



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:10 PM GMT

PDB ID : 4NWN  
Title : Computationally Designed Two-Component Self-Assembling Tetrahedral Cage T32-28  
Authors : McNamara, D.E.; King, N.P.; Bale, J.B.; Sheffler, W.; Baker, D.; Yeates, T.O.  
Deposited on : 2013-12-06  
Resolution : 4.50 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

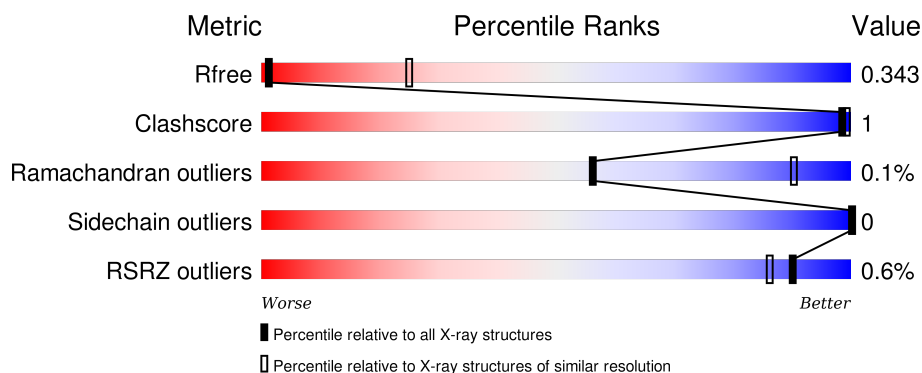
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.50 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.



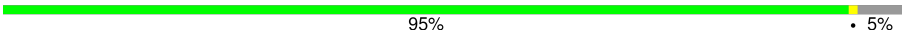
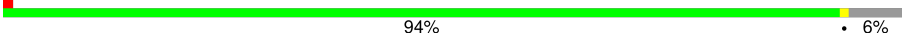

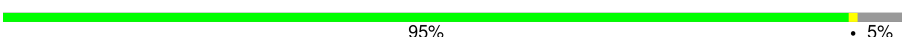

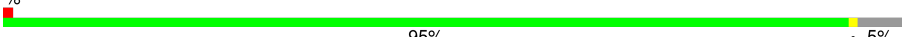




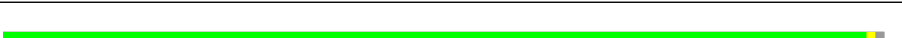


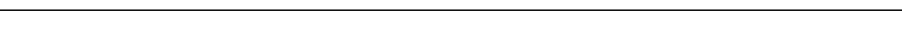
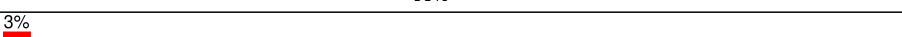
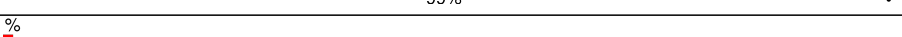
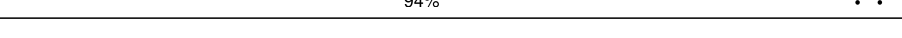
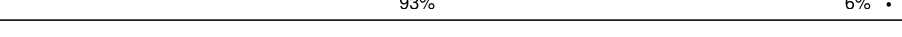
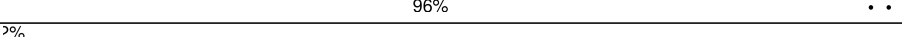
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1071 (5.40-3.60)
Clashscore	102246	1003 (5.30-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	192	<div> <div>95%</div> <div>5%</div> </div>
1	C	192	<div> <div>95%</div> <div>5%</div> </div>
1	E	192	<div> <div>95%</div> <div>• 5%</div> </div>
1	G	192	<div> <div>94%</div> <div>• 5%</div> </div>
1	I	192	<div> <div>95%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	192	 95% • 5%
1	M	192	 94% • 6%
1	O	192	 95% 5%
1	Q	192	 95% • 5%
1	S	192	 94% • 5%
1	U	192	 95% • 5%
1	W	192	 94% • 5%
2	B	159	 97% ..
2	D	159	 95% • •
2	F	159	 94% • •
2	H	159	 97% ..
2	J	159	 99% •
2	L	159	 96% • •
2	N	159	 96% • •
2	P	159	 99% •
2	R	159	 94% • •
2	T	159	 93% 6% •
2	V	159	 96% • •
2	X	159	 97% • •

