



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:19 PM UTC

PDB ID : 4NWN / pdb_00004nwn
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

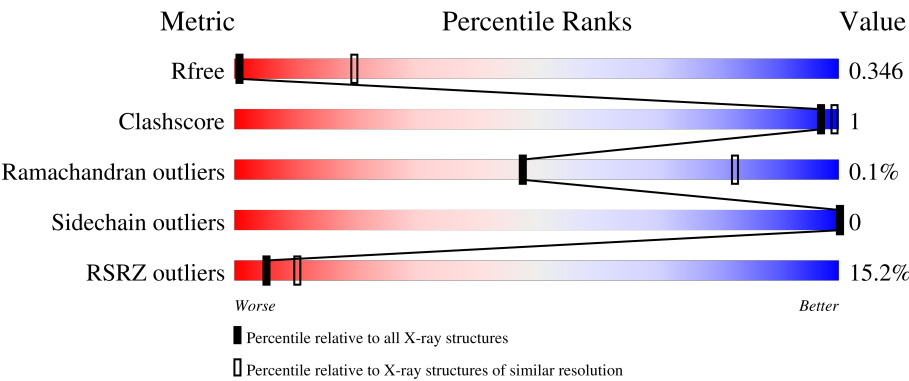
1 Overall quality at a glance i

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}	180053	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

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

Mol	Chain	Length	Quality of chain
1	A	192	9% 95% 5%
1	C	192	8% 95% 5%
1	E	192	10% 95% • 5%
1	G	192	14% 94% • 5%
1	I	192	14% 95% 5%

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Mol	Chain	Length	Quality of chain
1	K	192	
1	M	192	
1	O	192	
1	Q	192	
1	S	192	
1	U	192	
1	W	192	
2	B	159	
2	D	159	
2	F	159	
2	H	159	
2	J	159	
2	L	159	
2	N	159	
2	P	159	
2	R	159	
2	T	159	
2	V	159	
2	X	159	

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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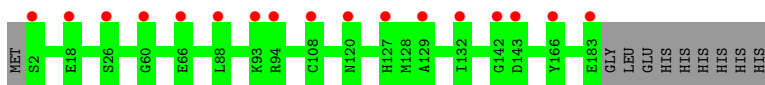
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Chain	Residue	Modelled	Actual	Comment	Reference
V	75	ALA	THR	engineered mutation	UNP A1W1R1
V	82	THR	ARG	engineered mutation	UNP A1W1R1
V	114	THR	ASN	engineered mutation	UNP A1W1R1
V	116	ALA	GLU	engineered mutation	UNP A1W1R1
V	120	LEU	TYR	engineered 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 [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

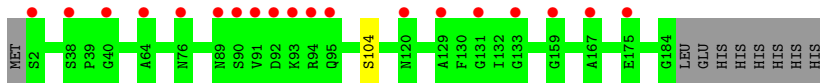
- Molecule 1: Uncharacterized protein



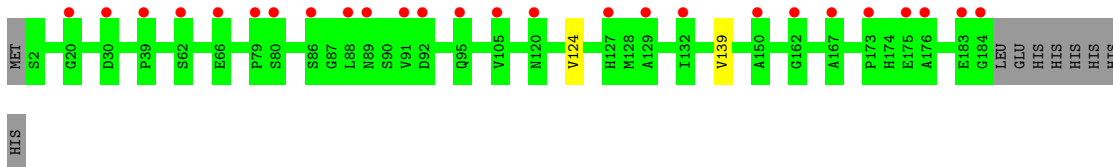
- Molecule 1: Uncharacterized protein



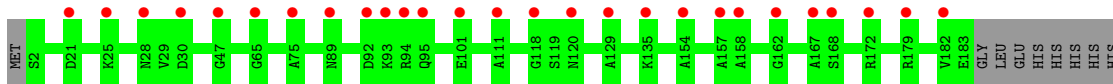
- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



