



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2016 – 01:59 PM EDT

PDB ID : 5L89  
Title : Crystal structure of Rhodospirillum rubrum Rru\_A0973 mutant E32A  
Authors : He, D.; Hughes, S.; Vanden-Hehir, S.; Georgiev, A.; Altenbach, K.; Tarrant, E.; Mackay, C.L.; Waldron, K.J.; Clarke, D.J.; Marles-Wright, J.  
Deposited on : 2016-06-07  
Resolution : 2.59 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
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)	:	rb-20027939

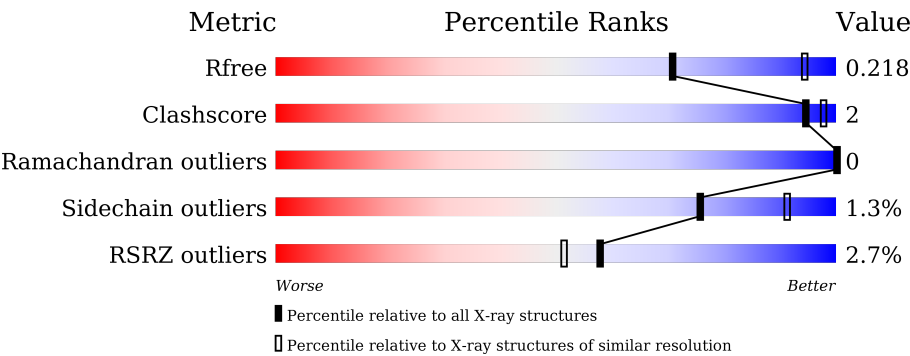
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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.



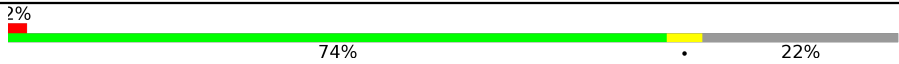

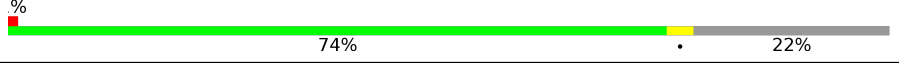
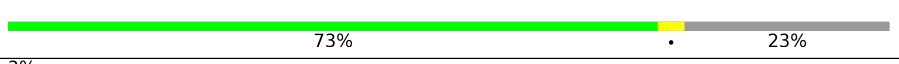

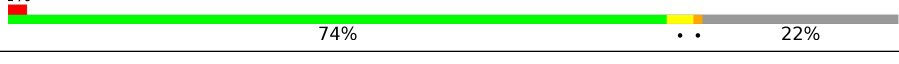


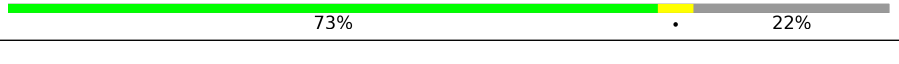


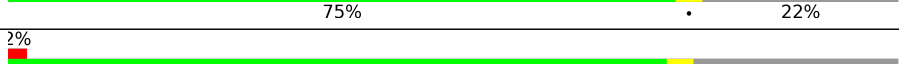

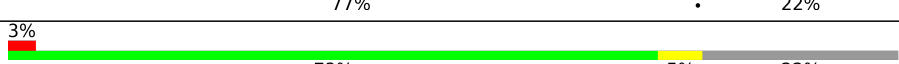
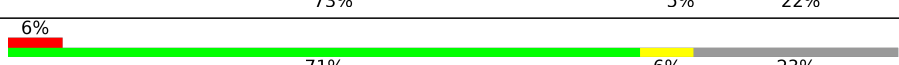
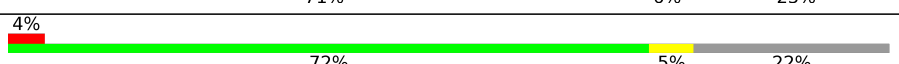
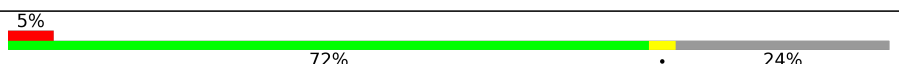
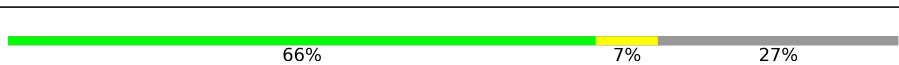
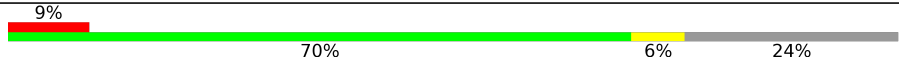



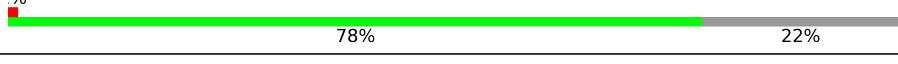

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	116	<div><div>4%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>76%</div><div></div><div>22%</div></div>
1	B	116	<div><div>3%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>73%</div><div></div><div>22%</div></div>
1	C	116	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>76%</div><div></div><div>22%</div></div>
1	D	116	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>74%</div><div></div><div>22%</div></div>
1	E	116	<div><div>2%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>72%</div><div>5%</div><div>22%</div></div>
1	F	116	<div><div>3%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>75%</div><div></div><div>22%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	116	
1	H	116	
1	I	116	
1	J	116	
1	K	116	
1	L	116	
1	M	116	
1	N	116	
1	O	116	
1	P	116	
1	Q	116	
1	R	116	
1	S	116	
1	T	116	
1	U	116	
1	V	116	
1	W	116	
1	X	116	
1	Y	116	
1	Z	116	
1	a	116	
1	b	116	
1	c	116	
1	d	116	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CA	P	201	-	-	-	X
2	CA	V	201	-	-	-	X
2	CA	d	201	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 43360 atoms, of which 20998 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 Rru\_A0973.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	91	Total	C	H	N	O	S	0	0	0
			1450	462	708	132	146	2			
1	B	90	Total	C	H	N	O	S	0	0	0
			1440	459	703	131	145	2			
1	C	90	Total	C	H	N	O	S	0	0	0
			1440	459	703	131	145	2			
1	D	91	Total	C	H	N	O	S	0	0	0
			1450	462	708	132	146	2			
1	E	90	Total	C	H	N	O	S	0	0	0
			1441	459	704	131	145	2			
1	F	91	Total	C	H	N	O	S	0	0	0
			1450	462	708	132	146	2			
1	G	91	Total	C	H	N	O	S	0	0	0
			1450	462	708	132	146	2			
1	H	90	Total	C	H	N	O	S	0	0	0
			1440	459	704	131	144	2			
1	I	90	Total	C	H	N	O	S	0	0	0
			1441	459	704	131	145	2			
1	J	89	Total	C	H	N	O	S	0	0	0
			1430	456	698	130	144	2			
1	K	89	Total	C	H	N	O	S	0	0	0
			1430	456	698	130	144	2			
1	L	91	Total	C	H	N	O	S	0	0	0
			1450	462	708	132	146	2			
1	M	89	Total	C	H	N	O	S	0	0	0
			1430	456	698	130	144	2			
1	N	91	Total	C	H	N	O	S	0	0	0
			1450	462	708	132	146	2			
1	O	90	Total	C	H	N	O	S	0	0	0
			1440	459	703	131	145	2			
1	P	91	Total	C	H	N	O	S	0	0	0
			1450	462	708	132	146	2			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	89	Total	C	H	N	O	S	0	0	0
			1430	456	698	130	144	2			
1	R	90	Total	C	H	N	O	S	0	0	0
			1440	459	703	131	145	2			
1	S	89	Total	C	H	N	O	S	0	0	0
			1430	456	698	130	144	2			
1	T	90	Total	C	H	N	O	S	0	0	0
			1440	459	704	131	144	2			
1	U	91	Total	C	H	N	O	S	0	0	0
			1450	462	708	132	146	2			
1	V	89	Total	C	H	N	O	S	0	0	0
			1430	456	699	130	143	2			
1	W	90	Total	C	H	N	O	S	0	0	0
			1440	459	703	131	145	2			
1	X	88	Total	C	H	N	O	S	0	0	0
			1420	453	694	129	142	2			
1	Y	85	Total	C	H	N	O	S	0	0	0
			1376	439	670	126	139	2			
1	Z	88	Total	C	H	N	O	S	0	0	0
			1420	453	694	129	142	2			
1	a	90	Total	C	H	N	O	S	0	0	0
			1439	459	703	131	144	2			
1	b	88	Total	C	H	N	O	S	0	0	0
			1419	453	693	129	142	2			
1	c	83	Total	C	H	N	O	S	0	0	0
			1347	430	657	124	134	2			
1	d	90	Total	C	H	N	O	S	0	0	0
			1440	459	703	131	145	2			