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20307 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	0	0	0
			902	538	182	182			
1	C	183	Total	C	N	O	0	0	0
			906	540	183	183			
1	E	183	Total	C	N	O	0	0	0
			906	540	183	183			
1	G	183	Total	C	N	O	0	0	0
			906	540	183	183			
1	I	182	Total	C	N	O	0	0	0
			902	538	182	182			
1	K	183	Total	C	N	O	0	0	0
			906	540	183	183			
1	M	181	Total	C	N	O	0	0	0
			897	535	181	181			
1	O	182	Total	C	N	O	0	0	0
			902	538	182	182			
1	Q	183	Total	C	N	O	0	0	0
			906	540	183	183			
1	S	183	Total	C	N	O	0	0	0
			906	540	183	183			
1	U	183	Total	C	N	O	0	0	0
			906	540	183	183			
1	W	183	Total	C	N	O	0	0	0
			906	540	183	183			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	SER	CYS	ENGINEERED MUTATION	UNP K8VQB8
A	114	LEU	ARG	ENGINEERED MUTATION	UNP K8VQB8
A	145	LEU	SER	ENGINEERED MUTATION	UNP K8VQB8
A	148	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8
A	149	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	152	ALA	THR	ENGINEERED MUTATION	UNP K8VQB8
A	153	THR	VAL	ENGINEERED MUTATION	UNP K8VQB8
A	156	LEU	GLU	ENGINEERED MUTATION	UNP K8VQB8
A	157	ALA	SER	ENGINEERED MUTATION	UNP K8VQB8
A	160	ALA	GLU	ENGINEERED MUTATION	UNP K8VQB8
A	167	ALA	ARG	ENGINEERED MUTATION	UNP K8VQB8
A	169	ILE	VAL	ENGINEERED MUTATION	UNP K8VQB8
A	185	LEU	-	EXPRESSION TAG	UNP K8VQB8
A	186	GLU	-	EXPRESSION TAG	UNP K8VQB8
A	187	HIS	-	EXPRESSION TAG	UNP K8VQB8
A	188	HIS	-	EXPRESSION TAG	UNP K8VQB8
A	189	HIS	-	EXPRESSION TAG	UNP K8VQB8
A	190	HIS	-	EXPRESSION TAG	UNP K8VQB8
A	191	HIS	-	EXPRESSION TAG	UNP K8VQB8
A	192	HIS	-	EXPRESSION TAG	UNP K8VQB8
C	38	SER	CYS	ENGINEERED MUTATION	UNP K8VQB8
C	114	LEU	ARG	ENGINEERED MUTATION	UNP K8VQB8
C	145	LEU	SER	ENGINEERED MUTATION	UNP K8VQB8
C	148	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8
C	149	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8
C	152	ALA	THR	ENGINEERED MUTATION	UNP K8VQB8
C	153	THR	VAL	ENGINEERED MUTATION	UNP K8VQB8
C	156	LEU	GLU	ENGINEERED MUTATION	UNP K8VQB8
C	157	ALA	SER	ENGINEERED MUTATION	UNP K8VQB8
C	160	ALA	GLU	ENGINEERED MUTATION	UNP K8VQB8
C	167	ALA	ARG	ENGINEERED MUTATION	UNP K8VQB8
C	169	ILE	VAL	ENGINEERED MUTATION	UNP K8VQB8
C	185	LEU	-	EXPRESSION TAG	UNP K8VQB8
C	186	GLU	-	EXPRESSION TAG	UNP K8VQB8
C	187	HIS	-	EXPRESSION TAG	UNP K8VQB8
C	188	HIS	-	EXPRESSION TAG	UNP K8VQB8
C	189	HIS	-	EXPRESSION TAG	UNP K8VQB8
C	190	HIS	-	EXPRESSION TAG	UNP K8VQB8
C	191	HIS	-	EXPRESSION TAG	UNP K8VQB8
C	192	HIS	-	EXPRESSION TAG	UNP K8VQB8
E	38	SER	CYS	ENGINEERED MUTATION	UNP K8VQB8
E	114	LEU	ARG	ENGINEERED MUTATION	UNP K8VQB8
E	145	LEU	SER	ENGINEERED MUTATION	UNP K8VQB8
E	148	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8
E	149	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8
E	152	ALA	THR	ENGINEERED MUTATION	UNP K8VQB8
E	153	THR	VAL	ENGINEERED MUTATION	UNP K8VQB8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	156	LEU	GLU	ENGINEERED MUTATION	UNP K8VQB8
E	157	ALA	SER	ENGINEERED MUTATION	UNP K8VQB8
E	160	ALA	GLU	ENGINEERED MUTATION	UNP K8VQB8
E	167	ALA	ARG	ENGINEERED MUTATION	UNP K8VQB8
E	169	ILE	VAL	ENGINEERED MUTATION	UNP K8VQB8
E	185	LEU	-	EXPRESSION TAG	UNP K8VQB8
E	186	GLU	-	EXPRESSION TAG	UNP K8VQB8
E	187	HIS	-	EXPRESSION TAG	UNP K8VQB8
E	188	HIS	-	EXPRESSION TAG	UNP K8VQB8
E	189	HIS	-	EXPRESSION TAG	UNP K8VQB8
E	190	HIS	-	EXPRESSION TAG	UNP K8VQB8
E	191	HIS	-	EXPRESSION TAG	UNP K8VQB8
E	192	HIS	-	EXPRESSION TAG	UNP K8VQB8
G	38	SER	CYS	ENGINEERED MUTATION	UNP K8VQB8
G	114	LEU	ARG	ENGINEERED MUTATION	UNP K8VQB8
G	145	LEU	SER	ENGINEERED MUTATION	UNP K8VQB8
G	148	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8
G	149	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8
G	152	ALA	THR	ENGINEERED MUTATION	UNP K8VQB8
G	153	THR	VAL	ENGINEERED MUTATION	UNP K8VQB8
G	156	LEU	GLU	ENGINEERED MUTATION	UNP K8VQB8
G	157	ALA	SER	ENGINEERED MUTATION	UNP K8VQB8
G	160	ALA	GLU	ENGINEERED MUTATION	UNP K8VQB8
G	167	ALA	ARG	ENGINEERED MUTATION	UNP K8VQB8
G	169	ILE	VAL	ENGINEERED MUTATION	UNP K8VQB8
G	185	LEU	-	EXPRESSION TAG	UNP K8VQB8
G	186	GLU	-	EXPRESSION TAG	UNP K8VQB8
G	187	HIS	-	EXPRESSION TAG	UNP K8VQB8
G	188	HIS	-	EXPRESSION TAG	UNP K8VQB8
G	189	HIS	-	EXPRESSION TAG	UNP K8VQB8
G	190	HIS	-	EXPRESSION TAG	UNP K8VQB8
G	191	HIS	-	EXPRESSION TAG	UNP K8VQB8
G	192	HIS	-	EXPRESSION TAG	UNP K8VQB8
I	38	SER	CYS	ENGINEERED MUTATION	UNP K8VQB8
I	114	LEU	ARG	ENGINEERED MUTATION	UNP K8VQB8
I	145	LEU	SER	ENGINEERED MUTATION	UNP K8VQB8
I	148	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8
I	149	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8
I	152	ALA	THR	ENGINEERED MUTATION	UNP K8VQB8
I	153	THR	VAL	ENGINEERED MUTATION	UNP K8VQB8
I	156	LEU	GLU	ENGINEERED MUTATION	UNP K8VQB8
I	157	ALA	SER	ENGINEERED MUTATION	UNP K8VQB8

