



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2016 – 11:04 AM EDT

PDB ID : 5L8G
Title : Crystal structure of Rhodospirillum rubrum Rru_A0973 mutant H65A
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 : 2.97 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

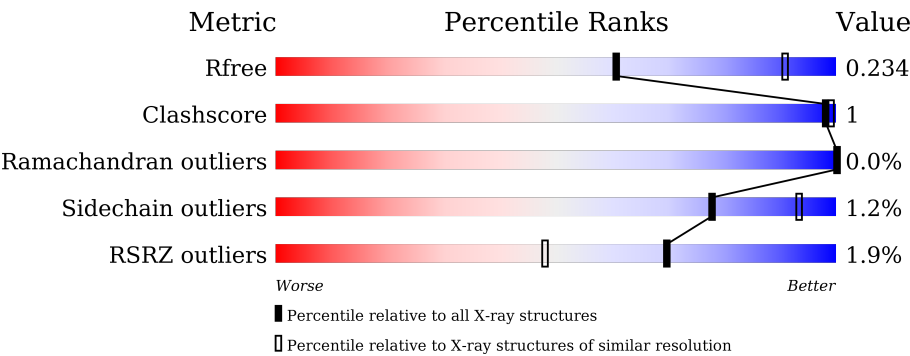
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.97 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.



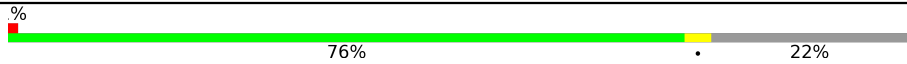

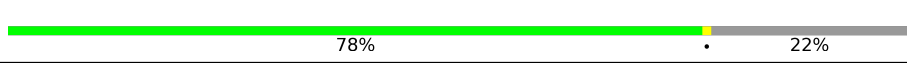
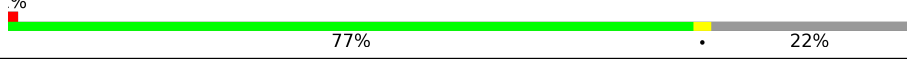

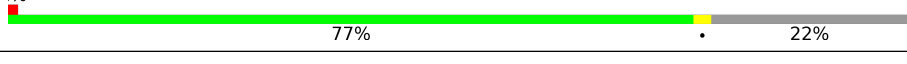


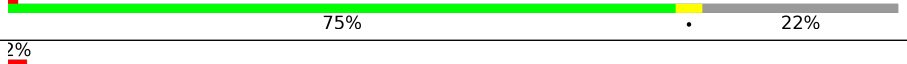


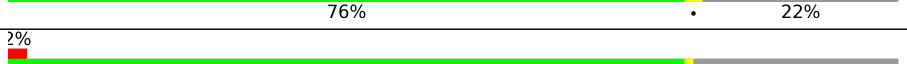

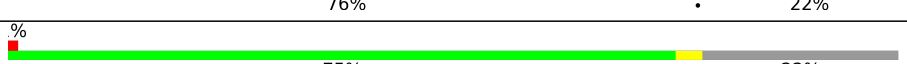
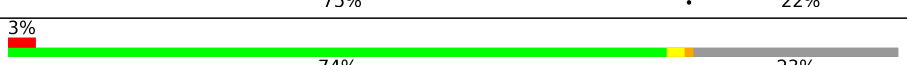
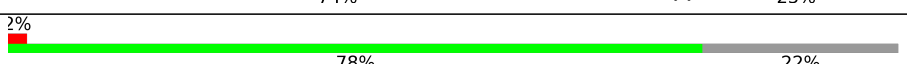
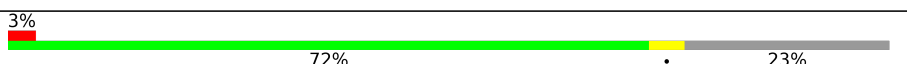
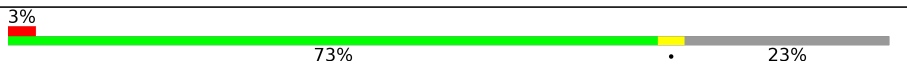
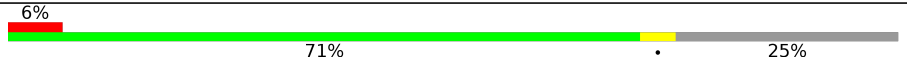