There are 630 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ALA	GLU	engineered mutation	UNP Q2RVS1
A	97	ALA	-	expression tag	UNP Q2RVS1
A	98	ASN	-	expression tag	UNP Q2RVS1
A	99	SER	-	expression tag	UNP Q2RVS1
A	100	SER	-	expression tag	UNP Q2RVS1
A	101	SER	-	expression tag	UNP Q2RVS1
A	102	VAL	-	expression tag	UNP Q2RVS1
A	103	ASP	-	expression tag	UNP Q2RVS1
A	104	LYS	-	expression tag	UNP Q2RVS1
A	105	LEU	-	expression tag	UNP Q2RVS1
A	106	ALA	-	expression tag	UNP Q2RVS1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	107	ALA	-	expression tag	UNP Q2RVS1
A	108	ALA	-	expression tag	UNP Q2RVS1
A	109	LEU	-	expression tag	UNP Q2RVS1
A	110	GLU	-	expression tag	UNP Q2RVS1
A	111	HIS	-	expression tag	UNP Q2RVS1
A	112	HIS	-	expression tag	UNP Q2RVS1
A	113	HIS	-	expression tag	UNP Q2RVS1
A	114	HIS	-	expression tag	UNP Q2RVS1
A	115	HIS	-	expression tag	UNP Q2RVS1
A	116	HIS	-	expression tag	UNP Q2RVS1
B	32	ALA	GLU	engineered mutation	UNP Q2RVS1
B	97	ALA	-	expression tag	UNP Q2RVS1
B	98	ASN	-	expression tag	UNP Q2RVS1
B	99	SER	-	expression tag	UNP Q2RVS1
B	100	SER	-	expression tag	UNP Q2RVS1
B	101	SER	-	expression tag	UNP Q2RVS1
B	102	VAL	-	expression tag	UNP Q2RVS1
B	103	ASP	-	expression tag	UNP Q2RVS1
B	104	LYS	-	expression tag	UNP Q2RVS1
B	105	LEU	-	expression tag	UNP Q2RVS1
B	106	ALA	-	expression tag	UNP Q2RVS1
B	107	ALA	-	expression tag	UNP Q2RVS1
B	108	ALA	-	expression tag	UNP Q2RVS1
B	109	LEU	-	expression tag	UNP Q2RVS1
B	110	GLU	-	expression tag	UNP Q2RVS1
B	111	HIS	-	expression tag	UNP Q2RVS1
B	112	HIS	-	expression tag	UNP Q2RVS1
B	113	HIS	-	expression tag	UNP Q2RVS1
B	114	HIS	-	expression tag	UNP Q2RVS1
B	115	HIS	-	expression tag	UNP Q2RVS1
B	116	HIS	-	expression tag	UNP Q2RVS1
C	32	ALA	GLU	engineered mutation	UNP Q2RVS1
C	97	ALA	-	expression tag	UNP Q2RVS1
C	98	ASN	-	expression tag	UNP Q2RVS1
C	99	SER	-	expression tag	UNP Q2RVS1
C	100	SER	-	expression tag	UNP Q2RVS1
C	101	SER	-	expression tag	UNP Q2RVS1
C	102	VAL	-	expression tag	UNP Q2RVS1
C	103	ASP	-	expression tag	UNP Q2RVS1
C	104	LYS	-	expression tag	UNP Q2RVS1
C	105	LEU	-	expression tag	UNP Q2RVS1
C	106	ALA	-	expression tag	UNP Q2RVS1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	107	ALA	-	expression tag	UNP Q2RVS1
C	108	ALA	-	expression tag	UNP Q2RVS1
C	109	LEU	-	expression tag	UNP Q2RVS1
C	110	GLU	-	expression tag	UNP Q2RVS1
C	111	HIS	-	expression tag	UNP Q2RVS1
C	112	HIS	-	expression tag	UNP Q2RVS1
C	113	HIS	-	expression tag	UNP Q2RVS1
C	114	HIS	-	expression tag	UNP Q2RVS1
C	115	HIS	-	expression tag	UNP Q2RVS1
C	116	HIS	-	expression tag	UNP Q2RVS1
D	32	ALA	GLU	engineered mutation	UNP Q2RVS1
D	97	ALA	-	expression tag	UNP Q2RVS1
D	98	ASN	-	expression tag	UNP Q2RVS1
D	99	SER	-	expression tag	UNP Q2RVS1
D	100	SER	-	expression tag	UNP Q2RVS1
D	101	SER	-	expression tag	UNP Q2RVS1
D	102	VAL	-	expression tag	UNP Q2RVS1
D	103	ASP	-	expression tag	UNP Q2RVS1
D	104	LYS	-	expression tag	UNP Q2RVS1
D	105	LEU	-	expression tag	UNP Q2RVS1
D	106	ALA	-	expression tag	UNP Q2RVS1
D	107	ALA	-	expression tag	UNP Q2RVS1
D	108	ALA	-	expression tag	UNP Q2RVS1
D	109	LEU	-	expression tag	UNP Q2RVS1
D	110	GLU	-	expression tag	UNP Q2RVS1
D	111	HIS	-	expression tag	UNP Q2RVS1
D	112	HIS	-	expression tag	UNP Q2RVS1
D	113	HIS	-	expression tag	UNP Q2RVS1
D	114	HIS	-	expression tag	UNP Q2RVS1
D	115	HIS	-	expression tag	UNP Q2RVS1
D	116	HIS	-	expression tag	UNP Q2RVS1
E	32	ALA	GLU	engineered mutation	UNP Q2RVS1
E	97	ALA	-	expression tag	UNP Q2RVS1
E	98	ASN	-	expression tag	UNP Q2RVS1
E	99	SER	-	expression tag	UNP Q2RVS1
E	100	SER	-	expression tag	UNP Q2RVS1
E	101	SER	-	expression tag	UNP Q2RVS1
E	102	VAL	-	expression tag	UNP Q2RVS1
E	103	ASP	-	expression tag	UNP Q2RVS1
E	104	LYS	-	expression tag	UNP Q2RVS1
E	105	LEU	-	expression tag	UNP Q2RVS1
E	106	ALA	-	expression tag	UNP Q2RVS1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	107	ALA	-	expression tag	UNP Q2RVS1
E	108	ALA	-	expression tag	UNP Q2RVS1
E	109	LEU	-	expression tag	UNP Q2RVS1
E	110	GLU	-	expression tag	UNP Q2RVS1
E	111	HIS	-	expression tag	UNP Q2RVS1
E	112	HIS	-	expression tag	UNP Q2RVS1
E	113	HIS	-	expression tag	UNP Q2RVS1
E	114	HIS	-	expression tag	UNP Q2RVS1
E	115	HIS	-	expression tag	UNP Q2RVS1
E	116	HIS	-	expression tag	UNP Q2RVS1
F	32	ALA	GLU	engineered mutation	UNP Q2RVS1
F	97	ALA	-	expression tag	UNP Q2RVS1
F	98	ASN	-	expression tag	UNP Q2RVS1
F	99	SER	-	expression tag	UNP Q2RVS1
F	100	SER	-	expression tag	UNP Q2RVS1
F	101	SER	-	expression tag	UNP Q2RVS1
F	102	VAL	-	expression tag	UNP Q2RVS1
F	103	ASP	-	expression tag	UNP Q2RVS1
F	104	LYS	-	expression tag	UNP Q2RVS1
F	105	LEU	-	expression tag	UNP Q2RVS1
F	106	ALA	-	expression tag	UNP Q2RVS1
F	107	ALA	-	expression tag	UNP Q2RVS1
F	108	ALA	-	expression tag	UNP Q2RVS1
F	109	LEU	-	expression tag	UNP Q2RVS1
F	110	GLU	-	expression tag	UNP Q2RVS1
F	111	HIS	-	expression tag	UNP Q2RVS1
F	112	HIS	-	expression tag	UNP Q2RVS1
F	113	HIS	-	expression tag	UNP Q2RVS1
F	114	HIS	-	expression tag	UNP Q2RVS1
F	115	HIS	-	expression tag	UNP Q2RVS1
F	116	HIS	-	expression tag	UNP Q2RVS1
G	32	ALA	GLU	engineered mutation	UNP Q2RVS1
G	97	ALA	-	expression tag	UNP Q2RVS1
G	98	ASN	-	expression tag	UNP Q2RVS1
G	99	SER	-	expression tag	UNP Q2RVS1
G	100	SER	-	expression tag	UNP Q2RVS1
G	101	SER	-	expression tag	UNP Q2RVS1
G	102	VAL	-	expression tag	UNP Q2RVS1
G	103	ASP	-	expression tag	UNP Q2RVS1
G	104	LYS	-	expression tag	UNP Q2RVS1
G	105	LEU	-	expression tag	UNP Q2RVS1
G	106	ALA	-	expression tag	UNP Q2RVS1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	107	ALA	-	expression tag	UNP Q2RVS1
G	108	ALA	-	expression tag	UNP Q2RVS1
G	109	LEU	-	expression tag	UNP Q2RVS1
G	110	GLU	-	expression tag	UNP Q2RVS1
G	111	HIS	-	expression tag	UNP Q2RVS1
G	112	HIS	-	expression tag	UNP Q2RVS1
G	113	HIS	-	expression tag	UNP Q2RVS1
G	114	HIS	-	expression tag	UNP Q2RVS1
G	115	HIS	-	expression tag	UNP Q2RVS1
G	116	HIS	-	expression tag	UNP Q2RVS1
H	32	ALA	GLU	engineered mutation	UNP Q2RVS1
H	97	ALA	-	expression tag	UNP Q2RVS1
H	98	ASN	-	expression tag	UNP Q2RVS1
H	99	SER	-	expression tag	UNP Q2RVS1
H	100	SER	-	expression tag	UNP Q2RVS1
H	101	SER	-	expression tag	UNP Q2RVS1
H	102	VAL	-	expression tag	UNP Q2RVS1
H	103	ASP	-	expression tag	UNP Q2RVS1
H	104	LYS	-	expression tag	UNP Q2RVS1
H	105	LEU	-	expression tag	UNP Q2RVS1
H	106	ALA	-	expression tag	UNP Q2RVS1
H	107	ALA	-	expression tag	UNP Q2RVS1
H	108	ALA	-	expression tag	UNP Q2RVS1
H	109	LEU	-	expression tag	UNP Q2RVS1
H	110	GLU	-	expression tag	UNP Q2RVS1
H	111	HIS	-	expression tag	UNP Q2RVS1
H	112	HIS	-	expression tag	UNP Q2RVS1
H	113	HIS	-	expression tag	UNP Q2RVS1
H	114	HIS	-	expression tag	UNP Q2RVS1
H	115	HIS	-	expression tag	UNP Q2RVS1
H	116	HIS	-	expression tag	UNP Q2RVS1
I	32	ALA	GLU	engineered mutation	UNP Q2RVS1
I	97	ALA	-	expression tag	UNP Q2RVS1
I	98	ASN	-	expression tag	UNP Q2RVS1
I	99	SER	-	expression tag	UNP Q2RVS1
I	100	SER	-	expression tag	UNP Q2RVS1
I	101	SER	-	expression tag	UNP Q2RVS1
I	102	VAL	-	expression tag	UNP Q2RVS1
I	103	ASP	-	expression tag	UNP Q2RVS1
I	104	LYS	-	expression tag	UNP Q2RVS1
I	105	LEU	-	expression tag	UNP Q2RVS1
I	106	ALA	-	expression tag	UNP Q2RVS1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	107	ALA	-	expression tag	UNP Q2RVS1
I	108	ALA	-	expression tag	UNP Q2RVS1
I	109	LEU	-	expression tag	UNP Q2RVS1
I	110	GLU	-	expression tag	UNP Q2RVS1
I	111	HIS	-	expression tag	UNP Q2RVS1
I	112	HIS	-	expression tag	UNP Q2RVS1
I	113	HIS	-	expression tag	UNP Q2RVS1
I	114	HIS	-	expression tag	UNP Q2RVS1
I	115	HIS	-	expression tag	UNP Q2RVS1
I	116	HIS	-	expression tag	UNP Q2RVS1
J	32	ALA	GLU	engineered mutation	UNP Q2RVS1
J	97	ALA	-	expression tag	UNP Q2RVS1
J	98	ASN	-	expression tag	UNP Q2RVS1
J	99	SER	-	expression tag	UNP Q2RVS1
J	100	SER	-	expression tag	UNP Q2RVS1
J	101	SER	-	expression tag	UNP Q2RVS1
J	102	VAL	-	expression tag	UNP Q2RVS1
J	103	ASP	-	expression tag	UNP Q2RVS1
J	104	LYS	-	expression tag	UNP Q2RVS1
J	105	LEU	-	expression tag	UNP Q2RVS1
J	106	ALA	-	expression tag	UNP Q2RVS1
J	107	ALA	-	expression tag	UNP Q2RVS1
J	108	ALA	-	expression tag	UNP Q2RVS1
J	109	LEU	-	expression tag	UNP Q2RVS1
J	110	GLU	-	expression tag	UNP Q2RVS1
J	111	HIS	-	expression tag	UNP Q2RVS1
J	112	HIS	-	expression tag	UNP Q2RVS1
J	113	HIS	-	expression tag	UNP Q2RVS1
J	114	HIS	-	expression tag	UNP Q2RVS1
J	115	HIS	-	expression tag	UNP Q2RVS1
J	116	HIS	-	expression tag	UNP Q2RVS1
K	32	ALA	GLU	engineered mutation	UNP Q2RVS1
K	97	ALA	-	expression tag	UNP Q2RVS1
K	98	ASN	-	expression tag	UNP Q2RVS1
K	99	SER	-	expression tag	UNP Q2RVS1
K	100	SER	-	expression tag	UNP Q2RVS1
K	101	SER	-	expression tag	UNP Q2RVS1
K	102	VAL	-	expression tag	UNP Q2RVS1
K	103	ASP	-	expression tag	UNP Q2RVS1
K	104	LYS	-	expression tag	UNP Q2RVS1
K	105	LEU	-	expression tag	UNP Q2RVS1
K	106	ALA	-	expression tag	UNP Q2RVS1