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Chain	Residue	Modelled	Actual	Comment	Reference
I	160	ALA	GLU	ENGINEERED MUTATION	UNP K8VQB8
I	167	ALA	ARG	ENGINEERED MUTATION	UNP K8VQB8
I	169	ILE	VAL	ENGINEERED MUTATION	UNP K8VQB8
I	185	LEU	-	EXPRESSION TAG	UNP K8VQB8
I	186	GLU	-	EXPRESSION TAG	UNP K8VQB8
I	187	HIS	-	EXPRESSION TAG	UNP K8VQB8
I	188	HIS	-	EXPRESSION TAG	UNP K8VQB8
I	189	HIS	-	EXPRESSION TAG	UNP K8VQB8
I	190	HIS	-	EXPRESSION TAG	UNP K8VQB8
I	191	HIS	-	EXPRESSION TAG	UNP K8VQB8
I	192	HIS	-	EXPRESSION TAG	UNP K8VQB8
K	38	SER	CYS	ENGINEERED MUTATION	UNP K8VQB8
K	114	LEU	ARG	ENGINEERED MUTATION	UNP K8VQB8
K	145	LEU	SER	ENGINEERED MUTATION	UNP K8VQB8
K	148	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8
K	149	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8
K	152	ALA	THR	ENGINEERED MUTATION	UNP K8VQB8
K	153	THR	VAL	ENGINEERED MUTATION	UNP K8VQB8
K	156	LEU	GLU	ENGINEERED MUTATION	UNP K8VQB8
K	157	ALA	SER	ENGINEERED MUTATION	UNP K8VQB8
K	160	ALA	GLU	ENGINEERED MUTATION	UNP K8VQB8
K	167	ALA	ARG	ENGINEERED MUTATION	UNP K8VQB8
K	169	ILE	VAL	ENGINEERED MUTATION	UNP K8VQB8
K	185	LEU	-	EXPRESSION TAG	UNP K8VQB8
K	186	GLU	-	EXPRESSION TAG	UNP K8VQB8
K	187	HIS	-	EXPRESSION TAG	UNP K8VQB8
K	188	HIS	-	EXPRESSION TAG	UNP K8VQB8
K	189	HIS	-	EXPRESSION TAG	UNP K8VQB8
K	190	HIS	-	EXPRESSION TAG	UNP K8VQB8
K	191	HIS	-	EXPRESSION TAG	UNP K8VQB8
K	192	HIS	-	EXPRESSION TAG	UNP K8VQB8
M	38	SER	CYS	ENGINEERED MUTATION	UNP K8VQB8
M	114	LEU	ARG	ENGINEERED MUTATION	UNP K8VQB8
M	145	LEU	SER	ENGINEERED MUTATION	UNP K8VQB8
M	148	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8
M	149	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8
M	152	ALA	THR	ENGINEERED MUTATION	UNP K8VQB8
M	153	THR	VAL	ENGINEERED MUTATION	UNP K8VQB8
M	156	LEU	GLU	ENGINEERED MUTATION	UNP K8VQB8
M	157	ALA	SER	ENGINEERED MUTATION	UNP K8VQB8
M	160	ALA	GLU	ENGINEERED MUTATION	UNP K8VQB8
M	167	ALA	ARG	ENGINEERED MUTATION	UNP K8VQB8

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Chain	Residue	Modelled	Actual	Comment	Reference
M	169	ILE	VAL	ENGINEERED MUTATION	UNP K8VQB8
M	185	LEU	-	EXPRESSION TAG	UNP K8VQB8
M	186	GLU	-	EXPRESSION TAG	UNP K8VQB8
M	187	HIS	-	EXPRESSION TAG	UNP K8VQB8
M	188	HIS	-	EXPRESSION TAG	UNP K8VQB8
M	189	HIS	-	EXPRESSION TAG	UNP K8VQB8
M	190	HIS	-	EXPRESSION TAG	UNP K8VQB8
M	191	HIS	-	EXPRESSION TAG	UNP K8VQB8
M	192	HIS	-	EXPRESSION TAG	UNP K8VQB8
O	38	SER	CYS	ENGINEERED MUTATION	UNP K8VQB8
O	114	LEU	ARG	ENGINEERED MUTATION	UNP K8VQB8
O	145	LEU	SER	ENGINEERED MUTATION	UNP K8VQB8
O	148	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8
O	149	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8
O	152	ALA	THR	ENGINEERED MUTATION	UNP K8VQB8
O	153	THR	VAL	ENGINEERED MUTATION	UNP K8VQB8
O	156	LEU	GLU	ENGINEERED MUTATION	UNP K8VQB8
O	157	ALA	SER	ENGINEERED MUTATION	UNP K8VQB8
O	160	ALA	GLU	ENGINEERED MUTATION	UNP K8VQB8
O	167	ALA	ARG	ENGINEERED MUTATION	UNP K8VQB8
O	169	ILE	VAL	ENGINEERED MUTATION	UNP K8VQB8
O	185	LEU	-	EXPRESSION TAG	UNP K8VQB8
O	186	GLU	-	EXPRESSION TAG	UNP K8VQB8
O	187	HIS	-	EXPRESSION TAG	UNP K8VQB8
O	188	HIS	-	EXPRESSION TAG	UNP K8VQB8
O	189	HIS	-	EXPRESSION TAG	UNP K8VQB8
O	190	HIS	-	EXPRESSION TAG	UNP K8VQB8
O	191	HIS	-	EXPRESSION TAG	UNP K8VQB8
O	192	HIS	-	EXPRESSION TAG	UNP K8VQB8
Q	38	SER	CYS	ENGINEERED MUTATION	UNP K8VQB8
Q	114	LEU	ARG	ENGINEERED MUTATION	UNP K8VQB8
Q	145	LEU	SER	ENGINEERED MUTATION	UNP K8VQB8
Q	148	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8
Q	149	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8
Q	152	ALA	THR	ENGINEERED MUTATION	UNP K8VQB8
Q	153	THR	VAL	ENGINEERED MUTATION	UNP K8VQB8
Q	156	LEU	GLU	ENGINEERED MUTATION	UNP K8VQB8
Q	157	ALA	SER	ENGINEERED MUTATION	UNP K8VQB8
Q	160	ALA	GLU	ENGINEERED MUTATION	UNP K8VQB8
Q	167	ALA	ARG	ENGINEERED MUTATION	UNP K8VQB8
Q	169	ILE	VAL	ENGINEERED MUTATION	UNP K8VQB8
Q	185	LEU	-	EXPRESSION TAG	UNP K8VQB8