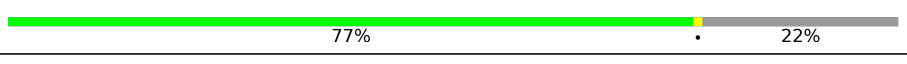

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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 ≥ 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></div><div><div></div><div></div><div></div><div></div></div><div>75%•22%</div></div>
1	B	116	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>76%•22%</div></div>
1	C	116	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>73%5%22%</div></div>
1	D	116	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>75%•22%</div></div>
1	E	116	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>72%5%22%</div></div>
1	F	116	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>77%•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	A	202	-	-	-	X
2	CA	D	203	-	-	-	X
2	CA	F	203	-	-	-	X
2	CA	I	201	-	-	-	X
2	CA	K	203	-	-	-	X
2	CA	O	202	-	-	-	X
2	CA	Q	202	-	-	-	X
2	CA	U	201	-	-	-	X
2	CA	V	201	-	-	-	X
2	CA	W	203	-	-	-	X
2	CA	X	201	-	-	-	X
2	CA	Z	204	-	-	-	X
2	CA	a	201	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 43188 atoms, of which 21043 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	91	Total	C	H	N	O	S	0	0	0
			1448	461	707	130	148	2			
1	B	91	Total	C	H	N	O	S	0	0	0
			1448	461	707	130	148	2			
1	C	91	Total	C	H	N	O	S	0	0	0
			1448	461	707	130	148	2			
1	D	91	Total	C	H	N	O	S	0	0	0
			1447	461	706	130	148	2			
1	E	90	Total	C	H	N	O	S	0	0	0
			1438	458	702	129	147	2			
1	F	91	Total	C	H	N	O	S	0	0	0
			1448	461	707	130	148	2			
1	G	91	Total	C	H	N	O	S	0	0	0
			1448	461	707	130	148	2			
1	H	91	Total	C	H	N	O	S	0	0	0
			1447	461	706	130	148	2			
1	I	91	Total	C	H	N	O	S	0	0	0
			1448	461	707	130	148	2			
1	J	91	Total	C	H	N	O	S	0	0	0
			1448	461	707	130	148	2			
1	K	91	Total	C	H	N	O	S	0	0	0
			1448	461	707	130	148	2			
1	L	91	Total	C	H	N	O	S	0	0	0
			1447	461	706	130	148	2			
1	M	89	Total	C	H	N	O	S	0	0	0
			1428	455	697	128	146	2			
1	N	91	Total	C	H	N	O	S	0	0	0
			1447	461	706	130	148	2			
1	O	90	Total	C	H	N	O	S	0	0	0
			1437	458	701	129	147	2			
1	P	91	Total	C	H	N	O	S	0	0	0
			1448	461	707	130	148	2			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	90	Total	C	H	N	O	S	0	0	0
			1438	458	702	129	147	2			
1	R	90	Total	C	H	N	O	S	0	0	0
			1438	458	702	129	147	2			
1	S	89	Total	C	H	N	O	S	0	0	0
			1428	455	697	128	146	2			
1	T	91	Total	C	H	N	O	S	0	0	0
			1448	461	707	130	148	2			
1	U	91	Total	C	H	N	O	S	0	0	0
			1448	461	707	130	148	2			
1	V	89	Total	C	H	N	O	S	0	0	0
			1428	455	697	128	146	2			
1	W	90	Total	C	H	N	O	S	0	0	0
			1438	458	702	129	147	2			
1	X	89	Total	C	H	N	O	S	0	0	0
			1427	455	696	128	146	2			
1	Y	89	Total	C	H	N	O	S	0	0	0
			1428	455	697	128	146	2			
1	Z	87	Total	C	H	N	O	S	0	0	0
			1403	448	685	126	142	2			
1	a	91	Total	C	H	N	O	S	0	0	0
			1448	461	707	130	148	2			
1	b	88	Total	C	H	N	O	S	0	0	0
			1417	452	692	127	144	2			
1	c	84	Total	C	H	N	O	S	0	0	0
			1359	433	663	123	138	2			
1	d	90	Total	C	H	N	O	S	0	0	0
			1438	458	702	129	147	2			

There are 630 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	65	ALA	HIS	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	4	Total Ca 4 4	0	0
2	K	3	Total Ca 3 3	0	0
2	B	3	Total Ca 3 3	0	0
2	c	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	W	3	Total 3	Ca 3	0	0
2	N	4	Total 4	Ca 4	0	0
2	X	3	Total 3	Ca 3	0	0
2	S	1	Total 1	Ca 1	0	0
2	J	3	Total 3	Ca 3	0	0
2	E	1	Total 1	Ca 1	0	0
2	b	1	Total 1	Ca 1	0	0
2	V	3	Total 3	Ca 3	0	0
2	A	3	Total 3	Ca 3	0	0
2	M	4	Total 4	Ca 4	0	0
2	D	4	Total 4	Ca 4	0	0
2	I	1	Total 1	Ca 1	0	0
2	Z	4	Total 4	Ca 4	0	0
2	a	4	Total 4	Ca 4	0	0
2	U	3	Total 3	Ca 3	0	0
2	L	1	Total 1	Ca 1	0	0
2	G	4	Total 4	Ca 4	0	0
2	Q	2	Total 2	Ca 2	0	0
2	d	2	Total 2	Ca 2	0	0
2	H	2	Total 2	Ca 2	0	0
2	C	3	Total 3	Ca 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	T	2	Total 2	Ca 2	0	0
2	O	2	Total 2	Ca 2	0	0
2	F	3	Total 3	Ca 3	0	0

