eutS

Chain A:  91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain B:  91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain C:  91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain D:  91% 7%




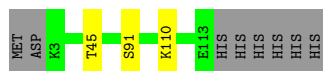
- Molecule 1: Ethanolamine utilization protein eutS

Chain E:  91% 7%



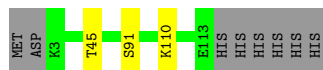
- Molecule 1: Ethanolamine utilization protein eutS

Chain F:  91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain G: 91% 7%



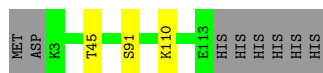
- Molecule 1: Ethanolamine utilization protein eutS

Chain H: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain I: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain J: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain K: 92% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain L: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain M: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain N: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain O: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain P: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain Q: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain R: 91% 7%



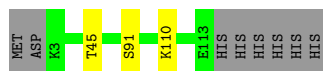
- Molecule 1: Ethanolamine utilization protein eutS

Chain S: 91% 7%



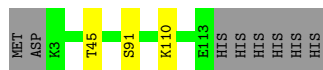
- Molecule 1: Ethanolamine utilization protein eutS

Chain T: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain U: 91% 7%



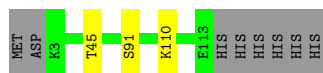
- Molecule 1: Ethanolamine utilization protein eutS

Chain V: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain W: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain X: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain Y: 91% 7%



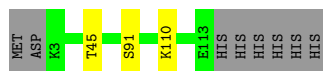
- Molecule 1: Ethanolamine utilization protein eutS

Chain Z: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain a: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain b: 91% 7%



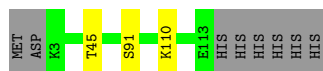
- Molecule 1: Ethanolamine utilization protein eutS

Chain c: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain d: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain e: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain f: 91% 7%



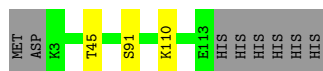
- Molecule 1: Ethanolamine utilization protein eutS

Chain g: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain h: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain i: 92% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain j: 92% 7%



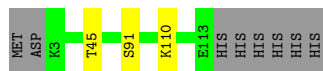
- Molecule 1: Ethanolamine utilization protein eutS

Chain k: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain l: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain m: 92% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain n: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain o: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain p: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain q: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain r: 92% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain s: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain t: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

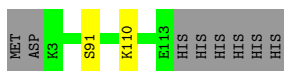
Chain u: 91% 7%



- Molecule 1: Ethanolamine utilization protein eutS

Chain v: 92% 7%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.58Å 151.39Å 127.46Å 90.00° 90.39° 90.00°	Depositor
Resolution (Å)	58.88 – 2.50 58.88 – 2.49	Depositor EDS
% Data completeness (in resolution range)	80.2 (58.88-2.50) 88.7 (58.88-2.49)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.4 _4	Depositor
R, $R_{free}$	0.217 , 0.239 0.272 , 0.263	Depositor DCC
$R_{free}$ test set	8725 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.2	Xtriage
Anisotropy	0.760	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 51.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.408 for h,-k,-l 0.408 for -h,-k,l 0.388 for -h,k,-l	Xtriage
Reported twinning fraction	0.463 for -h,-k,l	Depositor
Outliers	0 of 173036 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	39312	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	0.31	0/830	0.51	0/1123
1	B	0.30	0/830	0.51	0/1123
1	C	0.32	0/830	0.51	0/1123
1	D	0.30	0/830	0.51	0/1123
1	E	0.30	0/830	0.51	0/1123
1	F	0.31	0/830	0.51	0/1123
1	G	0.32	0/830	0.51	0/1123
1	H	0.31	0/830	0.50	0/1123
1	I	0.31	0/830	0.51	0/1123
1	J	0.31	0/830	0.51	0/1123
1	K	0.31	0/830	0.51	0/1123
1	L	0.32	0/830	0.51	0/1123
1	M	0.33	0/830	0.51	0/1123
1	N	0.32	0/830	0.51	0/1123
1	O	0.30	0/830	0.51	0/1123
1	P	0.31	0/830	0.51	0/1123
1	Q	0.32	0/830	0.51	0/1123
1	R	0.31	0/830	0.51	0/1123
1	S	0.31	0/830	0.51	0/1123
1	T	0.30	0/830	0.50	0/1123
1	U	0.31	0/830	0.51	0/1123
1	V	0.31	0/830	0.51	0/1123
1	W	0.32	0/830	0.50	0/1123
1	X	0.30	0/830	0.50	0/1123
1	Y	0.31	0/830	0.51	0/1123
1	Z	0.31	0/830	0.51	0/1123
1	a	0.30	0/830	0.51	0/1123
1	b	0.32	0/830	0.51	0/1123
1	c	0.31	0/830	0.51	0/1123
1	d	0.30	0/830	0.50	0/1123
1	e	0.30	0/830	0.51	0/1123
1	f	0.31	0/830	0.51	0/1123
1	g	0.30	0/830	0.50	0/1123
1	h	0.30	0/830	0.51	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	i	0.30	0/830	0.50	0/1123
1	j	0.31	0/830	0.50	0/1123
1	k	0.31	0/830	0.51	0/1123
1	l	0.31	0/830	0.51	0/1123
1	m	0.31	0/830	0.51	0/1123
1	n	0.30	0/830	0.50	0/1123
1	o	0.32	0/830	0.51	0/1123
1	p	0.31	0/830	0.51	0/1123
1	q	0.31	0/830	0.51	0/1123
1	r	0.30	0/830	0.51	0/1123
1	s	0.29	0/830	0.51	0/1123
1	t	0.31	0/830	0.51	0/1123
1	u	0.31	0/830	0.51	0/1123
1	v	0.31	0/830	0.51	0/1123
All	All	0.31	0/39840	0.51	0/53904