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	186	GLU	-	EXPRESSION TAG	UNP K8VQB8
Q	187	HIS	-	EXPRESSION TAG	UNP K8VQB8
Q	188	HIS	-	EXPRESSION TAG	UNP K8VQB8
Q	189	HIS	-	EXPRESSION TAG	UNP K8VQB8
Q	190	HIS	-	EXPRESSION TAG	UNP K8VQB8
Q	191	HIS	-	EXPRESSION TAG	UNP K8VQB8
Q	192	HIS	-	EXPRESSION TAG	UNP K8VQB8
S	38	SER	CYS	ENGINEERED MUTATION	UNP K8VQB8
S	114	LEU	ARG	ENGINEERED MUTATION	UNP K8VQB8
S	145	LEU	SER	ENGINEERED MUTATION	UNP K8VQB8
S	148	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8
S	149	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8
S	152	ALA	THR	ENGINEERED MUTATION	UNP K8VQB8
S	153	THR	VAL	ENGINEERED MUTATION	UNP K8VQB8
S	156	LEU	GLU	ENGINEERED MUTATION	UNP K8VQB8
S	157	ALA	SER	ENGINEERED MUTATION	UNP K8VQB8
S	160	ALA	GLU	ENGINEERED MUTATION	UNP K8VQB8
S	167	ALA	ARG	ENGINEERED MUTATION	UNP K8VQB8
S	169	ILE	VAL	ENGINEERED MUTATION	UNP K8VQB8
S	185	LEU	-	EXPRESSION TAG	UNP K8VQB8
S	186	GLU	-	EXPRESSION TAG	UNP K8VQB8
S	187	HIS	-	EXPRESSION TAG	UNP K8VQB8
S	188	HIS	-	EXPRESSION TAG	UNP K8VQB8
S	189	HIS	-	EXPRESSION TAG	UNP K8VQB8
S	190	HIS	-	EXPRESSION TAG	UNP K8VQB8
S	191	HIS	-	EXPRESSION TAG	UNP K8VQB8
S	192	HIS	-	EXPRESSION TAG	UNP K8VQB8
U	38	SER	CYS	ENGINEERED MUTATION	UNP K8VQB8
U	114	LEU	ARG	ENGINEERED MUTATION	UNP K8VQB8
U	145	LEU	SER	ENGINEERED MUTATION	UNP K8VQB8
U	148	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8
U	149	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8
U	152	ALA	THR	ENGINEERED MUTATION	UNP K8VQB8
U	153	THR	VAL	ENGINEERED MUTATION	UNP K8VQB8
U	156	LEU	GLU	ENGINEERED MUTATION	UNP K8VQB8
U	157	ALA	SER	ENGINEERED MUTATION	UNP K8VQB8
U	160	ALA	GLU	ENGINEERED MUTATION	UNP K8VQB8
U	167	ALA	ARG	ENGINEERED MUTATION	UNP K8VQB8
U	169	ILE	VAL	ENGINEERED MUTATION	UNP K8VQB8
U	185	LEU	-	EXPRESSION TAG	UNP K8VQB8
U	186	GLU	-	EXPRESSION TAG	UNP K8VQB8
U	187	HIS	-	EXPRESSION TAG	UNP K8VQB8

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Chain	Residue	Modelled	Actual	Comment	Reference
U	188	HIS	-	EXPRESSION TAG	UNP K8VQB8
U	189	HIS	-	EXPRESSION TAG	UNP K8VQB8
U	190	HIS	-	EXPRESSION TAG	UNP K8VQB8
U	191	HIS	-	EXPRESSION TAG	UNP K8VQB8
U	192	HIS	-	EXPRESSION TAG	UNP K8VQB8
W	38	SER	CYS	ENGINEERED MUTATION	UNP K8VQB8
W	114	LEU	ARG	ENGINEERED MUTATION	UNP K8VQB8
W	145	LEU	SER	ENGINEERED MUTATION	UNP K8VQB8
W	148	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8
W	149	ALA	ASN	ENGINEERED MUTATION	UNP K8VQB8
W	152	ALA	THR	ENGINEERED MUTATION	UNP K8VQB8
W	153	THR	VAL	ENGINEERED MUTATION	UNP K8VQB8
W	156	LEU	GLU	ENGINEERED MUTATION	UNP K8VQB8
W	157	ALA	SER	ENGINEERED MUTATION	UNP K8VQB8
W	160	ALA	GLU	ENGINEERED MUTATION	UNP K8VQB8
W	167	ALA	ARG	ENGINEERED MUTATION	UNP K8VQB8
W	169	ILE	VAL	ENGINEERED MUTATION	UNP K8VQB8
W	185	LEU	-	EXPRESSION TAG	UNP K8VQB8
W	186	GLU	-	EXPRESSION TAG	UNP K8VQB8
W	187	HIS	-	EXPRESSION TAG	UNP K8VQB8
W	188	HIS	-	EXPRESSION TAG	UNP K8VQB8
W	189	HIS	-	EXPRESSION TAG	UNP K8VQB8
W	190	HIS	-	EXPRESSION TAG	UNP K8VQB8
W	191	HIS	-	EXPRESSION TAG	UNP K8VQB8
W	192	HIS	-	EXPRESSION TAG	UNP K8VQB8