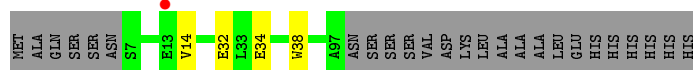
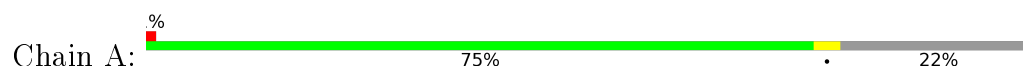
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total 1	O 1	0	0
3	P	2	Total 2	O 2	0	0
3	T	1	Total 1	O 1	0	0
3	d	1	Total 1	O 1	0	0

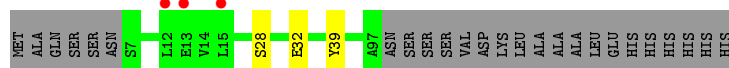
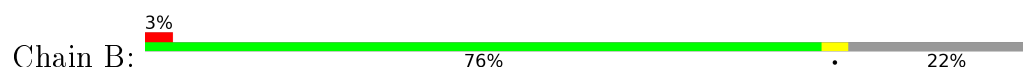
3 Residue-property plots [i](#)

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: Uncharacterized protein



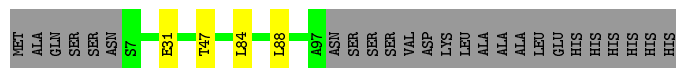
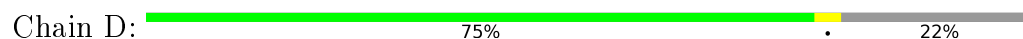
- Molecule 1: Uncharacterized protein



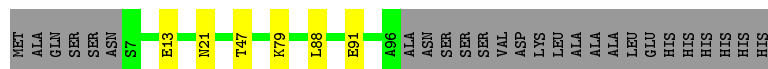
- Molecule 1: Uncharacterized protein



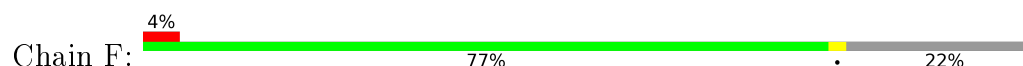
- Molecule 1: Uncharacterized protein

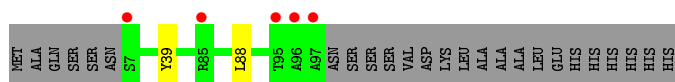


- Molecule 1: Uncharacterized protein

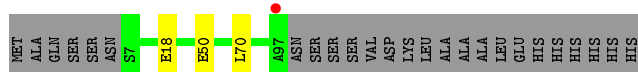
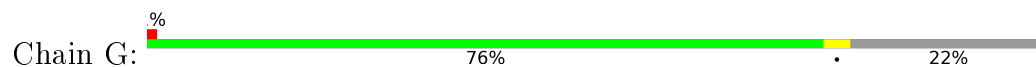


- Molecule 1: Uncharacterized protein

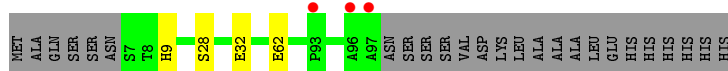
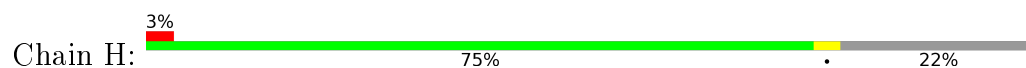




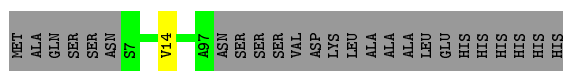
- Molecule 1: Uncharacterized protein



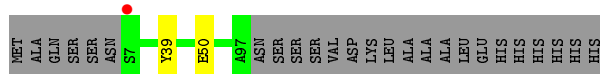
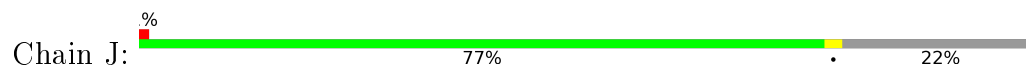
- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



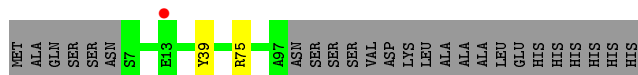
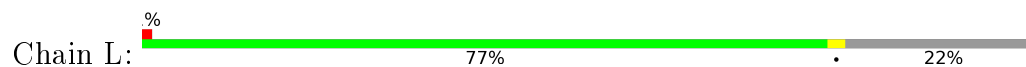
- Molecule 1: Uncharacterized protein