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Chain	Residue	Modelled	Actual	Comment	Reference
K	107	ALA	-	expression tag	UNP Q2RVS1
K	108	ALA	-	expression tag	UNP Q2RVS1
K	109	LEU	-	expression tag	UNP Q2RVS1
K	110	GLU	-	expression tag	UNP Q2RVS1
K	111	HIS	-	expression tag	UNP Q2RVS1
K	112	HIS	-	expression tag	UNP Q2RVS1
K	113	HIS	-	expression tag	UNP Q2RVS1
K	114	HIS	-	expression tag	UNP Q2RVS1
K	115	HIS	-	expression tag	UNP Q2RVS1
K	116	HIS	-	expression tag	UNP Q2RVS1
L	32	ALA	GLU	engineered mutation	UNP Q2RVS1
L	97	ALA	-	expression tag	UNP Q2RVS1
L	98	ASN	-	expression tag	UNP Q2RVS1
L	99	SER	-	expression tag	UNP Q2RVS1
L	100	SER	-	expression tag	UNP Q2RVS1
L	101	SER	-	expression tag	UNP Q2RVS1
L	102	VAL	-	expression tag	UNP Q2RVS1
L	103	ASP	-	expression tag	UNP Q2RVS1
L	104	LYS	-	expression tag	UNP Q2RVS1
L	105	LEU	-	expression tag	UNP Q2RVS1
L	106	ALA	-	expression tag	UNP Q2RVS1
L	107	ALA	-	expression tag	UNP Q2RVS1
L	108	ALA	-	expression tag	UNP Q2RVS1
L	109	LEU	-	expression tag	UNP Q2RVS1
L	110	GLU	-	expression tag	UNP Q2RVS1
L	111	HIS	-	expression tag	UNP Q2RVS1
L	112	HIS	-	expression tag	UNP Q2RVS1
L	113	HIS	-	expression tag	UNP Q2RVS1
L	114	HIS	-	expression tag	UNP Q2RVS1
L	115	HIS	-	expression tag	UNP Q2RVS1
L	116	HIS	-	expression tag	UNP Q2RVS1
M	32	ALA	GLU	engineered mutation	UNP Q2RVS1
M	97	ALA	-	expression tag	UNP Q2RVS1
M	98	ASN	-	expression tag	UNP Q2RVS1
M	99	SER	-	expression tag	UNP Q2RVS1
M	100	SER	-	expression tag	UNP Q2RVS1
M	101	SER	-	expression tag	UNP Q2RVS1
M	102	VAL	-	expression tag	UNP Q2RVS1
M	103	ASP	-	expression tag	UNP Q2RVS1
M	104	LYS	-	expression tag	UNP Q2RVS1
M	105	LEU	-	expression tag	UNP Q2RVS1
M	106	ALA	-	expression tag	UNP Q2RVS1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	107	ALA	-	expression tag	UNP Q2RVS1
M	108	ALA	-	expression tag	UNP Q2RVS1
M	109	LEU	-	expression tag	UNP Q2RVS1
M	110	GLU	-	expression tag	UNP Q2RVS1
M	111	HIS	-	expression tag	UNP Q2RVS1
M	112	HIS	-	expression tag	UNP Q2RVS1
M	113	HIS	-	expression tag	UNP Q2RVS1
M	114	HIS	-	expression tag	UNP Q2RVS1
M	115	HIS	-	expression tag	UNP Q2RVS1
M	116	HIS	-	expression tag	UNP Q2RVS1
N	32	ALA	GLU	engineered mutation	UNP Q2RVS1
N	97	ALA	-	expression tag	UNP Q2RVS1
N	98	ASN	-	expression tag	UNP Q2RVS1
N	99	SER	-	expression tag	UNP Q2RVS1
N	100	SER	-	expression tag	UNP Q2RVS1
N	101	SER	-	expression tag	UNP Q2RVS1
N	102	VAL	-	expression tag	UNP Q2RVS1
N	103	ASP	-	expression tag	UNP Q2RVS1
N	104	LYS	-	expression tag	UNP Q2RVS1
N	105	LEU	-	expression tag	UNP Q2RVS1
N	106	ALA	-	expression tag	UNP Q2RVS1
N	107	ALA	-	expression tag	UNP Q2RVS1
N	108	ALA	-	expression tag	UNP Q2RVS1
N	109	LEU	-	expression tag	UNP Q2RVS1
N	110	GLU	-	expression tag	UNP Q2RVS1
N	111	HIS	-	expression tag	UNP Q2RVS1
N	112	HIS	-	expression tag	UNP Q2RVS1
N	113	HIS	-	expression tag	UNP Q2RVS1
N	114	HIS	-	expression tag	UNP Q2RVS1
N	115	HIS	-	expression tag	UNP Q2RVS1
N	116	HIS	-	expression tag	UNP Q2RVS1
O	32	ALA	GLU	engineered mutation	UNP Q2RVS1
O	97	ALA	-	expression tag	UNP Q2RVS1
O	98	ASN	-	expression tag	UNP Q2RVS1
O	99	SER	-	expression tag	UNP Q2RVS1
O	100	SER	-	expression tag	UNP Q2RVS1
O	101	SER	-	expression tag	UNP Q2RVS1
O	102	VAL	-	expression tag	UNP Q2RVS1
O	103	ASP	-	expression tag	UNP Q2RVS1
O	104	LYS	-	expression tag	UNP Q2RVS1
O	105	LEU	-	expression tag	UNP Q2RVS1
O	106	ALA	-	expression tag	UNP Q2RVS1

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Chain	Residue	Modelled	Actual	Comment	Reference
O	107	ALA	-	expression tag	UNP Q2RVS1
O	108	ALA	-	expression tag	UNP Q2RVS1
O	109	LEU	-	expression tag	UNP Q2RVS1
O	110	GLU	-	expression tag	UNP Q2RVS1
O	111	HIS	-	expression tag	UNP Q2RVS1
O	112	HIS	-	expression tag	UNP Q2RVS1
O	113	HIS	-	expression tag	UNP Q2RVS1
O	114	HIS	-	expression tag	UNP Q2RVS1
O	115	HIS	-	expression tag	UNP Q2RVS1
O	116	HIS	-	expression tag	UNP Q2RVS1
P	32	ALA	GLU	engineered mutation	UNP Q2RVS1
P	97	ALA	-	expression tag	UNP Q2RVS1
P	98	ASN	-	expression tag	UNP Q2RVS1
P	99	SER	-	expression tag	UNP Q2RVS1
P	100	SER	-	expression tag	UNP Q2RVS1
P	101	SER	-	expression tag	UNP Q2RVS1
P	102	VAL	-	expression tag	UNP Q2RVS1
P	103	ASP	-	expression tag	UNP Q2RVS1
P	104	LYS	-	expression tag	UNP Q2RVS1
P	105	LEU	-	expression tag	UNP Q2RVS1
P	106	ALA	-	expression tag	UNP Q2RVS1
P	107	ALA	-	expression tag	UNP Q2RVS1
P	108	ALA	-	expression tag	UNP Q2RVS1
P	109	LEU	-	expression tag	UNP Q2RVS1
P	110	GLU	-	expression tag	UNP Q2RVS1
P	111	HIS	-	expression tag	UNP Q2RVS1
P	112	HIS	-	expression tag	UNP Q2RVS1
P	113	HIS	-	expression tag	UNP Q2RVS1
P	114	HIS	-	expression tag	UNP Q2RVS1
P	115	HIS	-	expression tag	UNP Q2RVS1
P	116	HIS	-	expression tag	UNP Q2RVS1
Q	32	ALA	GLU	engineered mutation	UNP Q2RVS1
Q	97	ALA	-	expression tag	UNP Q2RVS1
Q	98	ASN	-	expression tag	UNP Q2RVS1
Q	99	SER	-	expression tag	UNP Q2RVS1
Q	100	SER	-	expression tag	UNP Q2RVS1
Q	101	SER	-	expression tag	UNP Q2RVS1
Q	102	VAL	-	expression tag	UNP Q2RVS1
Q	103	ASP	-	expression tag	UNP Q2RVS1
Q	104	LYS	-	expression tag	UNP Q2RVS1
Q	105	LEU	-	expression tag	UNP Q2RVS1
Q	106	ALA	-	expression tag	UNP Q2RVS1