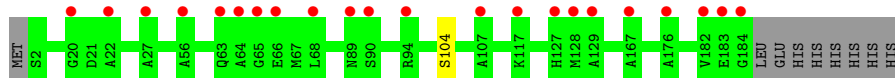
- Molecule 1: Uncharacterized protein



HIS

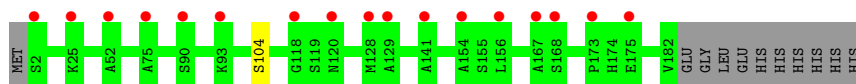
- Molecule 1: Uncharacterized protein

Chain K:  11% 95% 5%



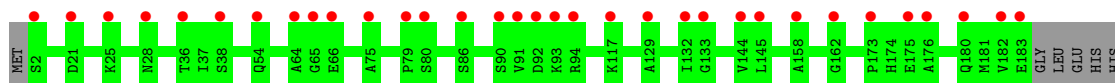
- Molecule 1: Uncharacterized protein

Chain M:  9% 94% 6%



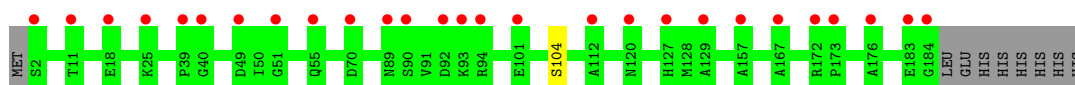
- Molecule 1: Uncharacterized protein

Chain O:  17% 95% 5%

HIS
HIS
HIS
HIS

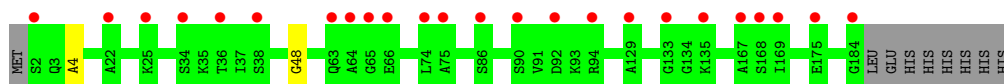
- Molecule 1: Uncharacterized protein

Chain Q:  14% 95% 5%



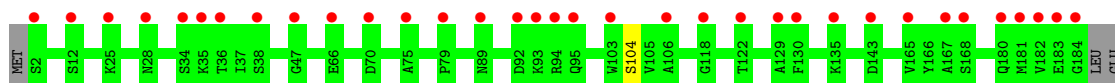
- Molecule 1: Uncharacterized protein

Chain S:  12% 94% 5%



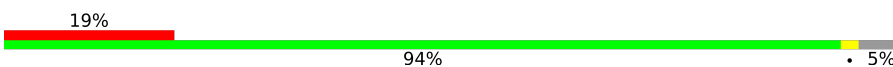
- Molecule 1: Uncharacterized protein

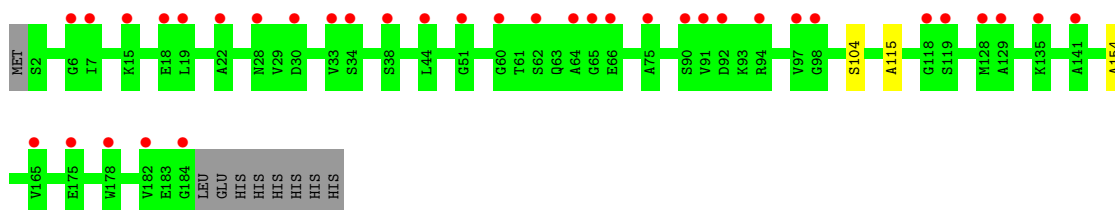
Chain U:  18% 95% 5%



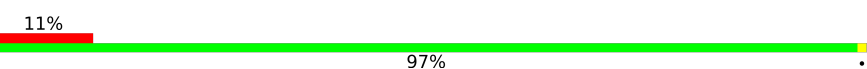
HIS
HIS
HIS
HIS
HIS
HIS

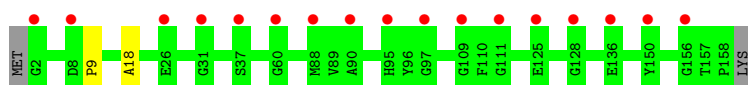
- Molecule 1: Uncharacterized protein

Chain W:  19% 94% 5%

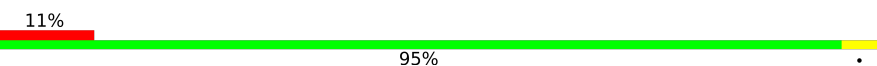


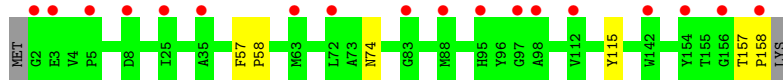
- Molecule 2: Propanediol utilization: polyhedral bodies pduT

Chain B:  11% 97% ..

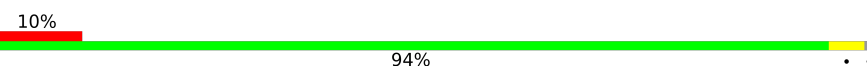


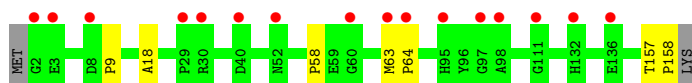
- Molecule 2: Propanediol utilization: polyhedral bodies pduT

Chain D:  11% 95% ..

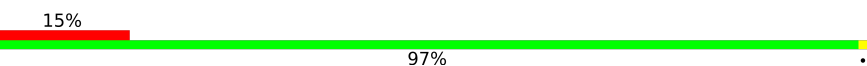


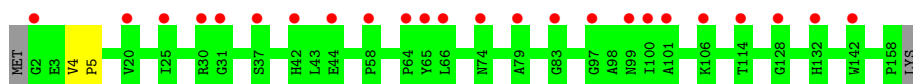
- Molecule 2: Propanediol utilization: polyhedral bodies pduT

Chain F:  10% 94% ..

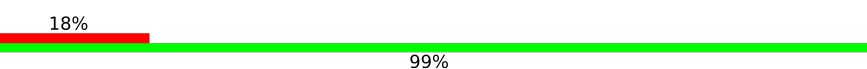


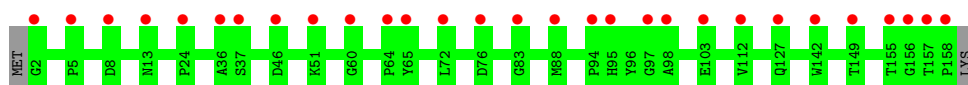
- Molecule 2: Propanediol utilization: polyhedral bodies pduT

Chain H:  15% 97% ..