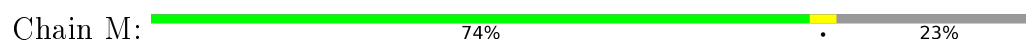
- Molecule 1: Uncharacterized protein

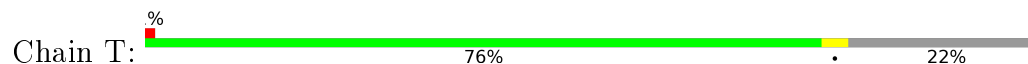


- Molecule 1: Uncharacterized protein



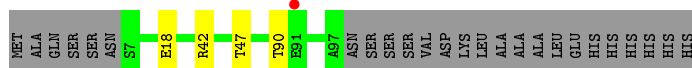
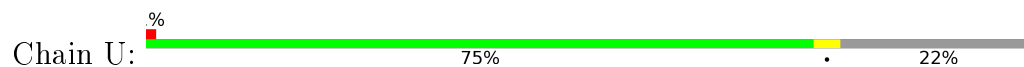
- Molecule 1: Uncharacterized protein



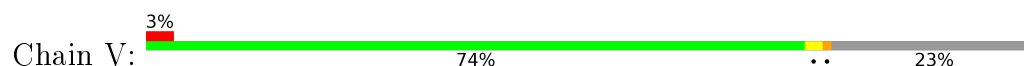




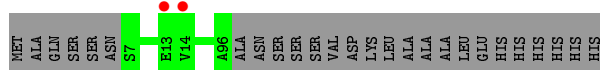
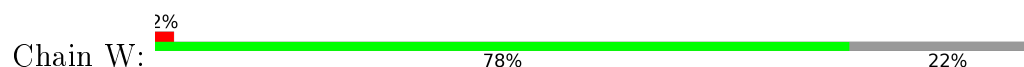
- Molecule 1: Uncharacterized protein



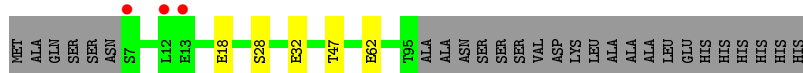
- Molecule 1: Uncharacterized protein



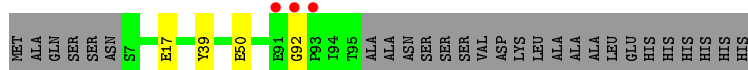
- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



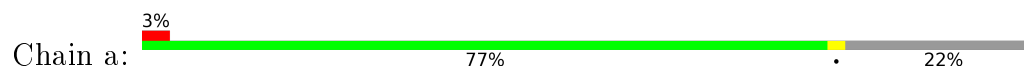
- Molecule 1: Uncharacterized protein

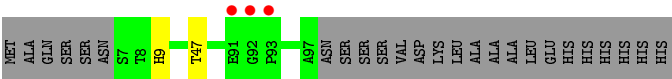


- Molecule 1: Uncharacterized protein

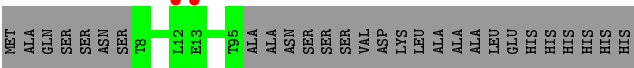
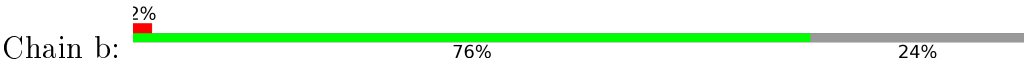


- Molecule 1: Uncharacterized protein





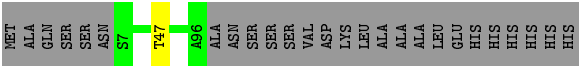
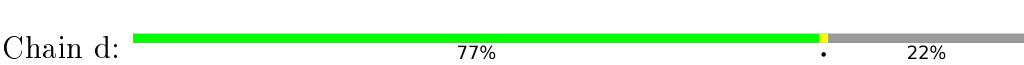
● Molecule 1: Uncharacterized protein



● Molecule 1: Uncharacterized protein



● Molecule 1: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.03Å 120.29Å 140.43Å 90.00° 95.39° 90.00°	Depositor
Resolution (Å)	48.86 – 2.97 48.87 – 2.97	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.86-2.97) 99.8 (48.87-2.97)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.196 , 0.242 0.184 , 0.234	Depositor DCC
R_{free} test set	3358 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	43188	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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

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	0.24	0/756	0.38	0/1029
1	B	0.23	0/756	0.39	0/1029
1	C	0.25	0/756	0.37	0/1029
1	D	0.23	0/756	0.37	0/1029
1	E	0.24	0/751	0.39	0/1022
1	F	0.23	0/756	0.37	0/1029
1	G	0.22	0/756	0.37	0/1029
1	H	0.23	0/756	0.37	0/1029
1	I	0.23	0/756	0.37	0/1029
1	J	0.23	0/756	0.37	0/1029
1	K	0.23	0/756	0.37	0/1029
1	L	0.24	0/756	0.37	0/1029
1	M	0.23	0/746	0.37	0/1015
1	N	0.23	0/756	0.37	0/1029
1	O	0.23	0/751	0.37	0/1022
1	P	0.24	0/756	0.38	0/1029
1	Q	0.23	0/751	0.36	0/1022
1	R	0.23	0/751	0.37	0/1022
1	S	0.22	0/746	0.38	0/1015
1	T	0.22	0/756	0.36	0/1029
1	U	0.23	0/756	0.38	0/1029
1	V	0.23	0/746	0.36	0/1015
1	W	0.23	0/751	0.37	0/1022
1	X	0.23	0/746	0.38	0/1015
1	Y	0.23	0/746	0.37	0/1015
1	Z	0.22	0/733	0.36	0/997
1	a	0.23	0/756	0.36	0/1029
1	b	0.23	0/740	0.37	0/1007
1	c	0.23	0/710	0.37	0/965
1	d	0.23	0/751	0.37	0/1022
All	All	0.23	0/22515	0.37	0/30640