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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	109/119 (92%)	109 (100%)	0	0	100	100
1	B	109/119 (92%)	107 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	109/119 (92%)	109 (100%)	0	0	100	100
1	D	109/119 (92%)	109 (100%)	0	0	100	100
1	E	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	F	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	G	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	H	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	I	109/119 (92%)	109 (100%)	0	0	100	100
1	J	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	K	109/119 (92%)	109 (100%)	0	0	100	100
1	L	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	M	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	N	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	O	109/119 (92%)	107 (98%)	2 (2%)	0	100	100
1	P	109/119 (92%)	109 (100%)	0	0	100	100
1	Q	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	R	109/119 (92%)	109 (100%)	0	0	100	100
1	S	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	T	109/119 (92%)	109 (100%)	0	0	100	100
1	U	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	V	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	W	109/119 (92%)	107 (98%)	2 (2%)	0	100	100
1	X	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	Y	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	Z	109/119 (92%)	109 (100%)	0	0	100	100
1	a	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	b	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	c	109/119 (92%)	109 (100%)	0	0	100	100
1	d	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	e	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	f	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	g	109/119 (92%)	108 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	h	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	i	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	j	109/119 (92%)	109 (100%)	0	0	100	100
1	k	109/119 (92%)	109 (100%)	0	0	100	100
1	l	109/119 (92%)	109 (100%)	0	0	100	100
1	m	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	n	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	o	109/119 (92%)	109 (100%)	0	0	100	100
1	p	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	q	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	r	109/119 (92%)	109 (100%)	0	0	100	100
1	s	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	t	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	u	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	v	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
All	All	5232/5712 (92%)	5196 (99%)	36 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	B	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	C	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	D	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	E	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	F	86/94 (92%)	83 (96%)	3 (4%)	36	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	H	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	I	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	J	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	K	86/94 (92%)	84 (98%)	2 (2%)	50	76
1	L	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	M	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	N	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	O	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	P	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	Q	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	R	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	S	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	T	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	U	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	V	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	W	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	X	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	Y	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	Z	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	a	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	b	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	c	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	d	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	e	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	f	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	g	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	h	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	i	86/94 (92%)	84 (98%)	2 (2%)	50	76
1	j	86/94 (92%)	84 (98%)	2 (2%)	50	76
1	k	86/94 (92%)	83 (96%)	3 (4%)	36	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	l	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	m	86/94 (92%)	84 (98%)	2 (2%)	50	76
1	n	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	o	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	p	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	q	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	r	86/94 (92%)	84 (98%)	2 (2%)	50	76
1	s	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	t	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	u	86/94 (92%)	83 (96%)	3 (4%)	36	62
1	v	86/94 (92%)	84 (98%)	2 (2%)	50	76
All	All	4128/4512 (92%)	3990 (97%)	138 (3%)	38	64