- Molecule 2 is a protein called Propanediol utilization: polyhedral bodies pduT.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	157	Total	C	N	O	0	0	0
			790	476	157	157			
2	D	157	Total	C	N	O	0	0	0
			790	476	157	157			
2	F	157	Total	C	N	O	0	0	0
			790	476	157	157			
2	H	157	Total	C	N	O	0	0	0
			790	476	157	157			
2	J	157	Total	C	N	O	0	0	0
			790	476	157	157			
2	L	157	Total	C	N	O	0	0	0
			790	476	157	157			
2	N	157	Total	C	N	O	0	0	0
			790	476	157	157			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	157	Total	C	N	O	0	0	0
			766	452	157	157			
2	R	157	Total	C	N	O	0	0	0
			790	476	157	157			
2	T	157	Total	C	N	O	0	0	0
			790	476	157	157			
2	V	157	Total	C	N	O	0	0	0
			790	476	157	157			
2	X	157	Total	C	N	O	0	0	0
			790	476	157	157			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	EXPRESSION TAG	UNP A1W1R1
B	71	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1
B	73	ALA	LYS	ENGINEERED MUTATION	UNP A1W1R1
B	75	ALA	THR	ENGINEERED MUTATION	UNP A1W1R1
B	82	THR	ARG	ENGINEERED MUTATION	UNP A1W1R1
B	114	THR	ASN	ENGINEERED MUTATION	UNP A1W1R1
B	116	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1
B	120	LEU	TYR	ENGINEERED MUTATION	UNP A1W1R1
B	147	VAL	LYS	ENGINEERED MUTATION	UNP A1W1R1
B	149	THR	ASP	ENGINEERED MUTATION	UNP A1W1R1
B	151	PHE	LYS	ENGINEERED MUTATION	UNP A1W1R1
D	1	MET	-	EXPRESSION TAG	UNP A1W1R1
D	71	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1
D	73	ALA	LYS	ENGINEERED MUTATION	UNP A1W1R1
D	75	ALA	THR	ENGINEERED MUTATION	UNP A1W1R1
D	82	THR	ARG	ENGINEERED MUTATION	UNP A1W1R1
D	114	THR	ASN	ENGINEERED MUTATION	UNP A1W1R1
D	116	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1
D	120	LEU	TYR	ENGINEERED MUTATION	UNP A1W1R1
D	147	VAL	LYS	ENGINEERED MUTATION	UNP A1W1R1
D	149	THR	ASP	ENGINEERED MUTATION	UNP A1W1R1
D	151	PHE	LYS	ENGINEERED MUTATION	UNP A1W1R1
F	1	MET	-	EXPRESSION TAG	UNP A1W1R1
F	71	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1
F	73	ALA	LYS	ENGINEERED MUTATION	UNP A1W1R1
F	75	ALA	THR	ENGINEERED MUTATION	UNP A1W1R1
F	82	THR	ARG	ENGINEERED MUTATION	UNP A1W1R1
F	114	THR	ASN	ENGINEERED MUTATION	UNP A1W1R1
F	116	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	120	LEU	TYR	ENGINEERED MUTATION	UNP A1W1R1
F	147	VAL	LYS	ENGINEERED MUTATION	UNP A1W1R1
F	149	THR	ASP	ENGINEERED MUTATION	UNP A1W1R1
F	151	PHE	LYS	ENGINEERED MUTATION	UNP A1W1R1
H	1	MET	-	EXPRESSION TAG	UNP A1W1R1
H	71	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1
H	73	ALA	LYS	ENGINEERED MUTATION	UNP A1W1R1
H	75	ALA	THR	ENGINEERED MUTATION	UNP A1W1R1
H	82	THR	ARG	ENGINEERED MUTATION	UNP A1W1R1
H	114	THR	ASN	ENGINEERED MUTATION	UNP A1W1R1
H	116	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1
H	120	LEU	TYR	ENGINEERED MUTATION	UNP A1W1R1
H	147	VAL	LYS	ENGINEERED MUTATION	UNP A1W1R1
H	149	THR	ASP	ENGINEERED MUTATION	UNP A1W1R1
H	151	PHE	LYS	ENGINEERED MUTATION	UNP A1W1R1
J	1	MET	-	EXPRESSION TAG	UNP A1W1R1
J	71	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1
J	73	ALA	LYS	ENGINEERED MUTATION	UNP A1W1R1
J	75	ALA	THR	ENGINEERED MUTATION	UNP A1W1R1
J	82	THR	ARG	ENGINEERED MUTATION	UNP A1W1R1
J	114	THR	ASN	ENGINEERED MUTATION	UNP A1W1R1
J	116	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1
J	120	LEU	TYR	ENGINEERED MUTATION	UNP A1W1R1
J	147	VAL	LYS	ENGINEERED MUTATION	UNP A1W1R1
J	149	THR	ASP	ENGINEERED MUTATION	UNP A1W1R1
J	151	PHE	LYS	ENGINEERED MUTATION	UNP A1W1R1
L	1	MET	-	EXPRESSION TAG	UNP A1W1R1
L	71	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1
L	73	ALA	LYS	ENGINEERED MUTATION	UNP A1W1R1
L	75	ALA	THR	ENGINEERED MUTATION	UNP A1W1R1
L	82	THR	ARG	ENGINEERED MUTATION	UNP A1W1R1
L	114	THR	ASN	ENGINEERED MUTATION	UNP A1W1R1
L	116	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1
L	120	LEU	TYR	ENGINEERED MUTATION	UNP A1W1R1
L	147	VAL	LYS	ENGINEERED MUTATION	UNP A1W1R1
L	149	THR	ASP	ENGINEERED MUTATION	UNP A1W1R1
L	151	PHE	LYS	ENGINEERED MUTATION	UNP A1W1R1
N	1	MET	-	EXPRESSION TAG	UNP A1W1R1
N	71	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1
N	73	ALA	LYS	ENGINEERED MUTATION	UNP A1W1R1
N	75	ALA	THR	ENGINEERED MUTATION	UNP A1W1R1
N	82	THR	ARG	ENGINEERED MUTATION	UNP A1W1R1