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	741	707	707	3	0
1	B	741	707	707	3	0
1	C	741	707	707	7	0
1	D	741	706	706	3	0
1	E	736	702	702	3	0
1	F	741	707	707	2	0
1	G	741	707	707	0	0
1	H	741	706	706	3	0
1	I	741	707	707	0	0
1	J	741	707	707	2	0
1	K	741	707	707	2	0
1	L	741	706	706	2	0
1	M	731	697	697	3	0
1	N	741	706	706	3	0
1	O	736	701	701	2	0
1	P	741	707	707	4	0
1	Q	736	702	702	1	0
1	R	736	702	702	1	0
1	S	731	697	697	1	0
1	T	741	707	707	1	0
1	U	741	707	707	3	0
1	V	731	697	697	2	0
1	W	736	702	701	0	0
1	X	731	696	696	3	0
1	Y	731	697	697	3	0
1	Z	718	685	684	2	0
1	a	741	707	707	0	0
1	b	725	692	692	0	0
1	c	696	663	663	0	0
1	d	736	702	702	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	4	0	0	0	0
2	E	1	0	0	0	0
2	F	3	0	0	0	0
2	G	4	0	0	0	0
2	H	2	0	0	0	0
2	I	1	0	0	0	0
2	J	3	0	0	0	0
2	K	3	0	0	0	0
2	L	1	0	0	0	0
2	M	4	0	0	0	0
2	N	4	0	0	0	0
2	O	2	0	0	0	0
2	P	4	0	0	0	0
2	Q	2	0	0	0	0
2	S	1	0	0	0	0
2	T	2	0	0	0	0
2	U	3	0	0	0	0
2	V	3	0	0	0	0
2	W	3	0	0	0	0
2	X	3	0	0	0	0
2	Z	4	0	0	0	0
2	a	4	0	0	0	0
2	b	1	0	0	0	0
2	c	1	0	0	0	0
2	d	2	0	0	0	0
3	E	1	0	0	0	0
3	P	2	0	0	0	0
3	T	1	0	0	0	0
3	d	1	0	0	0	0
All	All	22145	21043	21041	41	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 (41) 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:F:39:TYR:OH	1:H:32:GLU:OE2	2.02	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:TYR:OH	1:C:32:GLU:OE2	2.01	0.78
1:T:46:SER:HG	1:T:52:THR:HG1	1.32	0.76
1:V:13:GLU:OE1	1:V:13:GLU:N	2.25	0.70
1:A:32:GLU:OE1	1:J:39:TYR:OH	2.12	0.67
1:X:32:GLU:OE2	1:Y:39:TYR:OH	2.13	0.65
1:Y:92:GLY:O	1:Z:75:ARG:NH1	2.29	0.64
1:J:50:GLU:N	1:J:50:GLU:OE1	2.33	0.61
1:U:90:THR:O	1:V:75:ARG:NH2	2.34	0.60
1:K:46:SER:HG	1:K:52:THR:HG1	1.40	0.58
1:Y:50:GLU:OE1	1:Y:50:GLU:N	2.35	0.56
1:P:32:GLU:OE2	1:R:39:TYR:OH	2.28	0.52
1:C:28:SER:O	1:C:32:GLU:HG2	2.10	0.51
1:B:28:SER:O	1:B:32:GLU:HG2	2.13	0.49
1:O:38:TRP:CE2	1:P:9:HIS:HE1	2.29	0.49
1:K:90:THR:O	1:L:75:ARG:NH2	2.47	0.47
1:O:38:TRP:CD2	1:P:9:HIS:HE1	2.33	0.47
1:U:18:GLU:OE1	1:U:18:GLU:N	2.48	0.47
1:C:28:SER:O	1:C:32:GLU:HG3	3.25	0.46
1:E:88:LEU:HD13	1:F:88:LEU:HD13	1.98	0.45
1:H:28:SER:O	1:H:32:GLU:HG2	2.16	0.45
1:M:88:LEU:HD13	1:N:88:LEU:HD13	1.99	0.45
1:P:28:SER:O	1:P:32:GLU:HG2	2.17	0.45
1:Z:47:THR:O	1:Z:47:THR:CG2	2.66	0.44
1:C:47:THR:O	1:C:47:THR:CG2	3.01	0.43
1:L:39:TYR:OH	1:M:32:GLU:OE2	2.37	0.43
1:N:47:THR:CG2	1:N:47:THR:O	2.67	0.43
1:X:28:SER:O	1:X:32:GLU:HG2	2.18	0.43
1:A:14:VAL:O	1:A:14:VAL:HG22	2.19	0.42
1:X:32:GLU:OE1	1:X:62:GLU:OE1	2.37	0.42
1:B:32:GLU:OE2	1:C:39:TYR:OH	2.33	0.42
1:Q:21:ASN:ND2	1:S:47:THR:OG1	2.46	0.42
1:C:32:GLU:OE1	1:C:62:GLU:OE2	2.37	0.42
1:H:32:GLU:OE1	1:H:62:GLU:OE1	2.38	0.42
1:N:47:THR:HG22	1:N:47:THR:O	2.20	0.42
1:A:34:GLU:HG2	1:A:38:TRP:CE2	2.66	0.41
1:D:47:THR:OG1	1:E:21:ASN:ND2	2.46	0.41
1:E:79:LYS:NZ	1:M:43:VAL:O	2.45	0.41
1:C:47:THR:HG22	1:C:47:THR:O	2.37	0.41
1:D:84:LEU:O	1:D:88:LEU:HB2	2.21	0.40
1:D:31:GLU:OE2	1:U:42:ARG:NH2	68.12	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	89/116 (77%)	88 (99%)	1 (1%)	0	100	100
1	B	89/116 (77%)	88 (99%)	1 (1%)	0	100	100
1	C	89/116 (77%)	88 (99%)	1 (1%)	0	100	100
1	D	89/116 (77%)	88 (99%)	1 (1%)	0	100	100
1	E	88/116 (76%)	88 (100%)	0	0	100	100
1	F	89/116 (77%)	88 (99%)	1 (1%)	0	100	100
1	G	89/116 (77%)	86 (97%)	3 (3%)	0	100	100
1	H	89/116 (77%)	88 (99%)	1 (1%)	0	100	100
1	I	89/116 (77%)	88 (99%)	1 (1%)	0	100	100
1	J	89/116 (77%)	89 (100%)	0	0	100	100
1	K	89/116 (77%)	88 (99%)	1 (1%)	0	100	100
1	L	89/116 (77%)	89 (100%)	0	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%)	1 (1%)	1 (1%)	17	57
1	P	89/116 (77%)	88 (99%)	1 (1%)	0	100	100
1	Q	88/116 (76%)	88 (100%)	0	0	100	100
1	R	88/116 (76%)	87 (99%)	1 (1%)	0	100	100
1	S	87/116 (75%)	86 (99%)	1 (1%)	0	100	100
1	T	89/116 (77%)	89 (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	87/116 (75%)	86 (99%)	1 (1%)	0	100	100
1	Y	87/116 (75%)	86 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	85/116 (73%)	85 (100%)	0	0	100	100
1	a	89/116 (77%)	88 (99%)	1 (1%)	0	100	100
1	b	86/116 (74%)	86 (100%)	0	0	100	100
1	c	82/116 (71%)	81 (99%)	1 (1%)	0	100	100
1	d	88/116 (76%)	87 (99%)	1 (1%)	0	100	100
All	All	2640/3480 (76%)	2615 (99%)	24 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	95	THR