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	107	ALA	-	expression tag	UNP Q2RVS1
Q	108	ALA	-	expression tag	UNP Q2RVS1
Q	109	LEU	-	expression tag	UNP Q2RVS1
Q	110	GLU	-	expression tag	UNP Q2RVS1
Q	111	HIS	-	expression tag	UNP Q2RVS1
Q	112	HIS	-	expression tag	UNP Q2RVS1
Q	113	HIS	-	expression tag	UNP Q2RVS1
Q	114	HIS	-	expression tag	UNP Q2RVS1
Q	115	HIS	-	expression tag	UNP Q2RVS1
Q	116	HIS	-	expression tag	UNP Q2RVS1
R	32	ALA	GLU	engineered mutation	UNP Q2RVS1
R	97	ALA	-	expression tag	UNP Q2RVS1
R	98	ASN	-	expression tag	UNP Q2RVS1
R	99	SER	-	expression tag	UNP Q2RVS1
R	100	SER	-	expression tag	UNP Q2RVS1
R	101	SER	-	expression tag	UNP Q2RVS1
R	102	VAL	-	expression tag	UNP Q2RVS1
R	103	ASP	-	expression tag	UNP Q2RVS1
R	104	LYS	-	expression tag	UNP Q2RVS1
R	105	LEU	-	expression tag	UNP Q2RVS1
R	106	ALA	-	expression tag	UNP Q2RVS1
R	107	ALA	-	expression tag	UNP Q2RVS1
R	108	ALA	-	expression tag	UNP Q2RVS1
R	109	LEU	-	expression tag	UNP Q2RVS1
R	110	GLU	-	expression tag	UNP Q2RVS1
R	111	HIS	-	expression tag	UNP Q2RVS1
R	112	HIS	-	expression tag	UNP Q2RVS1
R	113	HIS	-	expression tag	UNP Q2RVS1
R	114	HIS	-	expression tag	UNP Q2RVS1
R	115	HIS	-	expression tag	UNP Q2RVS1
R	116	HIS	-	expression tag	UNP Q2RVS1
S	32	ALA	GLU	engineered mutation	UNP Q2RVS1
S	97	ALA	-	expression tag	UNP Q2RVS1
S	98	ASN	-	expression tag	UNP Q2RVS1
S	99	SER	-	expression tag	UNP Q2RVS1
S	100	SER	-	expression tag	UNP Q2RVS1
S	101	SER	-	expression tag	UNP Q2RVS1
S	102	VAL	-	expression tag	UNP Q2RVS1
S	103	ASP	-	expression tag	UNP Q2RVS1
S	104	LYS	-	expression tag	UNP Q2RVS1
S	105	LEU	-	expression tag	UNP Q2RVS1
S	106	ALA	-	expression tag	UNP Q2RVS1

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Chain	Residue	Modelled	Actual	Comment	Reference
S	107	ALA	-	expression tag	UNP Q2RVS1
S	108	ALA	-	expression tag	UNP Q2RVS1
S	109	LEU	-	expression tag	UNP Q2RVS1
S	110	GLU	-	expression tag	UNP Q2RVS1
S	111	HIS	-	expression tag	UNP Q2RVS1
S	112	HIS	-	expression tag	UNP Q2RVS1
S	113	HIS	-	expression tag	UNP Q2RVS1
S	114	HIS	-	expression tag	UNP Q2RVS1
S	115	HIS	-	expression tag	UNP Q2RVS1
S	116	HIS	-	expression tag	UNP Q2RVS1
T	32	ALA	GLU	engineered mutation	UNP Q2RVS1
T	97	ALA	-	expression tag	UNP Q2RVS1
T	98	ASN	-	expression tag	UNP Q2RVS1
T	99	SER	-	expression tag	UNP Q2RVS1
T	100	SER	-	expression tag	UNP Q2RVS1
T	101	SER	-	expression tag	UNP Q2RVS1
T	102	VAL	-	expression tag	UNP Q2RVS1
T	103	ASP	-	expression tag	UNP Q2RVS1
T	104	LYS	-	expression tag	UNP Q2RVS1
T	105	LEU	-	expression tag	UNP Q2RVS1
T	106	ALA	-	expression tag	UNP Q2RVS1
T	107	ALA	-	expression tag	UNP Q2RVS1
T	108	ALA	-	expression tag	UNP Q2RVS1
T	109	LEU	-	expression tag	UNP Q2RVS1
T	110	GLU	-	expression tag	UNP Q2RVS1
T	111	HIS	-	expression tag	UNP Q2RVS1
T	112	HIS	-	expression tag	UNP Q2RVS1
T	113	HIS	-	expression tag	UNP Q2RVS1
T	114	HIS	-	expression tag	UNP Q2RVS1
T	115	HIS	-	expression tag	UNP Q2RVS1
T	116	HIS	-	expression tag	UNP Q2RVS1
U	32	ALA	GLU	engineered mutation	UNP Q2RVS1
U	97	ALA	-	expression tag	UNP Q2RVS1
U	98	ASN	-	expression tag	UNP Q2RVS1
U	99	SER	-	expression tag	UNP Q2RVS1
U	100	SER	-	expression tag	UNP Q2RVS1
U	101	SER	-	expression tag	UNP Q2RVS1
U	102	VAL	-	expression tag	UNP Q2RVS1
U	103	ASP	-	expression tag	UNP Q2RVS1
U	104	LYS	-	expression tag	UNP Q2RVS1
U	105	LEU	-	expression tag	UNP Q2RVS1
U	106	ALA	-	expression tag	UNP Q2RVS1

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Chain	Residue	Modelled	Actual	Comment	Reference
U	107	ALA	-	expression tag	UNP Q2RVS1
U	108	ALA	-	expression tag	UNP Q2RVS1
U	109	LEU	-	expression tag	UNP Q2RVS1
U	110	GLU	-	expression tag	UNP Q2RVS1
U	111	HIS	-	expression tag	UNP Q2RVS1
U	112	HIS	-	expression tag	UNP Q2RVS1
U	113	HIS	-	expression tag	UNP Q2RVS1
U	114	HIS	-	expression tag	UNP Q2RVS1
U	115	HIS	-	expression tag	UNP Q2RVS1
U	116	HIS	-	expression tag	UNP Q2RVS1
V	32	ALA	GLU	engineered mutation	UNP Q2RVS1
V	97	ALA	-	expression tag	UNP Q2RVS1
V	98	ASN	-	expression tag	UNP Q2RVS1
V	99	SER	-	expression tag	UNP Q2RVS1
V	100	SER	-	expression tag	UNP Q2RVS1
V	101	SER	-	expression tag	UNP Q2RVS1
V	102	VAL	-	expression tag	UNP Q2RVS1
V	103	ASP	-	expression tag	UNP Q2RVS1
V	104	LYS	-	expression tag	UNP Q2RVS1
V	105	LEU	-	expression tag	UNP Q2RVS1
V	106	ALA	-	expression tag	UNP Q2RVS1
V	107	ALA	-	expression tag	UNP Q2RVS1
V	108	ALA	-	expression tag	UNP Q2RVS1
V	109	LEU	-	expression tag	UNP Q2RVS1
V	110	GLU	-	expression tag	UNP Q2RVS1
V	111	HIS	-	expression tag	UNP Q2RVS1
V	112	HIS	-	expression tag	UNP Q2RVS1
V	113	HIS	-	expression tag	UNP Q2RVS1
V	114	HIS	-	expression tag	UNP Q2RVS1
V	115	HIS	-	expression tag	UNP Q2RVS1
V	116	HIS	-	expression tag	UNP Q2RVS1
W	32	ALA	GLU	engineered mutation	UNP Q2RVS1
W	97	ALA	-	expression tag	UNP Q2RVS1
W	98	ASN	-	expression tag	UNP Q2RVS1
W	99	SER	-	expression tag	UNP Q2RVS1
W	100	SER	-	expression tag	UNP Q2RVS1
W	101	SER	-	expression tag	UNP Q2RVS1
W	102	VAL	-	expression tag	UNP Q2RVS1
W	103	ASP	-	expression tag	UNP Q2RVS1
W	104	LYS	-	expression tag	UNP Q2RVS1
W	105	LEU	-	expression tag	UNP Q2RVS1
W	106	ALA	-	expression tag	UNP Q2RVS1

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Chain	Residue	Modelled	Actual	Comment	Reference
W	107	ALA	-	expression tag	UNP Q2RVS1
W	108	ALA	-	expression tag	UNP Q2RVS1
W	109	LEU	-	expression tag	UNP Q2RVS1
W	110	GLU	-	expression tag	UNP Q2RVS1
W	111	HIS	-	expression tag	UNP Q2RVS1
W	112	HIS	-	expression tag	UNP Q2RVS1
W	113	HIS	-	expression tag	UNP Q2RVS1
W	114	HIS	-	expression tag	UNP Q2RVS1
W	115	HIS	-	expression tag	UNP Q2RVS1
W	116	HIS	-	expression tag	UNP Q2RVS1
X	32	ALA	GLU	engineered mutation	UNP Q2RVS1
X	97	ALA	-	expression tag	UNP Q2RVS1
X	98	ASN	-	expression tag	UNP Q2RVS1
X	99	SER	-	expression tag	UNP Q2RVS1
X	100	SER	-	expression tag	UNP Q2RVS1
X	101	SER	-	expression tag	UNP Q2RVS1
X	102	VAL	-	expression tag	UNP Q2RVS1
X	103	ASP	-	expression tag	UNP Q2RVS1
X	104	LYS	-	expression tag	UNP Q2RVS1
X	105	LEU	-	expression tag	UNP Q2RVS1
X	106	ALA	-	expression tag	UNP Q2RVS1
X	107	ALA	-	expression tag	UNP Q2RVS1
X	108	ALA	-	expression tag	UNP Q2RVS1
X	109	LEU	-	expression tag	UNP Q2RVS1
X	110	GLU	-	expression tag	UNP Q2RVS1
X	111	HIS	-	expression tag	UNP Q2RVS1
X	112	HIS	-	expression tag	UNP Q2RVS1
X	113	HIS	-	expression tag	UNP Q2RVS1
X	114	HIS	-	expression tag	UNP Q2RVS1
X	115	HIS	-	expression tag	UNP Q2RVS1
X	116	HIS	-	expression tag	UNP Q2RVS1
Y	32	ALA	GLU	engineered mutation	UNP Q2RVS1
Y	97	ALA	-	expression tag	UNP Q2RVS1
Y	98	ASN	-	expression tag	UNP Q2RVS1
Y	99	SER	-	expression tag	UNP Q2RVS1
Y	100	SER	-	expression tag	UNP Q2RVS1
Y	101	SER	-	expression tag	UNP Q2RVS1
Y	102	VAL	-	expression tag	UNP Q2RVS1
Y	103	ASP	-	expression tag	UNP Q2RVS1
Y	104	LYS	-	expression tag	UNP Q2RVS1
Y	105	LEU	-	expression tag	UNP Q2RVS1
Y	106	ALA	-	expression tag	UNP Q2RVS1