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Chain	Residue	Modelled	Actual	Comment	Reference
N	114	THR	ASN	ENGINEERED MUTATION	UNP A1W1R1
N	116	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1
N	120	LEU	TYR	ENGINEERED MUTATION	UNP A1W1R1
N	147	VAL	LYS	ENGINEERED MUTATION	UNP A1W1R1
N	149	THR	ASP	ENGINEERED MUTATION	UNP A1W1R1
N	151	PHE	LYS	ENGINEERED MUTATION	UNP A1W1R1
P	1	MET	-	EXPRESSION TAG	UNP A1W1R1
P	71	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1
P	73	ALA	LYS	ENGINEERED MUTATION	UNP A1W1R1
P	75	ALA	THR	ENGINEERED MUTATION	UNP A1W1R1
P	82	THR	ARG	ENGINEERED MUTATION	UNP A1W1R1
P	114	THR	ASN	ENGINEERED MUTATION	UNP A1W1R1
P	116	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1
P	120	LEU	TYR	ENGINEERED MUTATION	UNP A1W1R1
P	147	VAL	LYS	ENGINEERED MUTATION	UNP A1W1R1
P	149	THR	ASP	ENGINEERED MUTATION	UNP A1W1R1
P	151	PHE	LYS	ENGINEERED MUTATION	UNP A1W1R1
R	1	MET	-	EXPRESSION TAG	UNP A1W1R1
R	71	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1
R	73	ALA	LYS	ENGINEERED MUTATION	UNP A1W1R1
R	75	ALA	THR	ENGINEERED MUTATION	UNP A1W1R1
R	82	THR	ARG	ENGINEERED MUTATION	UNP A1W1R1
R	114	THR	ASN	ENGINEERED MUTATION	UNP A1W1R1
R	116	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1
R	120	LEU	TYR	ENGINEERED MUTATION	UNP A1W1R1
R	147	VAL	LYS	ENGINEERED MUTATION	UNP A1W1R1
R	149	THR	ASP	ENGINEERED MUTATION	UNP A1W1R1
R	151	PHE	LYS	ENGINEERED MUTATION	UNP A1W1R1
T	1	MET	-	EXPRESSION TAG	UNP A1W1R1
T	71	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1
T	73	ALA	LYS	ENGINEERED MUTATION	UNP A1W1R1
T	75	ALA	THR	ENGINEERED MUTATION	UNP A1W1R1
T	82	THR	ARG	ENGINEERED MUTATION	UNP A1W1R1
T	114	THR	ASN	ENGINEERED MUTATION	UNP A1W1R1
T	116	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1
T	120	LEU	TYR	ENGINEERED MUTATION	UNP A1W1R1
T	147	VAL	LYS	ENGINEERED MUTATION	UNP A1W1R1
T	149	THR	ASP	ENGINEERED MUTATION	UNP A1W1R1
T	151	PHE	LYS	ENGINEERED MUTATION	UNP A1W1R1
V	1	MET	-	EXPRESSION TAG	UNP A1W1R1
V	71	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1
V	73	ALA	LYS	ENGINEERED MUTATION	UNP A1W1R1

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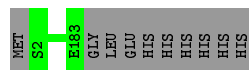
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Chain	Residue	Modelled	Actual	Comment	Reference
V	75	ALA	THR	ENGINEERED MUTATION	UNP A1W1R1
V	82	THR	ARG	ENGINEERED MUTATION	UNP A1W1R1
V	114	THR	ASN	ENGINEERED MUTATION	UNP A1W1R1
V	116	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1
V	120	LEU	TYR	ENGINEERED MUTATION	UNP A1W1R1
V	147	VAL	LYS	ENGINEERED MUTATION	UNP A1W1R1
V	149	THR	ASP	ENGINEERED MUTATION	UNP A1W1R1
V	151	PHE	LYS	ENGINEERED MUTATION	UNP A1W1R1
X	1	MET	-	EXPRESSION TAG	UNP A1W1R1
X	71	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1
X	73	ALA	LYS	ENGINEERED MUTATION	UNP A1W1R1
X	75	ALA	THR	ENGINEERED MUTATION	UNP A1W1R1
X	82	THR	ARG	ENGINEERED MUTATION	UNP A1W1R1
X	114	THR	ASN	ENGINEERED MUTATION	UNP A1W1R1
X	116	ALA	GLU	ENGINEERED MUTATION	UNP A1W1R1
X	120	LEU	TYR	ENGINEERED MUTATION	UNP A1W1R1
X	147	VAL	LYS	ENGINEERED MUTATION	UNP A1W1R1
X	149	THR	ASP	ENGINEERED MUTATION	UNP A1W1R1
X	151	PHE	LYS	ENGINEERED MUTATION	UNP A1W1R1

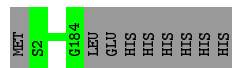
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: Uncharacterized protein



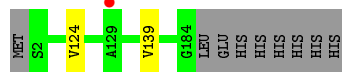
- Molecule 1: Uncharacterized protein



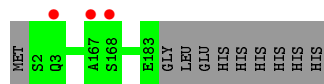
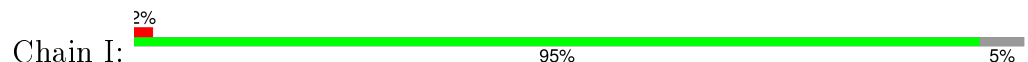
- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein

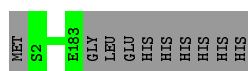




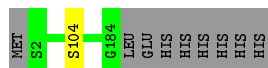
- Molecule 1: Uncharacterized protein



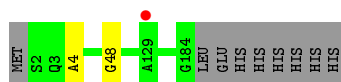
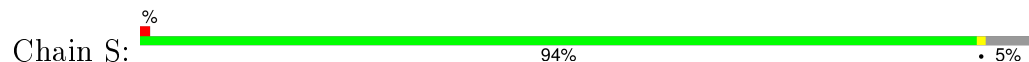
- Molecule 1: Uncharacterized protein



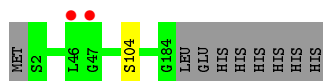
- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



- Molecule 2: Propanediol utilization: polyhedral bodies pduT







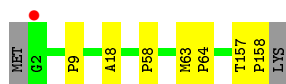
- Molecule 2: Propanediol utilization: polyhedral bodies pduT

Chain D: 95%



- Molecule 2: Propanediol utilization: polyhedral bodies pduT

Chain F: 94%



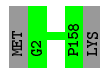
- Molecule 2: Propanediol utilization: polyhedral bodies pduT

Chain H: 97%



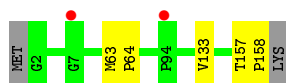
- Molecule 2: Propanediol utilization: polyhedral bodies pduT

Chain J: 99%



- Molecule 2: Propanediol utilization: polyhedral bodies pduT

Chain L: 96%



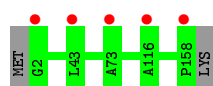
- Molecule 2: Propanediol utilization: polyhedral bodies pduT

Chain N: 96%

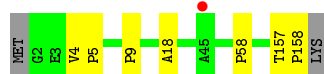


- Molecule 2: Propanediol utilization: polyhedral bodies pduT

Chain P: 99%



- Molecule 2: Propanediol utilization: polyhedral bodies pduT



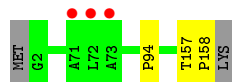
- Molecule 2: Propanediol utilization: polyhedral bodies pduT