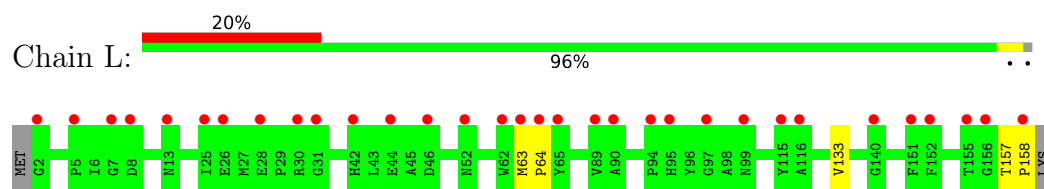


- Molecule 2: Propanediol utilization: polyhedral bodies pduT

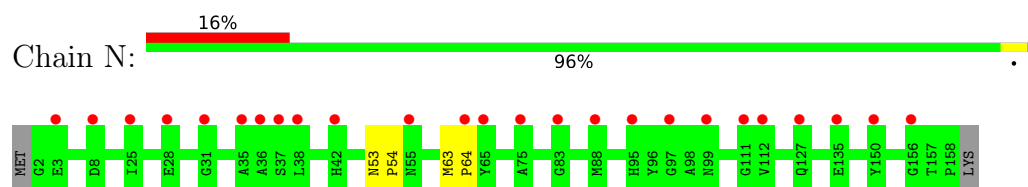
Chain J:  18% 99% .



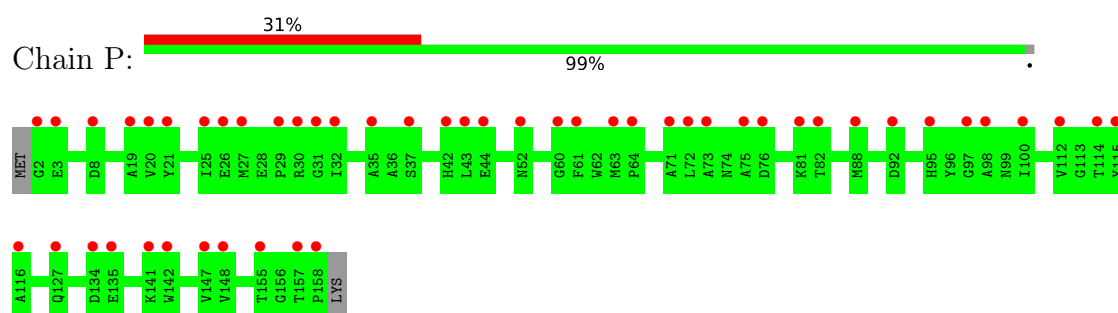
- Molecule 2: Propanediol utilization: polyhedral bodies pduT



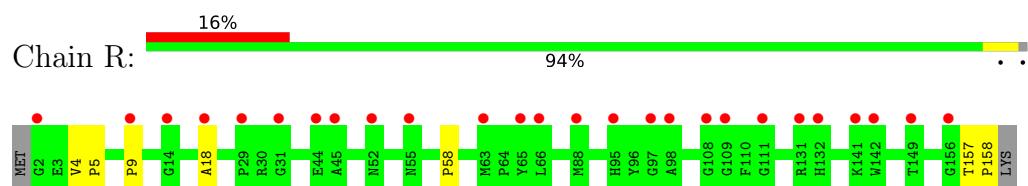
- Molecule 2: Propanediol utilization: polyhedral bodies pduT



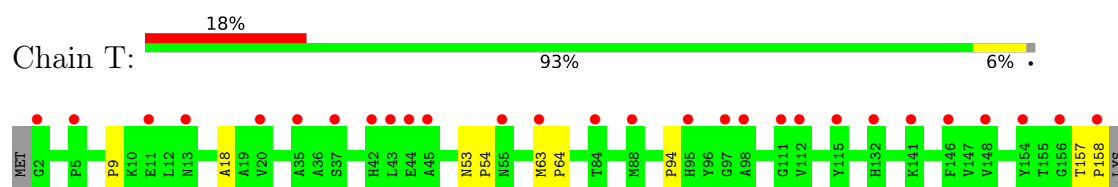
- Molecule 2: Propanediol utilization: polyhedral bodies pduT



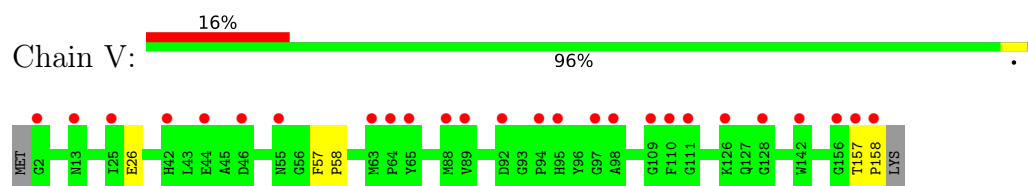
- Molecule 2: Propanediol utilization: polyhedral bodies pduT



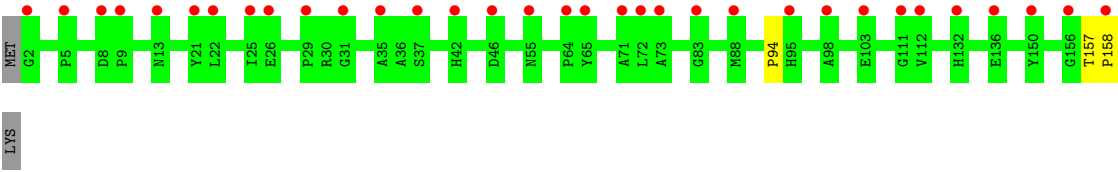
- Molecule 2: Propanediol utilization: polyhedral bodies pduT