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	107	ALA	-	expression tag	UNP Q2RVS1
Y	108	ALA	-	expression tag	UNP Q2RVS1
Y	109	LEU	-	expression tag	UNP Q2RVS1
Y	110	GLU	-	expression tag	UNP Q2RVS1
Y	111	HIS	-	expression tag	UNP Q2RVS1
Y	112	HIS	-	expression tag	UNP Q2RVS1
Y	113	HIS	-	expression tag	UNP Q2RVS1
Y	114	HIS	-	expression tag	UNP Q2RVS1
Y	115	HIS	-	expression tag	UNP Q2RVS1
Y	116	HIS	-	expression tag	UNP Q2RVS1
Z	32	ALA	GLU	engineered mutation	UNP Q2RVS1
Z	97	ALA	-	expression tag	UNP Q2RVS1
Z	98	ASN	-	expression tag	UNP Q2RVS1
Z	99	SER	-	expression tag	UNP Q2RVS1
Z	100	SER	-	expression tag	UNP Q2RVS1
Z	101	SER	-	expression tag	UNP Q2RVS1
Z	102	VAL	-	expression tag	UNP Q2RVS1
Z	103	ASP	-	expression tag	UNP Q2RVS1
Z	104	LYS	-	expression tag	UNP Q2RVS1
Z	105	LEU	-	expression tag	UNP Q2RVS1
Z	106	ALA	-	expression tag	UNP Q2RVS1
Z	107	ALA	-	expression tag	UNP Q2RVS1
Z	108	ALA	-	expression tag	UNP Q2RVS1
Z	109	LEU	-	expression tag	UNP Q2RVS1
Z	110	GLU	-	expression tag	UNP Q2RVS1
Z	111	HIS	-	expression tag	UNP Q2RVS1
Z	112	HIS	-	expression tag	UNP Q2RVS1
Z	113	HIS	-	expression tag	UNP Q2RVS1
Z	114	HIS	-	expression tag	UNP Q2RVS1
Z	115	HIS	-	expression tag	UNP Q2RVS1
Z	116	HIS	-	expression tag	UNP Q2RVS1
a	32	ALA	GLU	engineered mutation	UNP Q2RVS1
a	97	ALA	-	expression tag	UNP Q2RVS1
a	98	ASN	-	expression tag	UNP Q2RVS1
a	99	SER	-	expression tag	UNP Q2RVS1
a	100	SER	-	expression tag	UNP Q2RVS1
a	101	SER	-	expression tag	UNP Q2RVS1
a	102	VAL	-	expression tag	UNP Q2RVS1
a	103	ASP	-	expression tag	UNP Q2RVS1
a	104	LYS	-	expression tag	UNP Q2RVS1
a	105	LEU	-	expression tag	UNP Q2RVS1
a	106	ALA	-	expression tag	UNP Q2RVS1

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Chain	Residue	Modelled	Actual	Comment	Reference
a	107	ALA	-	expression tag	UNP Q2RVS1
a	108	ALA	-	expression tag	UNP Q2RVS1
a	109	LEU	-	expression tag	UNP Q2RVS1
a	110	GLU	-	expression tag	UNP Q2RVS1
a	111	HIS	-	expression tag	UNP Q2RVS1
a	112	HIS	-	expression tag	UNP Q2RVS1
a	113	HIS	-	expression tag	UNP Q2RVS1
a	114	HIS	-	expression tag	UNP Q2RVS1
a	115	HIS	-	expression tag	UNP Q2RVS1
a	116	HIS	-	expression tag	UNP Q2RVS1
b	32	ALA	GLU	engineered mutation	UNP Q2RVS1
b	97	ALA	-	expression tag	UNP Q2RVS1
b	98	ASN	-	expression tag	UNP Q2RVS1
b	99	SER	-	expression tag	UNP Q2RVS1
b	100	SER	-	expression tag	UNP Q2RVS1
b	101	SER	-	expression tag	UNP Q2RVS1
b	102	VAL	-	expression tag	UNP Q2RVS1
b	103	ASP	-	expression tag	UNP Q2RVS1
b	104	LYS	-	expression tag	UNP Q2RVS1
b	105	LEU	-	expression tag	UNP Q2RVS1
b	106	ALA	-	expression tag	UNP Q2RVS1
b	107	ALA	-	expression tag	UNP Q2RVS1
b	108	ALA	-	expression tag	UNP Q2RVS1
b	109	LEU	-	expression tag	UNP Q2RVS1
b	110	GLU	-	expression tag	UNP Q2RVS1
b	111	HIS	-	expression tag	UNP Q2RVS1
b	112	HIS	-	expression tag	UNP Q2RVS1
b	113	HIS	-	expression tag	UNP Q2RVS1
b	114	HIS	-	expression tag	UNP Q2RVS1
b	115	HIS	-	expression tag	UNP Q2RVS1
b	116	HIS	-	expression tag	UNP Q2RVS1
c	32	ALA	GLU	engineered mutation	UNP Q2RVS1
c	97	ALA	-	expression tag	UNP Q2RVS1
c	98	ASN	-	expression tag	UNP Q2RVS1
c	99	SER	-	expression tag	UNP Q2RVS1
c	100	SER	-	expression tag	UNP Q2RVS1
c	101	SER	-	expression tag	UNP Q2RVS1
c	102	VAL	-	expression tag	UNP Q2RVS1
c	103	ASP	-	expression tag	UNP Q2RVS1
c	104	LYS	-	expression tag	UNP Q2RVS1
c	105	LEU	-	expression tag	UNP Q2RVS1
c	106	ALA	-	expression tag	UNP Q2RVS1

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Chain	Residue	Modelled	Actual	Comment	Reference
c	107	ALA	-	expression tag	UNP Q2RVS1
c	108	ALA	-	expression tag	UNP Q2RVS1
c	109	LEU	-	expression tag	UNP Q2RVS1
c	110	GLU	-	expression tag	UNP Q2RVS1
c	111	HIS	-	expression tag	UNP Q2RVS1
c	112	HIS	-	expression tag	UNP Q2RVS1
c	113	HIS	-	expression tag	UNP Q2RVS1
c	114	HIS	-	expression tag	UNP Q2RVS1
c	115	HIS	-	expression tag	UNP Q2RVS1
c	116	HIS	-	expression tag	UNP Q2RVS1
d	32	ALA	GLU	engineered mutation	UNP Q2RVS1
d	97	ALA	-	expression tag	UNP Q2RVS1
d	98	ASN	-	expression tag	UNP Q2RVS1
d	99	SER	-	expression tag	UNP Q2RVS1
d	100	SER	-	expression tag	UNP Q2RVS1
d	101	SER	-	expression tag	UNP Q2RVS1
d	102	VAL	-	expression tag	UNP Q2RVS1
d	103	ASP	-	expression tag	UNP Q2RVS1
d	104	LYS	-	expression tag	UNP Q2RVS1
d	105	LEU	-	expression tag	UNP Q2RVS1
d	106	ALA	-	expression tag	UNP Q2RVS1
d	107	ALA	-	expression tag	UNP Q2RVS1
d	108	ALA	-	expression tag	UNP Q2RVS1
d	109	LEU	-	expression tag	UNP Q2RVS1
d	110	GLU	-	expression tag	UNP Q2RVS1
d	111	HIS	-	expression tag	UNP Q2RVS1
d	112	HIS	-	expression tag	UNP Q2RVS1
d	113	HIS	-	expression tag	UNP Q2RVS1
d	114	HIS	-	expression tag	UNP Q2RVS1
d	115	HIS	-	expression tag	UNP Q2RVS1
d	116	HIS	-	expression tag	UNP Q2RVS1

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	1	Total Ca 1 1	0	0
2	G	1	Total Ca 1 1	0	0
2	Q	1	Total Ca 1 1	0	0
2	d	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total 1	Ca 1	0	0
2	V	1	Total 1	Ca 1	0	0
2	N	1	Total 1	Ca 1	0	0
2	U	1	Total 1	Ca 1	0	0
2	L	1	Total 1	Ca 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total 17	O 17	0	0
3	B	11	Total 11	O 11	0	0
3	C	10	Total 10	O 10	0	0
3	D	19	Total 19	O 19	0	0
3	E	15	Total 15	O 15	0	0
3	F	16	Total 16	O 16	0	0
3	G	14	Total 14	O 14	0	0
3	H	8	Total 8	O 8	0	0
3	I	8	Total 8	O 8	0	0
3	J	9	Total 9	O 9	0	0
3	K	14	Total 14	O 14	0	0
3	L	11	Total 11	O 11	0	0
3	M	17	Total 17	O 17	0	0
3	N	21	Total 21	O 21	0	0

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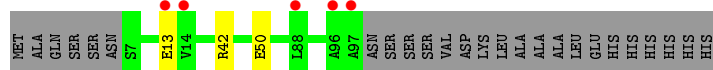
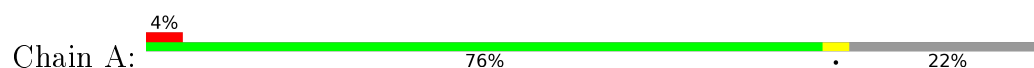
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	10	Total 10	O 10	0	0
3	P	14	Total 14	O 14	0	0
3	Q	13	Total 13	O 13	0	0
3	R	9	Total 9	O 9	0	0
3	S	11	Total 11	O 11	0	0
3	T	12	Total 12	O 12	0	0
3	U	9	Total 9	O 9	0	0
3	V	6	Total 6	O 6	0	0
3	W	4	Total 4	O 4	0	0
3	X	3	Total 3	O 3	0	0
3	Y	7	Total 7	O 7	0	0
3	Z	4	Total 4	O 4	0	0
3	a	19	Total 19	O 19	0	0
3	b	10	Total 10	O 10	0	0
3	c	16	Total 16	O 16	0	0
3	d	11	Total 11	O 11	0	0

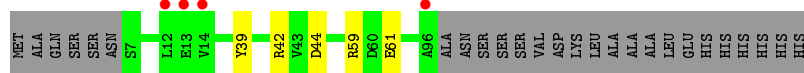
### 3 Residue-property plots [i](#)

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.