- Molecule 2: Propanediol utilization: polyhedral bodies pduT



- Molecule 2: Propanediol utilization: polyhedral bodies pduT



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	246.01Å 246.01Å 290.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	93.93 – 4.50 93.93 – 4.50	Depositor EDS
% Data completeness (in resolution range)	98.3 (93.93-4.50) 98.3 (93.93-4.50)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 4.47Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.297 , 0.343 0.297 , 0.343	Depositor DCC
$R_{free}$ test set	5980 reflections (10.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	184.0	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 1219.7	EDS
Estimated twinning fraction	0.055 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 59814 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	20307	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	216.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.19	0/906	0.38	0/1260
1	C	0.19	0/910	0.38	0/1265
1	E	0.19	0/910	0.38	0/1265
1	G	0.18	0/910	0.37	0/1265
1	I	0.18	0/906	0.38	0/1260
1	K	0.18	0/910	0.38	0/1265
1	M	0.18	0/901	0.37	0/1253
1	O	0.18	0/906	0.37	0/1260
1	Q	0.18	0/910	0.38	0/1265
1	S	0.18	0/910	0.38	0/1265
1	U	0.18	0/910	0.37	0/1265
1	W	0.18	0/910	0.38	0/1265
2	B	0.19	0/801	0.36	0/1118
2	D	0.19	0/801	0.36	0/1118
2	F	0.19	0/801	0.37	0/1118
2	H	0.19	0/801	0.36	0/1118
2	J	0.19	0/801	0.37	0/1118
2	L	0.19	0/801	0.36	0/1118
2	N	0.19	0/801	0.37	0/1118
2	P	0.18	0/765	0.34	0/1058
2	R	0.19	0/801	0.36	0/1118
2	T	0.19	0/801	0.36	0/1118
2	V	0.19	0/801	0.36	0/1118
2	X	0.19	0/801	0.36	0/1118
All	All	0.19	0/20475	0.37	0/28509

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 ⓘ

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	902	0	487	0	0
1	C	906	0	490	0	0
1	E	906	0	490	0	0
1	G	906	0	490	1	0
1	I	902	0	487	0	0
1	K	906	0	490	0	0
1	M	897	0	485	0	0
1	O	902	0	487	0	0
1	Q	906	0	490	0	0
1	S	906	0	490	1	0
1	U	906	0	490	0	0
1	W	906	0	490	1	0
2	B	790	0	440	1	0
2	D	790	0	440	3	0
2	F	790	0	440	4	0
2	H	790	0	440	1	0
2	J	790	0	440	0	0
2	L	790	0	440	3	0
2	N	790	0	440	2	0
2	P	766	0	368	0	0
2	R	790	0	440	4	0
2	T	790	0	440	5	0
2	V	790	0	440	3	0
2	X	790	0	440	2	0
All	All	20307	0	11074	28	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 1.

All (28) 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:T:9:PRO:HB3	2:T:18:ALA:HB2	1.96	0.48
2:F:58:PRO:HD3	2:T:94:PRO:HD3	1.95	0.47
2:B:9:PRO:HB3	2:B:18:ALA:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:124:VAL:N	1:G:139:VAL:O	2.43	0.47
2:R:157:THR:HA	2:R:158:PRO:HD3	1.81	0.46
2:F:9:PRO:HB3	2:F:18:ALA:HB2	1.97	0.46
1:W:115:ALA:HB2	1:W:154:ALA:HB2	1.98	0.46
2:D:74:ASN:HA	2:D:115:TYR:HA	1.98	0.45
2:V:157:THR:HA	2:V:158:PRO:HD3	1.81	0.44
2:F:63:MET:HA	2:F:64:PRO:HD3	1.83	0.44
2:L:133:VAL:N	2:V:26:GLU:O	2.49	0.44
2:H:4:VAL:HA	2:H:5:PRO:HD3	1.88	0.44
2:F:157:THR:HA	2:F:158:PRO:HD3	1.81	0.44
2:D:157:THR:HA	2:D:158:PRO:HD3	1.81	0.44
2:N:63:MET:HA	2:N:64:PRO:HD3	1.86	0.44
2:T:157:THR:HA	2:T:158:PRO:HD3	1.82	0.43
2:R:4:VAL:HA	2:R:5:PRO:HD3	1.89	0.43
2:R:58:PRO:HD3	2:X:94:PRO:HD3	2.01	0.43
2:V:57:PHE:HA	2:V:58:PRO:HD3	1.90	0.43
2:X:157:THR:HA	2:X:158:PRO:HD3	1.81	0.42
2:N:53:ASN:HA	2:N:54:PRO:HD3	1.93	0.41
2:R:9:PRO:HB3	2:R:18:ALA:HB2	2.02	0.41
2:D:57:PHE:HA	2:D:58:PRO:HD3	1.88	0.41
2:L:157:THR:HA	2:L:158:PRO:HD3	1.81	0.41
2:T:63:MET:HA	2:T:64:PRO:HD3	1.84	0.41
2:L:63:MET:HA	2:L:64:PRO:HD3	1.83	0.41
2:T:53:ASN:HA	2:T:54:PRO:HD3	1.93	0.41
1:S:4:ALA:N	1:S:48:GLY:O	2.48	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	180/192 (94%)	176 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	181/192 (94%)	175 (97%)	6 (3%)	0	100	100
1	E	181/192 (94%)	175 (97%)	5 (3%)	1 (1%)	30	74
1	G	181/192 (94%)	175 (97%)	6 (3%)	0	100	100
1	I	180/192 (94%)	175 (97%)	5 (3%)	0	100	100
1	K	181/192 (94%)	176 (97%)	4 (2%)	1 (1%)	30	74
1	M	179/192 (93%)	173 (97%)	5 (3%)	1 (1%)	30	74
1	O	180/192 (94%)	174 (97%)	6 (3%)	0	100	100
1	Q	181/192 (94%)	175 (97%)	5 (3%)	1 (1%)	30	74
1	S	181/192 (94%)	175 (97%)	6 (3%)	0	100	100
1	U	181/192 (94%)	175 (97%)	5 (3%)	1 (1%)	30	74
1	W	181/192 (94%)	176 (97%)	4 (2%)	1 (1%)	30	74
2	B	155/159 (98%)	152 (98%)	3 (2%)	0	100	100
2	D	155/159 (98%)	152 (98%)	3 (2%)	0	100	100
2	F	155/159 (98%)	152 (98%)	3 (2%)	0	100	100
2	H	155/159 (98%)	152 (98%)	3 (2%)	0	100	100
2	J	155/159 (98%)	152 (98%)	3 (2%)	0	100	100
2	L	155/159 (98%)	152 (98%)	3 (2%)	0	100	100
2	N	155/159 (98%)	152 (98%)	3 (2%)	0	100	100
2	P	155/159 (98%)	152 (98%)	3 (2%)	0	100	100
2	R	155/159 (98%)	152 (98%)	3 (2%)	0	100	100
2	T	155/159 (98%)	152 (98%)	3 (2%)	0	100	100
2	V	155/159 (98%)	152 (98%)	3 (2%)	0	100	100
2	X	155/159 (98%)	152 (98%)	3 (2%)	0	100	100
All	All	4027/4212 (96%)	3924 (97%)	97 (2%)	6 (0%)	56	90