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 4.47Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.297 , 0.343 0.309 , 0.346	Depositor DCC
R_{free} test set	5982 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	184.0	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.055 for -h,-k,l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	20307	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0/906	0.84	0/1260
1	C	0.32	0/910	0.82	0/1265
1	E	0.31	0/910	0.82	0/1265
1	G	0.31	0/910	0.83	0/1265
1	I	0.31	0/906	0.86	0/1260
1	K	0.31	0/910	0.84	0/1265
1	M	0.31	0/901	0.83	0/1253
1	O	0.31	0/906	0.84	0/1260
1	Q	0.31	0/910	0.84	0/1265
1	S	0.30	0/910	0.84	0/1265
1	U	0.31	0/910	0.84	0/1265
1	W	0.30	0/910	0.84	0/1265
2	B	0.30	0/801	0.76	0/1118
2	D	0.29	0/801	0.78	0/1118
2	F	0.29	0/801	0.79	0/1118
2	H	0.30	0/801	0.77	0/1118
2	J	0.29	0/801	0.78	0/1118
2	L	0.29	0/801	0.77	0/1118
2	N	0.29	0/801	0.77	0/1118
2	P	0.28	0/765	0.79	0/1058
2	R	0.29	0/801	0.77	0/1118
2	T	0.29	0/801	0.76	0/1118
2	V	0.29	0/801	0.77	0/1118
2	X	0.29	0/801	0.78	0/1118
All	All	0.30	0/20475	0.81	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:B:9:PRO:HB3	2:B:18:ALA:HB2	1.95	0.47
2:F:58:PRO:HD3	2:T:94:PRO:HD3	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:F:157:THR:HA	2:F:158:PRO:HD3	1.81	0.44
2:H:4:VAL:HA	2:H:5:PRO:HD3	1.88	0.44
2:L:133:VAL:N	2:V:26:GLU:O	2.49	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%)	21	58
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%)	21	58
1	M	179/192 (93%)	173 (97%)	5 (3%)	1 (1%)	21	58
1	O	180/192 (94%)	174 (97%)	6 (3%)	0	100	100
1	Q	181/192 (94%)	175 (97%)	5 (3%)	1 (1%)	21	58
1	S	181/192 (94%)	175 (97%)	6 (3%)	0	100	100
1	U	181/192 (94%)	175 (97%)	5 (3%)	1 (1%)	21	58
1	W	181/192 (94%)	176 (97%)	4 (2%)	1 (1%)	21	58
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%)	48	83

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.

Sometimes 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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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, 95th 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 ²)	Q<0.9
1	A	182/192 (94%)	0.42	17 (9%) 14 18	53, 139, 307, 477	0
1	C	183/192 (95%)	0.53	15 (8%) 17 21	111, 165, 325, 510	0
1	E	183/192 (95%)	0.54	19 (10%) 11 16	76, 141, 314, 495	0
1	G	183/192 (95%)	0.81	26 (14%) 6 11	138, 182, 381, 500	0
1	I	182/192 (94%)	0.67	27 (14%) 5 10	114, 200, 377, 504	0
1	K	183/192 (95%)	0.65	22 (12%) 9 13	82, 172, 308, 480	0
1	M	181/192 (94%)	0.67	17 (9%) 14 18	110, 163, 348, 484	0
1	O	182/192 (94%)	0.80	33 (18%) 3 8	135, 204, 368, 550	0
1	Q	183/192 (95%)	0.79	27 (14%) 5 10	98, 215, 389, 522	0
1	S	183/192 (95%)	0.86	24 (13%) 7 12	157, 240, 407, 540	0
1	U	183/192 (95%)	1.04	34 (18%) 3 8	210, 256, 424, 542	0
1	W	183/192 (95%)	1.00	36 (19%) 3 7	134, 274, 452, 511	0
2	B	157/159 (98%)	0.79	17 (10%) 11 15	89, 148, 299, 401	0
2	D	157/159 (98%)	0.81	18 (11%) 9 14	139, 173, 327, 543	0
2	F	157/159 (98%)	0.71	16 (10%) 12 16	95, 168, 326, 477	0
2	H	157/159 (98%)	0.80	24 (15%) 5 10	111, 155, 290, 407	0
2	J	157/159 (98%)	1.04	29 (18%) 3 8	158, 226, 391, 521	0
2	L	157/159 (98%)	1.19	32 (20%) 3 6	147, 219, 396, 560	0
2	N	157/159 (98%)	0.79	25 (15%) 5 9	92, 157, 266, 462	0
2	P	157/159 (98%)	1.50	50 (31%) 1 4	176, 283, 427, 573	0
2	R	157/159 (98%)	0.95	26 (16%) 4 9	146, 189, 379, 516	0
2	T	157/159 (98%)	1.02	28 (17%) 4 8	123, 197, 338, 482	0
2	V	157/159 (98%)	1.03	26 (16%) 4 9	153, 219, 359, 470	0
2	X	157/159 (98%)	1.20	33 (21%) 2 6	155, 233, 392, 467	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4075/4212 (96%)	0.85	621 (15%) 5 10	53, 198, 384, 573	0