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%)	77 (99%)	1 (1%)	76	93
1	D	78/99 (79%)	78 (100%)	0	100	100
1	E	78/99 (79%)	75 (96%)	3 (4%)	40	77
1	F	78/99 (79%)	78 (100%)	0	100	100
1	G	78/99 (79%)	75 (96%)	3 (4%)	40	77
1	H	78/99 (79%)	77 (99%)	1 (1%)	76	93
1	I	78/99 (79%)	77 (99%)	1 (1%)	76	93
1	J	78/99 (79%)	78 (100%)	0	100	100
1	K	78/99 (79%)	76 (97%)	2 (3%)	54	84
1	L	78/99 (79%)	78 (100%)	0	100	100
1	M	78/99 (79%)	78 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	78/99 (79%)	77 (99%)	1 (1%)	76	93
1	O	78/99 (79%)	77 (99%)	1 (1%)	76	93
1	P	78/99 (79%)	77 (99%)	1 (1%)	76	93
1	Q	78/99 (79%)	77 (99%)	1 (1%)	76	93
1	R	78/99 (79%)	77 (99%)	1 (1%)	76	93
1	S	78/99 (79%)	78 (100%)	0	100	100
1	T	78/99 (79%)	77 (99%)	1 (1%)	76	93
1	U	78/99 (79%)	77 (99%)	1 (1%)	76	93
1	V	78/99 (79%)	76 (97%)	2 (3%)	54	84
1	W	78/99 (79%)	78 (100%)	0	100	100
1	X	78/99 (79%)	76 (97%)	2 (3%)	54	84
1	Y	78/99 (79%)	77 (99%)	1 (1%)	76	93
1	Z	76/99 (77%)	73 (96%)	3 (4%)	39	76
1	a	78/99 (79%)	76 (97%)	2 (3%)	54	84
1	b	77/99 (78%)	77 (100%)	0	100	100
1	c	74/99 (75%)	74 (100%)	0	100	100
1	d	78/99 (79%)	77 (99%)	1 (1%)	76	93
All	All	2333/2970 (79%)	2304 (99%)	29 (1%)	78	93