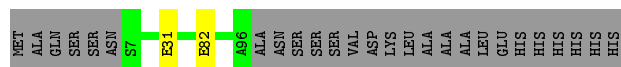
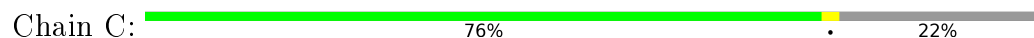
#### • Molecule 1: Rru\_A0973



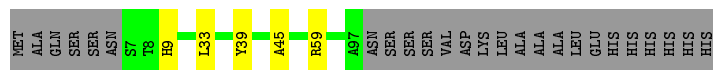
#### • Molecule 1: Rru\_A0973



#### • Molecule 1: Rru\_A0973



#### • Molecule 1: Rru\_A0973



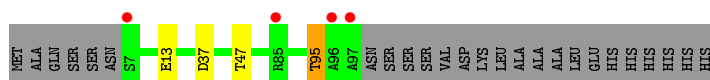
#### • Molecule 1: Rru\_A0973



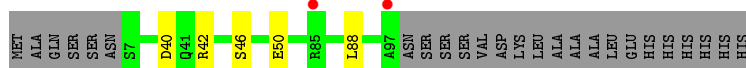
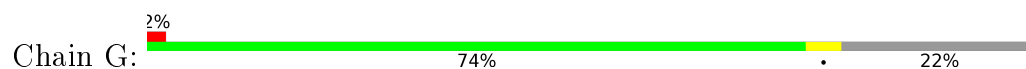
#### • Molecule 1: Rru\_A0973



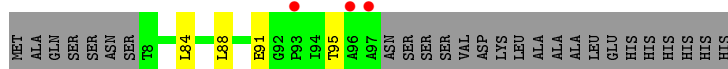
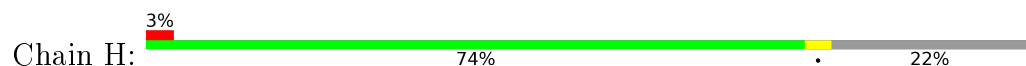




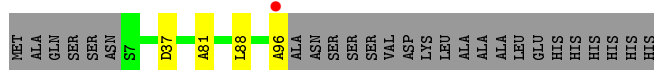
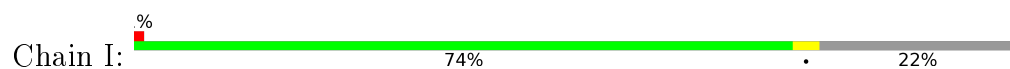
- Molecule 1: Rru\_A0973



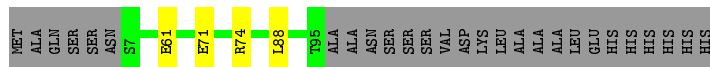
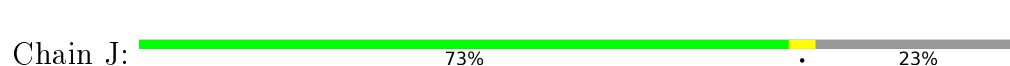
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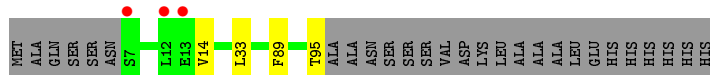
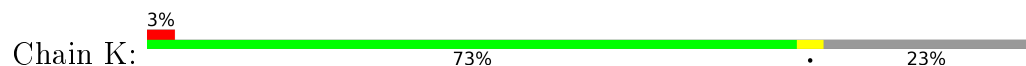
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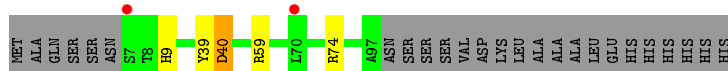
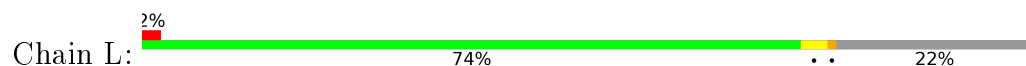
- Molecule 1: Rru\_A0973



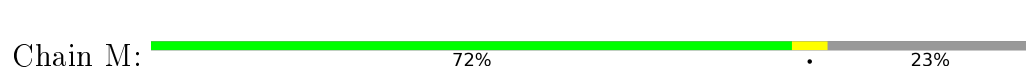
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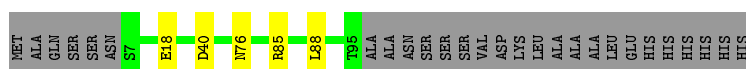


- Molecule 1: Rru\_A0973

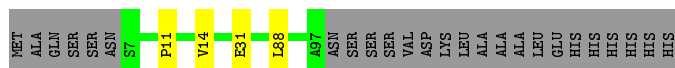


- Molecule 1: Rru\_A0973

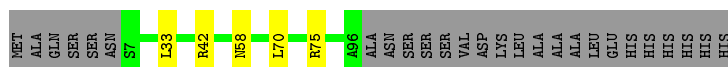




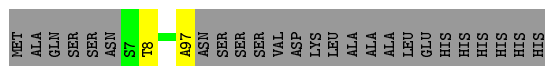
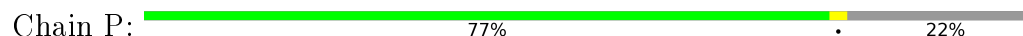
- Molecule 1: Rru\_A0973



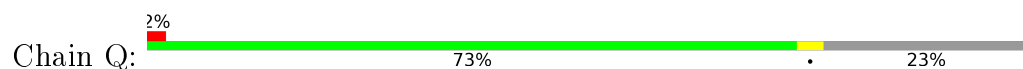
- Molecule 1: Rru\_A0973



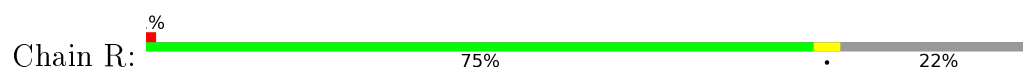
- Molecule 1: Rru\_A0973



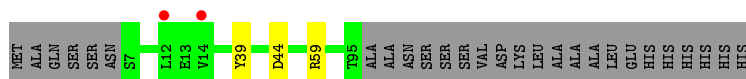
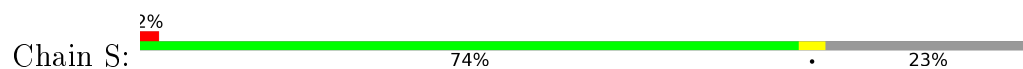
- Molecule 1: Rru\_A0973



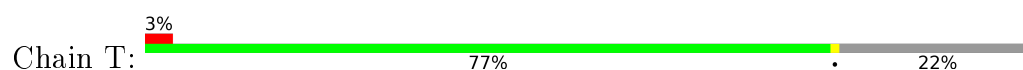
- Molecule 1: Rru\_A0973

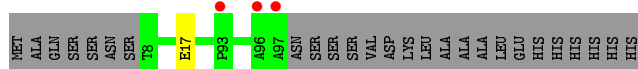


- Molecule 1: Rru\_A0973

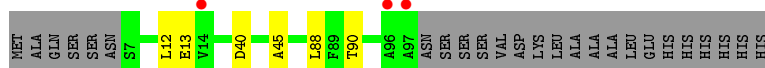
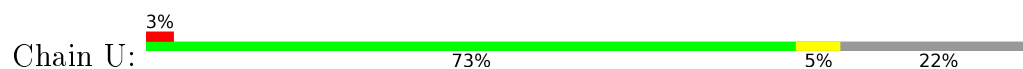


- Molecule 1: Rru\_A0973

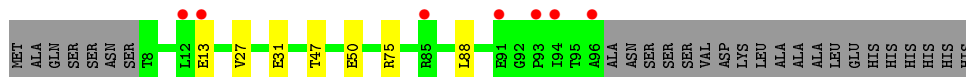




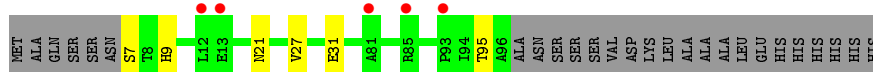
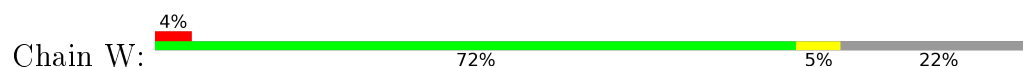
• Molecule 1: Rru\_A0973



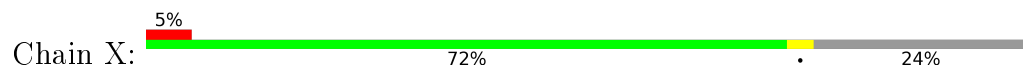
• Molecule 1: Rru\_A0973



• Molecule 1: Rru\_A0973



• Molecule 1: Rru\_A0973



• Molecule 1: Rru\_A0973

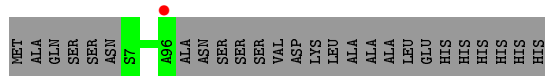


• Molecule 1: Rru\_A0973



• Molecule 1: Rru\_A0973





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.78Å 120.28Å 140.53Å 90.00° 95.41° 90.00°	Depositor
Resolution (Å)	48.84 – 2.59 49.59 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.84-2.59) 99.3 (49.59-2.59)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.20	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.186 , 0.221 0.181 , 0.218	Depositor DCC
$R_{free}$ test set	5002 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.7	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 36.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	43360	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.26	0/758	0.42	0/1032
1	B	0.25	0/753	0.42	0/1025
1	C	0.26	0/753	0.43	0/1025
1	D	0.26	0/758	0.42	0/1032
1	E	0.26	0/753	0.43	0/1025
1	F	0.26	0/758	0.43	0/1032
1	G	0.26	0/758	0.42	0/1032
1	H	0.26	0/752	0.43	0/1024
1	I	0.24	0/753	0.41	0/1025
1	J	0.25	0/748	0.43	0/1018
1	K	0.26	0/748	0.44	0/1018
1	L	0.26	0/758	0.41	0/1032
1	M	0.28	0/748	0.42	0/1018
1	N	0.26	0/758	0.43	0/1032
1	O	0.26	0/753	0.45	0/1025
1	P	0.25	0/758	0.42	0/1032
1	Q	0.26	0/748	0.42	0/1018
1	R	0.26	0/753	0.43	0/1025
1	S	0.26	0/748	0.41	0/1018
1	T	0.25	0/752	0.41	0/1024
1	U	0.25	0/758	0.42	0/1032
1	V	0.26	0/747	0.43	0/1017
1	W	0.25	0/753	0.41	0/1025
1	X	0.26	0/742	0.43	0/1010
1	Y	0.26	0/721	0.43	0/980
1	Z	0.27	0/742	0.42	0/1010
1	a	0.26	0/752	0.43	0/1024
1	b	0.27	0/742	0.42	0/1010
1	c	0.24	0/705	0.43	0/958
1	d	0.26	0/753	0.43	0/1025
All	All	0.26	0/22483	0.42	0/30603