All (621) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	97	GLY	10.0
2	R	97	GLY	9.3
2	F	97	GLY	9.3
1	S	184	GLY	8.6
2	B	97	GLY	8.5
2	V	97	GLY	7.7
2	P	157	THR	7.4
2	J	157	THR	7.3
2	N	88	MET	7.2
2	L	97	GLY	7.1
2	J	97	GLY	7.0
2	H	31	GLY	6.9
1	G	92	ASP	6.9
2	V	158	PRO	6.8
2	D	158	PRO	6.6
2	X	29	PRO	6.5
1	M	120	ASN	6.4
2	P	76	ASP	6.3
1	W	28	ASN	6.3
1	O	183	GLU	6.2
2	F	95	HIS	6.1
2	J	37	SER	5.9
1	A	143	ASP	5.9
2	X	72	LEU	5.7
2	H	142	TRP	5.7
2	T	97	GLY	5.6
1	Q	127	HIS	5.6
2	B	31	GLY	5.5
1	S	168	SER	5.5
2	X	9	PRO	5.5
1	W	184	GLY	5.4
2	V	44	GLU	5.4
1	G	184	GLY	5.3
2	L	65	TYR	5.3
2	N	42	HIS	5.2
2	P	98	ALA	5.2
2	P	97	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
1	W	15	LYS	5.2
1	W	18	GLU	5.1
2	R	44	GLU	5.1
2	F	98	ALA	5.1
1	K	90	SER	5.1
2	P	29	PRO	5.1
1	Q	184	GLY	5.1
1	I	167	ALA	5.0
2	T	88	MET	5.0
1	S	63	GLN	5.0
2	B	111	GLY	5.0
1	K	183	GLU	4.9
1	U	129	ALA	4.9
1	O	145	LEU	4.9
2	D	142	TRP	4.9
2	J	51	LYS	4.8
1	I	129	ALA	4.8
1	U	184	GLY	4.8
1	S	133	GLY	4.8
1	E	129	ALA	4.8
1	K	184	GLY	4.8
2	R	98	ALA	4.7
2	P	135	GLU	4.7
1	G	129	ALA	4.7
2	J	156	GLY	4.7
1	C	92	ASP	4.7
1	U	93	LYS	4.7
2	V	25	ILE	4.6
2	L	2	GLY	4.6
2	V	42	HIS	4.6
2	P	31	GLY	4.5
2	P	158	PRO	4.5
2	R	109	GLY	4.5
2	X	98	ALA	4.5
2	H	2	GLY	4.5
2	N	97	GLY	4.5
1	W	34	SER	4.5
1	G	176	ALA	4.4
1	S	129	ALA	4.4
2	R	31	GLY	4.4
2	R	156	GLY	4.4
1	M	175	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
2	P	72	LEU	4.4
1	A	2	SER	4.4
1	U	165	VAL	4.4
1	M	167	ALA	4.4
2	L	95	HIS	4.4
1	C	176	ALA	4.3
1	O	94	ARG	4.3
1	Q	90	SER	4.3
2	L	94	PRO	4.3
2	J	155	THR	4.3
1	W	92	ASP	4.3
1	O	162	GLY	4.3
1	S	135	LYS	4.3
2	J	13	ASN	4.3
2	L	63	MET	4.2
2	T	42	HIS	4.2
2	T	98	ALA	4.2
2	P	25	ILE	4.2
1	O	86	SER	4.2
2	F	132	HIS	4.2
1	U	2	SER	4.2
1	W	75	ALA	4.2
1	Q	18	GLU	4.2
2	F	111	GLY	4.1
2	X	42	HIS	4.1
2	X	5	PRO	4.1
2	P	116	ALA	4.1
2	X	2	GLY	4.1
1	Q	129	ALA	4.1
2	P	73	ALA	4.1
2	P	27	MET	4.1
2	D	8	ASP	4.1
2	R	132	HIS	4.1
1	M	2	SER	4.1
2	T	95	HIS	4.0
2	N	65	TYR	4.0
1	G	88	LEU	4.0
1	S	66	GLU	4.0
2	N	135	GLU	4.0
2	F	2	GLY	4.0
2	F	8	ASP	4.0
2	J	5	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
2	X	88	MET	4.0
1	M	75	ALA	4.0
2	B	8	ASP	4.0
2	R	29	PRO	4.0
2	L	26	GLU	3.9
1	O	133	GLY	3.9
2	V	156	GLY	3.9
2	V	157	THR	3.9
1	I	94	ARG	3.9
2	N	156	GLY	3.9
1	C	184	GLY	3.9
2	P	32	ILE	3.9
2	X	35	ALA	3.9
1	Q	183	GLU	3.9
1	O	92	ASP	3.9
1	Q	25	LYS	3.8
1	W	118	GLY	3.8
2	L	156	GLY	3.8
1	G	91	VAL	3.8
2	T	2	GLY	3.8
1	E	94	ARG	3.8
1	C	127	HIS	3.8
2	T	37	SER	3.8
2	R	63	MET	3.8
2	V	92	ASP	3.8
2	V	88	MET	3.7
1	G	150	ALA	3.7
1	C	120	ASN	3.7
1	Q	49	ASP	3.7