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	91	SER
1	A	110	LYS
1	B	45	THR
1	B	91	SER
1	B	110	LYS
1	C	45	THR
1	C	91	SER
1	C	110	LYS
1	D	45	THR
1	D	91	SER
1	D	110	LYS
1	E	45	THR
1	E	91	SER
1	E	110	LYS
1	F	45	THR
1	F	91	SER
1	F	110	LYS
1	G	45	THR
1	G	91	SER
1	G	110	LYS
1	H	45	THR

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Mol	Chain	Res	Type
1	H	91	SER
1	H	110	LYS
1	I	45	THR
1	I	91	SER
1	I	110	LYS
1	J	45	THR
1	J	91	SER
1	J	110	LYS
1	K	91	SER
1	K	110	LYS
1	L	45	THR
1	L	91	SER
1	L	110	LYS
1	M	45	THR
1	M	91	SER
1	M	110	LYS
1	N	45	THR
1	N	91	SER
1	N	110	LYS
1	O	45	THR
1	O	91	SER
1	O	110	LYS
1	P	45	THR
1	P	91	SER
1	P	110	LYS
1	Q	45	THR
1	Q	91	SER
1	Q	110	LYS
1	R	45	THR
1	R	91	SER
1	R	110	LYS
1	S	45	THR
1	S	91	SER
1	S	110	LYS
1	T	45	THR
1	T	91	SER
1	T	110	LYS
1	U	45	THR
1	U	91	SER
1	U	110	LYS
1	V	45	THR
1	V	91	SER

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Mol	Chain	Res	Type
1	V	110	LYS
1	W	45	THR
1	W	91	SER
1	W	110	LYS
1	X	45	THR
1	X	91	SER
1	X	110	LYS
1	Y	45	THR
1	Y	91	SER
1	Y	110	LYS
1	Z	45	THR
1	Z	91	SER
1	Z	110	LYS
1	a	45	THR
1	a	91	SER
1	a	110	LYS
1	b	45	THR
1	b	91	SER
1	b	110	LYS
1	c	45	THR
1	c	91	SER
1	c	110	LYS
1	d	45	THR
1	d	91	SER
1	d	110	LYS
1	e	45	THR
1	e	91	SER
1	e	110	LYS
1	f	45	THR
1	f	91	SER
1	f	110	LYS
1	g	45	THR
1	g	91	SER
1	g	110	LYS
1	h	45	THR
1	h	91	SER
1	h	110	LYS
1	i	91	SER
1	i	110	LYS
1	j	91	SER
1	j	110	LYS
1	k	45	THR

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Mol	Chain	Res	Type
1	k	91	SER
1	k	110	LYS
1	l	45	THR
1	l	91	SER
1	l	110	LYS
1	m	91	SER
1	m	110	LYS
1	n	45	THR
1	n	91	SER
1	n	110	LYS
1	o	45	THR
1	o	91	SER
1	o	110	LYS
1	p	45	THR
1	p	91	SER
1	p	110	LYS
1	q	45	THR
1	q	91	SER
1	q	110	LYS
1	r	91	SER
1	r	110	LYS
1	s	45	THR
1	s	91	SER
1	s	110	LYS
1	t	45	THR
1	t	91	SER
1	t	110	LYS
1	u	45	THR
1	u	91	SER
1	u	110	LYS
1	v	91	SER
1	v	110	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	B	8	GLN
1	C	66	HIS
1	D	8	GLN
1	D	66	HIS
1	F	8	GLN

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Mol	Chain	Res	Type
1	F	66	HIS
1	G	8	GLN
1	I	8	GLN
1	I	66	HIS
1	J	66	HIS
1	K	8	GLN
1	L	66	HIS
1	M	8	GLN
1	M	66	HIS
1	O	8	GLN
1	O	66	HIS
1	Q	8	GLN
1	Q	66	HIS
1	R	66	HIS
1	T	8	GLN
1	V	8	GLN
1	V	66	HIS
1	W	66	HIS
1	X	8	GLN
1	Y	8	GLN
1	Y	66	HIS
1	Z	66	HIS
1	a	8	GLN
1	a	66	HIS
1	b	66	HIS
1	c	8	GLN
1	c	66	HIS
1	d	66	HIS
1	e	66	HIS
1	f	8	GLN
1	g	66	HIS
1	h	8	GLN
1	h	66	HIS
1	j	8	GLN
1	j	66	HIS
1	k	8	GLN
1	l	66	HIS
1	m	8	GLN
1	o	8	GLN
1	o	66	HIS
1	q	8	GLN
1	r	66	HIS

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Mol	Chain	Res	Type
1	s	8	GLN
1	t	66	HIS
1	u	8	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides 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 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.