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	104	SER
1	E	104	SER
1	M	104	SER
1	Q	104	SER
1	U	104	SER
1	W	104	SER

### 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	5/146 (3%)	5 (100%)	0	100	100
1	C	5/146 (3%)	5 (100%)	0	100	100
1	E	5/146 (3%)	5 (100%)	0	100	100
1	G	5/146 (3%)	5 (100%)	0	100	100
1	I	5/146 (3%)	5 (100%)	0	100	100
1	K	5/146 (3%)	5 (100%)	0	100	100
1	M	5/146 (3%)	5 (100%)	0	100	100
1	O	5/146 (3%)	5 (100%)	0	100	100
1	Q	5/146 (3%)	5 (100%)	0	100	100
1	S	5/146 (3%)	5 (100%)	0	100	100
1	U	5/146 (3%)	5 (100%)	0	100	100
1	W	5/146 (3%)	5 (100%)	0	100	100
2	B	12/124 (10%)	12 (100%)	0	100	100
2	D	12/124 (10%)	12 (100%)	0	100	100
2	F	12/124 (10%)	12 (100%)	0	100	100
2	H	12/124 (10%)	12 (100%)	0	100	100
2	J	12/124 (10%)	12 (100%)	0	100	100
2	L	12/124 (10%)	12 (100%)	0	100	100
2	N	12/124 (10%)	12 (100%)	0	100	100
2	R	12/124 (10%)	12 (100%)	0	100	100
2	T	12/124 (10%)	12 (100%)	0	100	100
2	V	12/124 (10%)	12 (100%)	0	100	100
2	X	12/124 (10%)	12 (100%)	0	100	100
All	All	192/3116 (6%)	192 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no



such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	182/192 (94%)	-0.59	0 100 100	53, 139, 307, 477	0
1	C	183/192 (95%)	-0.58	0 100 100	111, 165, 325, 510	0
1	E	183/192 (95%)	-0.54	0 100 100	76, 141, 314, 495	0
1	G	183/192 (95%)	-0.45	1 (0%) 91 88	138, 182, 381, 500	0
1	I	182/192 (94%)	-0.49	3 (1%) 74 65	114, 200, 377, 504	0
1	K	183/192 (95%)	-0.53	0 100 100	82, 172, 308, 480	0
1	M	181/192 (94%)	-0.48	1 (0%) 90 86	110, 163, 348, 484	0
1	O	182/192 (94%)	-0.56	0 100 100	135, 204, 368, 550	0
1	Q	183/192 (95%)	-0.54	0 100 100	98, 215, 389, 522	0
1	S	183/192 (95%)	-0.44	1 (0%) 91 88	157, 240, 407, 540	0
1	U	183/192 (95%)	-0.35	2 (1%) 82 76	210, 256, 424, 542	0
1	W	183/192 (95%)	-0.29	4 (2%) 65 56	134, 274, 452, 511	0
2	B	157/159 (98%)	-0.56	0 100 100	89, 148, 299, 401	0
2	D	157/159 (98%)	-0.65	0 100 100	139, 173, 327, 543	0
2	F	157/159 (98%)	-0.66	1 (0%) 90 86	95, 168, 326, 477	0
2	H	157/159 (98%)	-0.68	0 100 100	111, 155, 290, 407	0
2	J	157/159 (98%)	-0.63	0 100 100	158, 227, 391, 521	0
2	L	157/159 (98%)	-0.39	2 (1%) 79 71	147, 219, 396, 560	0
2	N	157/159 (98%)	-0.57	0 100 100	92, 157, 266, 462	0
2	P	157/159 (98%)	-0.26	5 (3%) 51 40	176, 283, 427, 573	0
2	R	157/159 (98%)	-0.56	1 (0%) 90 86	146, 189, 379, 516	0
2	T	157/159 (98%)	-0.59	0 100 100	123, 197, 338, 482	0
2	V	157/159 (98%)	-0.57	0 100 100	153, 219, 359, 470	0
2	X	157/159 (98%)	-0.35	3 (1%) 70 61	155, 233, 392, 467	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	4075/4212 (96%)	-0.51	24 (0%) 90 86	53, 198, 384, 573	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	X	72	LEU	4.4
1	U	47	GLY	3.5
1	G	129	ALA	3.5
2	P	116	ALA	3.5
1	W	75	ALA	3.3
2	P	73	ALA	3.1
1	W	97	VAL	3.0
1	I	167	ALA	2.9
2	L	7	GLY	2.8
2	P	2	GLY	2.8
2	P	158	PRO	2.7
2	X	71	ALA	2.6
1	U	46	LEU	2.5
1	W	44	LEU	2.3
1	W	30	ASP	2.3
2	R	45	ALA	2.3
1	M	168	SER	2.2
1	I	168	SER	2.2
2	X	73	ALA	2.1
2	P	43	LEU	2.1
1	S	129	ALA	2.0
2	L	94	PRO	2.0
2	F	2	GLY	2.0
1	I	3	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.