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	742	708	708	3	0
1	B	737	703	703	5	0
1	C	737	703	703	3	0
1	D	742	708	708	2	0
1	E	737	704	703	2	0
1	F	742	708	708	4	0
1	G	742	708	708	4	0
1	H	736	704	703	3	0
1	I	737	704	703	5	0
1	J	732	698	698	3	0
1	K	732	698	698	2	0
1	L	742	708	708	3	0
1	M	732	698	698	6	0
1	N	742	708	708	5	0
1	O	737	703	703	3	0
1	P	742	708	708	2	0
1	Q	732	698	698	3	0
1	R	737	703	703	2	0
1	S	732	698	698	2	0
1	T	736	704	703	0	0
1	U	742	708	708	4	0
1	V	731	699	698	5	0
1	W	737	703	703	4	0
1	X	726	694	693	3	0
1	Y	706	670	670	7	0
1	Z	726	694	693	6	0
1	a	736	703	703	0	0
1	b	726	693	693	0	0
1	c	690	657	657	0	0
1	d	737	703	703	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	G	1	0	0	0	0
2	L	1	0	0	0	0
2	N	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	U	1	0	0	0	0
2	V	1	0	0	0	0
2	d	1	0	0	0	0
3	A	17	0	0	0	0
3	B	11	0	0	1	0
3	C	10	0	0	1	0
3	D	19	0	0	1	0
3	E	15	0	0	1	0
3	F	16	0	0	3	0
3	G	14	0	0	3	0
3	H	8	0	0	1	0
3	I	8	0	0	4	0
3	J	9	0	0	1	0
3	K	14	0	0	0	0
3	L	11	0	0	1	0
3	M	17	0	0	3	0
3	N	21	0	0	0	0
3	O	10	0	0	2	0
3	P	14	0	0	2	0
3	Q	13	0	0	3	0
3	R	9	0	0	1	0
3	S	11	0	0	1	0
3	T	12	0	0	0	0
3	U	9	0	0	2	1
3	V	6	0	0	0	0
3	W	4	0	0	1	0
3	X	3	0	0	0	0
3	Y	7	0	0	0	0
3	Z	4	0	0	1	0
3	a	19	0	0	0	1
3	b	10	0	0	0	0
3	c	16	0	0	0	0
3	d	11	0	0	0	0
All	All	22362	20998	20991	73	1

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 2.



All (73) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:46:SER:O	3:G:301:HOH:O	1.81	0.99
1:S:44:ASP:OD1	3:S:201:HOH:O	1.81	0.96
1:B:44:ASP:OD1	3:B:201:HOH:O	2.36	0.94
1:Z:64:GLU:OE1	3:Z:201:HOH:O	1.97	0.83
1:Q:44:ASP:OD1	3:Q:301:HOH:O	1.98	0.81
1:D:45:ALA:O	3:D:201:HOH:O	1.99	0.80
1:I:37:ASP:OD1	3:I:201:HOH:O	1.99	0.80
1:X:31:GLU:OE2	1:Y:42:ARG:NH2	2.17	0.76
1:E:48:ASP:OD2	3:E:201:HOH:O	2.04	0.76
1:X:57:HIS:NE2	1:X:61:GLU:OE2	2.19	0.75
1:F:37:ASP:OD1	3:F:201:HOH:O	2.03	0.75
1:M:85:ARG:O	3:M:301:HOH:O	2.04	0.75
1:G:40:ASP:OD2	3:G:302:HOH:O	2.04	0.74
1:I:81:ALA:O	3:I:202:HOH:O	2.04	0.74
1:G:42:ARG:NH2	3:G:303:HOH:O	2.23	0.72
1:U:12:LEU:O	3:U:301:HOH:O	2.05	0.72
1:U:90:THR:O	1:V:75:ARG:NH2	2.23	0.71
1:X:61:GLU:OE1	1:Y:65:HIS:NE2	2.24	0.69
1:C:82:GLU:OE2	3:C:301:HOH:O	2.12	0.68
1:Q:7:SER:O	3:Q:302:HOH:O	2.10	0.68
1:B:42:ARG:NH2	1:C:31:GLU:OE2	2.28	0.67
1:Q:8:THR:HA	3:Q:302:HOH:O	1.95	0.67
1:L:40:ASP:OD2	3:L:301:HOH:O	2.14	0.65
1:N:31:GLU:OE2	1:O:42:ARG:NH2	2.30	0.63
1:O:58:ASN:ND2	3:O:202:HOH:O	2.28	0.63
1:P:97:ALA:O	3:P:301:HOH:O	2.14	0.63
1:F:95:THR:OG1	3:F:202:HOH:O	2.16	0.62
1:F:47:THR:O	3:F:203:HOH:O	2.16	0.61
1:H:91:GLU:OE2	3:H:201:HOH:O	2.15	0.59
1:I:88:LEU:HD13	1:J:88:LEU:HD13	1.85	0.58
1:U:45:ALA:O	3:U:302:HOH:O	2.17	0.58
1:R:13:GLU:N	1:R:13:GLU:OE1	2.36	0.57
1:G:88:LEU:HD13	1:H:88:LEU:HD13	1.86	0.57
1:M:40:ASP:OD2	3:M:302:HOH:O	2.18	0.57
1:U:88:LEU:HD13	1:V:88:LEU:HD13	1.89	0.55
1:W:7:SER:N	3:W:201:HOH:O	2.40	0.55
1:A:50:GLU:OE1	1:A:50:GLU:N	2.40	0.54
1:A:42:ARG:NH2	1:C:31:GLU:OE2	26.25	0.53
1:R:7:SER:N	3:R:201:HOH:O	2.42	0.53
1:J:71:GLU:OE2	1:J:74:ARG:NH2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:47:THR:OG1	1:W:21:ASN:ND2	2.43	0.51
1:B:61:GLU:CD	1:Z:61:GLU:OE2	57.77	0.51
1:W:27:VAL:O	1:W:31:GLU:HG2	2.11	0.51
1:A:13:GLU:N	1:A:13:GLU:OE1	2.45	0.49
1:Y:88:LEU:HD13	1:Z:88:LEU:HD13	1.94	0.49
1:I:96:ALA:N	3:I:203:HOH:O	2.45	0.49
1:M:18:GLU:N	1:M:18:GLU:OE1	2.43	0.49
1:Y:57:HIS:NE2	1:Y:61:GLU:OE1	2.46	0.48
1:J:61:GLU:OE2	3:J:201:HOH:O	2.20	0.47
1:K:14:VAL:HG22	1:K:14:VAL:O	2.14	0.47
1:M:76:ASN:O	3:M:303:HOH:O	2.20	0.45
1:B:61:GLU:CG	1:Z:61:GLU:OE2	58.63	0.45
1:Y:87:TYR:OH	1:Z:64:GLU:OE2	2.30	0.45
1:S:39:TYR:HB3	1:S:59:ARG:HB2	1.99	0.44
1:O:75:ARG:NH1	3:O:204:HOH:O	2.30	0.44
1:D:39:TYR:HB3	1:D:59:ARG:HB2	2.08	0.44
1:I:81:ALA:CA	3:I:202:HOH:O	2.65	0.44
1:M:88:LEU:HD22	1:N:88:LEU:HD13	2.00	0.44
1:N:11:PRO:O	1:N:14:VAL:HG12	2.19	0.43
1:K:89:PHE:CE1	1:L:74:ARG:HD2	2.54	0.42
1:V:13:GLU:N	1:V:13:GLU:OE1	2.46	0.42
1:F:13:GLU:N	1:F:13:GLU:OE1	2.53	0.42
1:P:8:THR:HA	3:P:303:HOH:O	2.19	0.42
1:W:95:THR:HG21	1:Y:53:ALA:HB1	2.02	0.42
1:V:27:VAL:O	1:V:31:GLU:HG2	2.19	0.41
1:H:84:LEU:HD22	1:H:88:LEU:HD11	2.03	0.41
1:E:27:VAL:O	1:E:31:GLU:HG2	2.20	0.41
1:L:39:TYR:HB3	1:L:59:ARG:HB2	2.03	0.41
1:Y:14:VAL:O	1:Y:14:VAL:HG22	2.21	0.41
1:M:88:LEU:CD2	1:N:88:LEU:HD13	2.51	0.41
1:Z:39:TYR:HB3	1:Z:59:ARG:HB2	2.02	0.41
1:N:14:VAL:HG22	1:N:14:VAL:O	2.21	0.41
1:B:39:TYR:HB3	1:B:59:ARG:HB2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:301:HOH:O	3:a:214:HOH:O[2_555]	1.83	0.37