2	T	11	GLU	3.7
1	U	95	GLN	3.7
2	P	37	SER	3.7
1	G	175	GLU	3.7
2	P	75	ALA	3.7
1	S	75	ALA	3.7
2	L	5	PRO	3.6
1	S	175	GLU	3.6
2	P	44	GLU	3.6
2	T	148	VAL	3.6
1	E	38	SER	3.6
1	O	79	PRO	3.6
1	O	66	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	142	GLY	3.6
2	L	90	ALA	3.6
1	I	135	LYS	3.6
1	S	167	ALA	3.6
2	N	95	HIS	3.6
2	N	64	PRO	3.6
2	N	36	ALA	3.6
2	X	112	VAL	3.6
2	V	2	GLY	3.6
1	E	133	GLY	3.5
1	I	95	GLN	3.5
1	Q	94	ARG	3.5
1	O	129	ALA	3.5
1	U	75	ALA	3.5
1	C	25	LYS	3.5
2	P	3	GLU	3.5
2	D	112	VAL	3.5
2	R	88	MET	3.5
1	C	133	GLY	3.5
2	L	62	TRP	3.5
2	V	64	PRO	3.5
2	N	38	LEU	3.4
2	L	42	HIS	3.4
1	I	101	GLU	3.4
1	M	129	ALA	3.4
2	L	140	GLY	3.4
1	W	182	VAL	3.4
2	H	65	TYR	3.4
1	K	89	ASN	3.4
2	X	71	ALA	3.4
2	V	94	PRO	3.4
2	D	35	ALA	3.3
2	L	44	GLU	3.3
1	A	127	HIS	3.3
2	J	2	GLY	3.3
2	X	8	ASP	3.3
2	F	63	MET	3.3
1	O	65	GLY	3.3
2	F	60	GLY	3.3
2	R	108	GLY	3.3
1	M	25	LYS	3.3
1	I	120	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	154	TYR	3.3
1	K	20	GLY	3.3
2	L	46	ASP	3.3
2	V	98	ALA	3.3
1	C	91	VAL	3.3
1	M	168	SER	3.3
2	L	155	THR	3.3
2	H	97	GLY	3.3
1	Q	55	GLN	3.3
1	M	128	MET	3.3
2	J	46	ASP	3.3
2	T	44	GLU	3.2
2	J	64	PRO	3.2
1	I	168	SER	3.2
1	A	93	LYS	3.2
2	P	114	THR	3.2
1	E	90	SER	3.2
2	H	44	GLU	3.2
1	W	22	ALA	3.2
1	G	162	GLY	3.2
1	I	65	GLY	3.2
1	U	143	ASP	3.2
1	A	120	ASN	3.2
1	E	64	ALA	3.2
2	H	101	ALA	3.2
1	S	169	ILE	3.2
2	J	127	GLN	3.2
1	W	60	GLY	3.2
2	P	20	VAL	3.2
1	W	30	ASP	3.2
2	R	52	ASN	3.1
2	X	37	SER	3.1
1	W	94	ARG	3.1
1	E	92	ASP	3.1
2	T	156	GLY	3.1
1	E	76	ASN	3.1
1	Q	89	ASN	3.1
1	K	129	ALA	3.1
2	R	141	LYS	3.1
2	L	7	GLY	3.1
1	O	176	ALA	3.1
2	X	95	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	O	144	VAL	3.1
1	E	131	GLY	3.0
2	D	95	HIS	3.0
1	G	66	GLU	3.0
2	V	65	TYR	3.0
2	V	109	GLY	3.0
1	S	38	SER	3.0
2	P	82	THR	3.0
1	K	127	HIS	3.0
2	P	88	MET	3.0
2	L	158	PRO	3.0
1	S	2	SER	3.0
1	W	135	LYS	3.0
2	L	99	ASN	3.0
2	V	95	HIS	3.0
2	D	5	PRO	3.0
1	Q	176	ALA	3.0
1	S	94	ARG	3.0
1	U	118	GLY	3.0
2	D	2	GLY	3.0
1	W	175	GLU	3.0
2	B	90	ALA	3.0
1	O	38	SER	3.0
1	G	120	ASN	3.0
2	J	65	TYR	3.0
2	L	151	PHE	3.0
2	R	18	ALA	3.0
2	V	110	PHE	3.0
2	B	128	GLY	3.0
1	W	97	VAL	3.0
2	D	72	LEU	2.9
2	V	142	TRP	2.9
1	E	93	LYS	2.9
1	I	75	ALA	2.9
1	G	132	ILE	2.9
2	B	156	GLY	2.9
2	B	95	HIS	2.9
2	L	13	ASN	2.9
2	V	55	ASN	2.9
1	E	40	GLY	2.9
1	U	94	ARG	2.9
2	H	42	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
2	P	42	HIS	2.9
1	A	183	GLU	2.9
2	H	99	ASN	2.9
1	K	117	LYS	2.9
2	D	83	GLY	2.9
1	Q	167	ALA	2.9
2	H	132	HIS	2.9
2	N	83	GLY	2.9
2	V	111	GLY	2.9
2	D	25	ILE	2.9
2	B	60	GLY	2.9
1	G	127	HIS	2.8
2	D	3	GLU	2.8