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	38	TRP
1	E	13	GLU
1	E	47	THR
1	E	91	GLU
1	G	18	GLU
1	G	50	GLU
1	G	70	LEU
1	H	9	HIS
1	I	14	VAL
1	K	13	GLU
1	K	47	THR
1	N	85	ARG
1	O	47	THR
1	P	47	THR

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Mol	Chain	Res	Type
1	Q	13	GLU
1	R	17	GLU
1	T	47	THR
1	U	47	THR
1	V	13	GLU
1	V	47	THR
1	X	18	GLU
1	X	47	THR
1	Y	17	GLU
1	Z	17	GLU
1	Z	50	GLU
1	Z	74	ARG
1	a	9	HIS
1	a	47	THR
1	d	47	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	9	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 74 ligands modelled in this entry, 74 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, 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	91/116 (78%)	0.18	1 (1%) 82 64	35, 45, 65, 74	0
1	B	91/116 (78%)	0.31	3 (3%) 50 29	33, 43, 67, 76	0
1	C	91/116 (78%)	0.27	4 (4%) 38 21	31, 39, 59, 64	0
1	D	91/116 (78%)	-0.02	0 100 100	30, 39, 62, 69	0
1	E	90/116 (77%)	0.02	0 100 100	30, 37, 58, 65	0
1	F	91/116 (78%)	0.24	5 (5%) 29 15	27, 38, 61, 67	0
1	G	91/116 (78%)	0.20	1 (1%) 82 64	33, 41, 58, 65	0
1	H	91/116 (78%)	0.30	3 (3%) 50 29	31, 39, 60, 72	0
1	I	91/116 (78%)	0.10	0 100 100	33, 45, 64, 82	0
1	J	91/116 (78%)	0.09	1 (1%) 82 64	36, 45, 64, 75	0
1	K	91/116 (78%)	0.16	0 100 100	34, 43, 64, 70	0
1	L	91/116 (78%)	0.06	1 (1%) 82 64	33, 40, 57, 66	0
1	M	89/116 (76%)	-0.04	0 100 100	28, 38, 56, 72	0
1	N	91/116 (78%)	-0.05	0 100 100	33, 40, 55, 69	0
1	O	90/116 (77%)	0.25	1 (1%) 82 64	28, 44, 68, 80	0
1	P	91/116 (78%)	0.36	2 (2%) 65 42	34, 45, 62, 71	0
1	Q	90/116 (77%)	0.09	0 100 100	35, 47, 65, 73	0
1	R	90/116 (77%)	0.13	1 (1%) 82 64	38, 46, 66, 79	0
1	S	89/116 (76%)	0.13	2 (2%) 65 42	33, 42, 64, 75	0
1	T	91/116 (78%)	0.07	1 (1%) 82 64	34, 43, 64, 77	0
1	U	91/116 (78%)	0.18	1 (1%) 82 64	36, 47, 68, 76	0
1	V	89/116 (76%)	0.35	3 (3%) 49 28	38, 49, 71, 82	0
1	W	90/116 (77%)	0.29	2 (2%) 65 42	40, 53, 78, 87	0
1	X	89/116 (76%)	0.40	3 (3%) 49 28	41, 55, 79, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	89/116 (76%)	0.37	3 (3%) 49 28	48, 60, 74, 87	0
1	Z	87/116 (75%)	0.32	7 (8%) 15 7	46, 57, 79, 85	0
1	a	91/116 (78%)	0.31	3 (3%) 50 29	35, 45, 67, 76	0
1	b	88/116 (75%)	0.18	2 (2%) 64 41	35, 49, 67, 85	0
1	c	84/116 (72%)	0.03	1 (1%) 81 61	34, 42, 64, 75	0
1	d	90/116 (77%)	0.13	0 100 100	34, 45, 63, 74	0
All	All	2700/3480 (77%)	0.18	51 (1%) 70 48	27, 45, 68, 88	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	b	13	GLU	3.3
1	H	97	ALA	3.3
1	a	93	PRO	3.2
1	G	97	ALA	3.1
1	H	96	ALA	3.1
1	X	13	GLU	3.1
1	V	13	GLU	3.0
1	Z	92	GLY	3.0
1	a	92	GLY	2.8
1	S	7	SER	2.8
1	Z	93	PRO	2.8
1	F	7	SER	2.7