## 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	89/116 (77%)	87 (98%)	2 (2%)	0	100	100
1	B	88/116 (76%)	88 (100%)	0	0	100	100
1	C	88/116 (76%)	88 (100%)	0	0	100	100
1	D	89/116 (77%)	88 (99%)	1 (1%)	0	100	100
1	E	88/116 (76%)	87 (99%)	1 (1%)	0	100	100
1	F	89/116 (77%)	88 (99%)	1 (1%)	0	100	100
1	G	89/116 (77%)	88 (99%)	1 (1%)	0	100	100
1	H	88/116 (76%)	87 (99%)	1 (1%)	0	100	100
1	I	88/116 (76%)	87 (99%)	1 (1%)	0	100	100
1	J	87/116 (75%)	87 (100%)	0	0	100	100
1	K	87/116 (75%)	87 (100%)	0	0	100	100
1	L	89/116 (77%)	88 (99%)	1 (1%)	0	100	100
1	M	87/116 (75%)	87 (100%)	0	0	100	100
1	N	89/116 (77%)	88 (99%)	1 (1%)	0	100	100
1	O	88/116 (76%)	86 (98%)	2 (2%)	0	100	100
1	P	89/116 (77%)	87 (98%)	2 (2%)	0	100	100
1	Q	87/116 (75%)	87 (100%)	0	0	100	100
1	R	88/116 (76%)	88 (100%)	0	0	100	100
1	S	87/116 (75%)	87 (100%)	0	0	100	100
1	T	88/116 (76%)	88 (100%)	0	0	100	100
1	U	89/116 (77%)	89 (100%)	0	0	100	100
1	V	87/116 (75%)	86 (99%)	1 (1%)	0	100	100
1	W	88/116 (76%)	86 (98%)	2 (2%)	0	100	100
1	X	86/116 (74%)	86 (100%)	0	0	100	100
1	Y	83/116 (72%)	82 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	86/116 (74%)	85 (99%)	1 (1%)	0	100	100
1	a	88/116 (76%)	87 (99%)	1 (1%)	0	100	100
1	b	86/116 (74%)	86 (100%)	0	0	100	100
1	c	81/116 (70%)	81 (100%)	0	0	100	100
1	d	88/116 (76%)	87 (99%)	1 (1%)	0	100	100
All	All	2624/3480 (75%)	2603 (99%)	21 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	78/99 (79%)	78 (100%)	0	100	100
1	B	78/99 (79%)	78 (100%)	0	100	100
1	C	78/99 (79%)	78 (100%)	0	100	100
1	D	78/99 (79%)	76 (97%)	2 (3%)	54	80
1	E	78/99 (79%)	75 (96%)	3 (4%)	40	68
1	F	78/99 (79%)	77 (99%)	1 (1%)	76	91
1	G	78/99 (79%)	77 (99%)	1 (1%)	76	91
1	H	77/99 (78%)	76 (99%)	1 (1%)	76	91
1	I	78/99 (79%)	78 (100%)	0	100	100
1	J	78/99 (79%)	78 (100%)	0	100	100
1	K	78/99 (79%)	76 (97%)	2 (3%)	54	80
1	L	78/99 (79%)	76 (97%)	2 (3%)	54	80
1	M	78/99 (79%)	78 (100%)	0	100	100
1	N	78/99 (79%)	78 (100%)	0	100	100
1	O	78/99 (79%)	76 (97%)	2 (3%)	54	80
1	P	78/99 (79%)	78 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	78/99 (79%)	77 (99%)	1 (1%)	76	91
1	R	78/99 (79%)	77 (99%)	1 (1%)	76	91
1	S	78/99 (79%)	78 (100%)	0	100	100
1	T	77/99 (78%)	76 (99%)	1 (1%)	76	91
1	U	78/99 (79%)	76 (97%)	2 (3%)	54	80
1	V	77/99 (78%)	76 (99%)	1 (1%)	76	91
1	W	78/99 (79%)	77 (99%)	1 (1%)	76	91
1	X	77/99 (78%)	76 (99%)	1 (1%)	76	91
1	Y	75/99 (76%)	75 (100%)	0	100	100
1	Z	77/99 (78%)	75 (97%)	2 (3%)	54	80
1	a	77/99 (78%)	74 (96%)	3 (4%)	39	68
1	b	77/99 (78%)	73 (95%)	4 (5%)	29	54
1	c	73/99 (74%)	73 (100%)	0	100	100
1	d	78/99 (79%)	78 (100%)	0	100	100
All	All	2325/2970 (78%)	2294 (99%)	31 (1%)	76	91

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	9	HIS
1	D	33	LEU
1	E	9	HIS
1	E	14	VAL
1	E	50	GLU
1	F	95	THR
1	G	50	GLU
1	H	95	THR
1	K	33	LEU
1	K	95	THR
1	L	9	HIS
1	L	40	ASP
1	O	33	LEU
1	O	70	LEU
1	Q	31	GLU
1	R	9	HIS
1	T	17	GLU
1	U	13	GLU

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Mol	Chain	Res	Type
1	U	40	ASP
1	V	50	GLU
1	W	9	HIS
1	X	85	ARG
1	Z	9	HIS
1	Z	17	GLU
1	a	9	HIS
1	a	17	GLU
1	a	33	LEU
1	b	13	GLU
1	b	50	GLU
1	b	61	GLU
1	b	91	GLU

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	91/116 (78%)	0.29	5 (5%) 29 21	29, 41, 61, 75	0
1	B	90/116 (77%)	0.30	4 (4%) 38 30	30, 40, 61, 69	0
1	C	90/116 (77%)	0.12	0 100 100	27, 35, 57, 64	0
1	D	91/116 (78%)	0.03	0 100 100	27, 34, 58, 63	0
1	E	90/116 (77%)	0.04	2 (2%) 65 59	24, 31, 53, 63	0
1	F	91/116 (78%)	0.35	4 (4%) 38 30	23, 31, 55, 69	0
1	G	91/116 (78%)	0.24	2 (2%) 65 59	26, 37, 55, 69	0
1	H	90/116 (77%)	0.33	3 (3%) 50 43	23, 35, 57, 69	0
1	I	90/116 (77%)	0.13	1 (1%) 82 79	28, 38, 58, 74	0
1	J	89/116 (76%)	0.02	0 100 100	33, 41, 56, 65	0
1	K	89/116 (76%)	0.14	3 (3%) 49 41	26, 34, 56, 74	0
1	L	91/116 (78%)	0.14	2 (2%) 65 59	26, 36, 56, 62	0
1	M	89/116 (76%)	0.02	0 100 100	25, 32, 50, 66	0
1	N	91/116 (78%)	0.10	0 100 100	23, 35, 52, 62	0
1	O	90/116 (77%)	0.24	0 100 100	28, 36, 67, 70	0
1	P	91/116 (78%)	0.24	0 100 100	29, 39, 58, 67	0
1	Q	89/116 (76%)	0.06	2 (2%) 65 59	27, 35, 56, 69	0
1	R	90/116 (77%)	0.21	1 (1%) 82 79	28, 38, 61, 66	0
1	S	89/116 (76%)	0.14	2 (2%) 65 59	25, 34, 54, 64	0
1	T	90/116 (77%)	0.11	3 (3%) 50 43	25, 35, 54, 64	0
1	U	91/116 (78%)	0.19	3 (3%) 50 43	24, 39, 66, 71	0
1	V	89/116 (76%)	0.45	7 (7%) 15 11	27, 44, 67, 72	0
1	W	90/116 (77%)	0.43	5 (5%) 28 21	32, 46, 72, 81	0
1	X	88/116 (75%)	0.45	6 (6%) 20 15	37, 49, 70, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	Y	85/116 (73%)	0.48	0 100 100	39, 57, 68, 72	0
1	Z	88/116 (75%)	0.68	10 (11%) 7 4	39, 54, 77, 87	0
1	a	90/116 (77%)	0.24	3 (3%) 50 43	25, 36, 63, 74	0
1	b	88/116 (75%)	0.12	2 (2%) 64 57	29, 41, 58, 76	0
1	c	83/116 (71%)	0.07	2 (2%) 62 56	24, 33, 53, 66	0
1	d	90/116 (77%)	0.11	1 (1%) 82 79	25, 35, 55, 64	0
All	All	2684/3480 (77%)	0.22	73 (2%) 58 51	23, 38, 63, 87	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	96	ALA	6.8
1	H	97	ALA	5.5
1	F	97	ALA	5.1
1	F	96	ALA	4.6
1	A	96	ALA	4.6
1	Z	14	VAL	4.1
1	b	13	GLU	4.1
1	W	13	GLU	4.0
1	I	96	ALA	3.7
1	T	96	ALA	3.6
1	Z	11	PRO	3.4
1	B	12	LEU	3.3
1	V	13	GLU	3.3
1	A	97	ALA	3.3
1	V	96	ALA	3.3
1	V	94	ILE	3.2
1	K	12	LEU	3.2
1	Z	13	GLU	3.1
1	A	14	VAL	3.1
1	Z	95	THR	3.1
1	W	81	ALA	3.1
1	G	97	ALA	3.0
1	X	13	GLU	3.0
1	V	85	ARG	3.0
1	Z	93	PRO	3.0
1	V	12	LEU	3.0
1	E	89	PHE	2.9
1	Z	15	LEU	2.9
1	Z	12	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	13	GLU	2.8
1	F	7	SER	2.7
1	X	14	VAL	2.7
1	a	13	GLU	2.7
1	W	12	LEU	2.7
1	B	14	VAL	2.7
1	X	15	LEU	2.6
1	a	14	VAL	2.6
1	V	93	PRO	2.6
1	E	96	ALA	2.5
1	F	85	ARG	2.5
1	Z	88	LEU	2.5
1	B	96	ALA	2.5
1	S	14	VAL	2.5
1	R	96	ALA	2.4
1	G	85	ARG	2.4
1	X	95	THR	2.4
1	a	91	GLU	2.4
1	L	70	LEU	2.4
1	Q	14	VAL	2.4
1	T	97	ALA	2.4
1	b	12	LEU	2.3
1	V	91	GLU	2.3
1	Z	92	GLY	2.3
1	A	88	LEU	2.3
1	U	96	ALA	2.3
1	X	56	ALA	2.3
1	T	93	PRO	2.3
1	B	13	GLU	2.3
1	X	12	LEU	2.3
1	K	7	SER	2.2
1	W	85	ARG	2.2
1	L	7	SER	2.2
1	c	13	GLU	2.2
1	S	12	LEU	2.2
1	U	97	ALA	2.1
1	K	13	GLU	2.1
1	W	93	PRO	2.1
1	d	96	ALA	2.1
1	H	93	PRO	2.1
1	U	14	VAL	2.0
1	Z	89	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	Q	13	GLU	2.0
1	c	7	SER	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	V	201	1/1	0.87	0.33	5.70	72,72,72,72	0
2	CA	P	201	1/1	0.92	0.37	3.45	91,91,91,91	0
2	CA	d	201	1/1	0.72	0.29	3.12	83,83,83,83	0
2	CA	U	201	1/1	0.95	0.21	1.83	40,40,40,40	1
2	CA	Q	201	1/1	0.85	0.18	-1.29	74,74,74,74	0
2	CA	G	201	1/1	0.86	0.17	-1.44	74,74,74,74	0
2	CA	C	201	1/1	0.94	0.15	-1.47	71,71,71,71	0
2	CA	N	201	1/1	0.84	0.13	-2.17	72,72,72,72	0
2	CA	L	201	1/1	0.87	0.10	-6.28	78,78,78,78	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.