2	J	60	GLY	2.8
2	J	83	GLY	2.8
1	I	89	ASN	2.8
2	R	45	ALA	2.8
1	U	36	THR	2.8
1	W	119	SER	2.8
1	U	103	TRP	2.8
1	I	182	VAL	2.8
1	K	22	ALA	2.8
2	X	13	ASN	2.8
2	P	95	HIS	2.8
1	S	90	SER	2.8
1	U	66	GLU	2.8
2	V	89	VAL	2.8
2	X	83	GLY	2.8
1	I	25	LYS	2.8
2	J	36	ALA	2.8
2	R	9	PRO	2.8
2	H	74	ASN	2.8
2	T	141	LYS	2.8
1	W	19	LEU	2.8
2	J	88	MET	2.8
1	Q	51	GLY	2.8
1	C	103	TRP	2.8
2	B	37	SER	2.8
2	F	136	GLU	2.8
2	R	149	THR	2.8
2	T	158	PRO	2.8
2	X	64	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	P	112	VAL	2.8
2	H	83	GLY	2.8
1	I	154	ALA	2.8
1	W	90	SER	2.8
2	P	35	ALA	2.8
2	F	29	PRO	2.8
1	O	21	ASP	2.8
2	P	92	ASP	2.8
1	I	28	ASN	2.7
1	K	66	GLU	2.7
1	W	62	SER	2.7
1	G	183	GLU	2.7
1	O	2	SER	2.7
1	W	91	VAL	2.7
2	B	2	GLY	2.7
2	L	52	ASN	2.7
2	R	111	GLY	2.7
1	A	129	ALA	2.7
2	R	131	ARG	2.7
1	S	36	THR	2.7
2	F	40	ASP	2.7
2	H	25	ILE	2.7
2	X	26	GLU	2.7
2	H	66	LEU	2.7
2	T	43	LEU	2.7
1	W	51	GLY	2.7
2	T	35	ALA	2.7
1	S	25	LYS	2.7
1	E	2	SER	2.7
1	U	92	ASP	2.6
1	W	64	ALA	2.6
2	X	46	ASP	2.6
2	F	64	PRO	2.6
2	J	112	VAL	2.6
2	L	152	PHE	2.6
1	K	94	ARG	2.6
2	X	132	HIS	2.6
1	C	2	SER	2.6
1	G	167	ALA	2.6
2	T	84	THR	2.6
1	S	92	ASP	2.6
2	N	8	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	Q	40	GLY	2.6
2	X	31	GLY	2.6
1	U	38	SER	2.6
2	H	30	ARG	2.6
1	I	21	ASP	2.6
2	B	136	GLU	2.6
1	C	93	LYS	2.6
2	T	111	GLY	2.6
2	L	25	ILE	2.6
1	A	88	LEU	2.6
1	W	44	LEU	2.6
1	W	128	MET	2.6
1	E	175	GLU	2.6
1	K	64	ALA	2.6
2	N	112	VAL	2.6
2	H	37	SER	2.6
1	U	183	GLU	2.6
2	P	100	ILE	2.6
1	U	79	PRO	2.6
1	U	25	LYS	2.5
1	M	118	GLY	2.5
1	S	65	GLY	2.5
2	P	60	GLY	2.5
1	K	107	ALA	2.5
1	O	64	ALA	2.5
2	J	98	ALA	2.5
2	L	64	PRO	2.5
1	C	90	SER	2.5
1	I	172	ARG	2.5
1	M	90	SER	2.5
2	P	141	LYS	2.5
1	W	6	GLY	2.5
2	V	128	GLY	2.5
1	O	117	LYS	2.5
2	P	115	TYR	2.5
2	P	134	ASP	2.5
2	T	146	PHE	2.5
1	S	74	LEU	2.5
2	N	55	ASN	2.5
2	T	55	ASN	2.5
2	N	35	ALA	2.5
1	W	38	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	64	PRO	2.5
1	O	182	VAL	2.5
2	P	63	MET	2.5
1	A	66	GLU	2.5
1	E	95	GLN	2.5
1	S	22	ALA	2.5
1	A	108	CYS	2.4
1	A	166	TYR	2.4
1	O	54	GLN	2.4
2	L	30	ARG	2.4
2	L	116	ALA	2.4
2	P	52	ASN	2.4
2	P	142	TRP	2.4
2	H	114	THR	2.4
1	U	180	GLN	2.4
2	N	37	SER	2.4
2	H	106	LYS	2.4
2	N	75	ALA	2.4
1	W	7	ILE	2.4
2	F	3	GLU	2.4
2	V	63	MET	2.4
2	N	111	GLY	2.4
1	U	167	ALA	2.4
2	X	21	TYR	2.4
2	B	88	MET	2.4
1	G	39	PRO	2.4
1	M	154	ALA	2.4
2	X	55	ASN	2.4
2	D	63	MET	2.4
2	L	28	GLU	2.4
1	E	159	GLY	2.4
2	N	31	GLY	2.4
1	Q	112	ALA	2.4
1	O	132	ILE	2.4
1	W	66	GLU	2.4
2	J	72	LEU	2.4
2	R	66	LEU	2.4
2	P	147	VAL	2.4
1	O	25	LYS	2.4
2	N	3	GLU	2.3
1	A	26	SER	2.3
1	U	181	MET	2.3

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Mol	Chain	Res	Type	RSRZ
2	J	8	ASP	2.3
2	L	115	TYR	2.3
2	F	52	ASN	2.3
1	W	141	ALA	2.3
2	P	19	ALA	2.3
1	E	91	VAL	2.3
1	U	34	SER	2.3
2	R	142	TRP	2.3
1	Q	70	ASP	2.3
1	W	65	GLY	2.3
1	K	167	ALA	2.3
1	U	106	ALA	2.3
1	O	36	THR	2.3
2	J	76	ASP	2.3
2	T	5	PRO	2.3
1	W	98	GLY	2.3
2	L	31	GLY	2.3
1	O	28	ASN	2.3
1	O	180	GLN	2.3
1	W	165	VAL	2.3
2	P	155	THR	2.3
2	J	95	HIS	2.3
2	V	46	ASP	2.3
1	I	157	ALA	2.3
1	O	75	ALA	2.3
1	G	105	VAL	2.3
2	J	103	GLU	2.3
2	L	89	VAL	2.3
1	C	76	ASN	2.3
1	Q	120	ASN	2.3
2	T	13	ASN	2.3
2	P	61	PHE	2.3
2	H	100	ILE	2.3
2	R	14	GLY	2.3
1	U	70	ASP	2.3
2	L	8	ASP	2.3
2	T	112	VAL	2.3
1	E	89	ASN	2.3
1	E	167	ALA	2.3
1	K	27	ALA	2.3
2	F	30	ARG	2.3
1	A	18	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	26	GLU	2.2
2	P	127	GLN	2.3
1	Q	39	PRO	2.2
2	D	156	GLY	2.2
2	X	111	GLY	2.2
1	I	111	ALA	2.2
1	O	158	ALA	2.2
2	N	28	GLU	2.2
1	A	132	ILE	2.2
1	U	35	LYS	2.2
1	M	156	LEU	2.2
2	J	149	THR	2.2
2	T	132	HIS	2.2
2	R	65	TYR	2.2
1	M	93	LYS	2.2
1	E	120	ASN	2.2
1	K	68	LEU	2.2
1	M	141	ALA	2.2
1	Q	157	ALA	2.2
1	U	12	SER	2.2
1	U	168	SER	2.2
2	N	127	GLN	2.2
2	X	25	ILE	2.2
1	Q	92	ASP	2.2
2	X	136	GLU	2.2
1	O	173	PRO	2.2
1	U	28	ASN	2.2
2	H	128	GLY	2.2
2	P	148	VAL	2.2
2	P	81	LYS	2.2
1	O	175	GLU	2.2
2	P	43	LEU	2.2
2	T	154	TYR	2.2
1	A	60	GLY	2.2
1	K	65	GLY	2.2
1	K	176	ALA	2.2
1	W	129	ALA	2.2
2	B	109	GLY	2.2
2	P	64	PRO	2.2
1	O	90	SER	2.2
2	R	95	HIS	2.2
2	X	103	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	X	150	TYR	2.2
1	K	182	VAL	2.2
2	J	142	TRP	2.2
1	G	20	GLY	2.2
2	N	99	ASN	2.2
1	C	153	THR	2.2
1	Q	93	LYS	2.2
1	U	122	THR	2.2
1	Q	101	GLU	2.2
1	U	182	VAL	2.2
2	B	150	TYR	2.2
1	G	79	PRO	2.1
1	K	56	ALA	2.1
2	D	98	ALA	2.1
2	P	8	ASP	2.1
1	U	135	LYS	2.1
2	V	126	LYS	2.1
1	G	80	SER	2.1
1	S	34	SER	2.1
1	C	75	ALA	2.1
1	I	162	GLY	2.1
2	X	73	ALA	2.1
2	J	24	PRO	2.1
2	X	22	LEU	2.1
1	G	89	ASN	2.1
1	U	89	ASN	2.1
2	V	13	ASN	2.1
1	I	179	ARG	2.1
1	O	80	SER	2.1
2	R	2	GLY	2.1
2	H	58	PRO	2.1
1	W	33	VAL	2.1
2	R	55	ASN	2.1
1	G	86	SER	2.1
1	I	47	GLY	2.1
1	I	118	GLY	2.1
1	K	63	GLN	2.1
1	M	52	ALA	2.1
1	S	64	ALA	2.1
2	P	26	GLU	2.1
2	P	71	ALA	2.1
2	T	45	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	173	PRO	2.1
2	N	25	ILE	2.1
1	G	30	ASP	2.1
1	I	30	ASP	2.1
2	T	20	VAL	2.1
1	Q	172	ARG	2.1
2	T	115	TYR	2.1
1	A	94	ARG	2.1
2	D	88	MET	2.1
1	I	93	LYS	2.1
1	Q	11	THR	2.1
1	U	47	GLY	2.1
1	Q	2	SER	2.1
1	S	86	SER	2.1
2	J	158	PRO	2.1
2	H	20	VAL	2.1
2	T	63	MET	2.1
1	O	91	VAL	2.1
1	I	92	ASP	2.0
2	X	156	GLY	2.0
1	Q	173	PRO	2.0
2	J	94	PRO	2.0
1	G	62	SER	2.0
2	N	150	TYR	2.0
2	P	2	GLY	2.0
1	M	173	PRO	2.0
1	W	178	TRP	2.0
2	P	30	ARG	2.0
1	U	130	PHE	2.0
2	P	21	TYR	2.0
2	X	65	TYR	2.0
1	I	158	ALA	2.0
2	H	79	ALA	2.0
2	X	158	PRO	2.0
1	G	95	GLN	2.0
1	K	128	MET	2.0
1	O	93	LYS	2.0
2	B	125	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.