1	Y	92	GLY	2.7
1	Y	91	GLU	2.6
1	H	93	PRO	2.6
1	F	97	ALA	2.5
1	V	14	VAL	2.4
1	Z	14	VAL	2.4
1	Z	69	THR	2.4
1	C	93	PRO	2.4
1	X	12	LEU	2.4
1	a	91	GLU	2.3
1	L	13	GLU	2.3
1	C	95	THR	2.3
1	b	12	LEU	2.3
1	A	13	GLU	2.3
1	W	13	GLU	2.2
1	B	13	GLU	2.2
1	B	12	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	95	THR	2.2
1	O	7	SER	2.2
1	X	7	SER	2.2
1	P	17	GLU	2.2
1	C	47	THR	2.2
1	U	91	GLU	2.2
1	Z	12	LEU	2.1
1	c	89	PHE	2.1
1	C	94	ILE	2.1
1	J	7	SER	2.1
1	S	12	LEU	2.1
1	V	15	LEU	2.1
1	F	85	ARG	2.1
1	B	15	LEU	2.1
1	W	14	VAL	2.1
1	P	91	GLU	2.0
1	Y	93	PRO	2.0
1	Z	85	ARG	2.0
1	T	96	ALA	2.0
1	F	96	ALA	2.0
1	Z	11	PRO	2.0
1	R	93	PRO	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, 95th 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(\AA^2)	Q<0.9
2	CA	W	203	1/1	0.87	0.76	25.76	89,89,89,89	0
2	CA	F	203	1/1	0.88	0.41	13.90	62,62,62,62	0
2	CA	V	201	1/1	0.84	0.42	8.76	74,74,74,74	0
2	CA	D	203	1/1	0.88	0.39	8.67	62,62,62,62	0
2	CA	X	201	1/1	0.82	0.45	6.65	84,84,84,84	0
2	CA	U	201	1/1	0.94	0.55	6.51	66,66,66,66	0
2	CA	O	202	1/1	0.91	0.30	3.57	71,71,71,71	0
2	CA	A	202	1/1	0.91	0.38	3.54	64,64,64,64	0
2	CA	I	201	1/1	0.92	0.40	3.47	55,55,55,55	0
2	CA	a	201	1/1	0.94	0.38	3.33	65,65,65,65	0
2	CA	K	203	1/1	0.90	0.31	3.26	65,65,65,65	0
2	CA	Z	204	1/1	0.80	0.29	3.07	63,63,63,63	0
2	CA	Q	202	1/1	0.90	0.32	2.93	61,61,61,61	0
2	CA	M	201	1/1	0.90	0.26	1.22	55,55,55,55	0
2	CA	H	201	1/1	0.85	0.20	0.35	53,53,53,53	0
2	CA	M	204	1/1	0.70	0.18	0.25	76,76,76,76	0
2	CA	a	204	1/1	0.77	0.18	0.13	79,79,79,79	0
2	CA	d	202	1/1	0.97	0.19	-0.26	64,64,64,64	0
2	CA	S	201	1/1	0.87	0.20	-0.37	74,74,74,74	0
2	CA	J	203	1/1	0.93	0.16	-1.10	59,59,59,59	0
2	CA	V	203	1/1	0.91	0.18	-1.15	72,72,72,72	0
2	CA	T	202	1/1	0.93	0.15	-1.16	73,73,73,73	0
2	CA	K	202	1/1	0.76	0.16	-1.44	68,68,68,68	0
2	CA	X	203	1/1	0.93	0.14	-1.53	72,72,72,72	0
2	CA	C	201	1/1	0.85	0.14	-1.54	64,64,64,64	0
2	CA	H	202	1/1	0.89	0.14	-1.69	71,71,71,71	0
2	CA	G	201	1/1	0.90	0.17	-1.72	66,66,66,66	0
2	CA	N	201	1/1	0.51	0.14	-1.80	70,70,70,70	0
2	CA	U	203	1/1	0.93	0.14	-1.98	82,82,82,82	0
2	CA	Q	201	1/1	0.92	0.11	-2.14	77,77,77,77	0
2	CA	G	202	1/1	0.98	0.14	-2.26	67,67,67,67	0
2	CA	X	202	1/1	0.84	0.09	-2.38	69,69,69,69	0
2	CA	V	202	1/1	0.92	0.13	-2.38	60,60,60,60	0
2	CA	Z	201	1/1	0.93	0.12	-2.51	78,78,78,78	0
2	CA	D	202	1/1	0.94	0.09	-2.79	62,62,62,62	0
2	CA	A	203	1/1	0.94	0.13	-2.85	66,66,66,66	0
2	CA	Z	202	1/1	0.93	0.06	-2.90	67,67,67,67	0
2	CA	D	201	1/1	0.86	0.09	-2.96	64,64,64,64	0
2	CA	M	203	1/1	0.97	0.11	-3.03	52,52,52,52	0
2	CA	A	201	1/1	0.76	0.09	-3.09	67,67,67,67	0
2	CA	P	201	1/1	0.91	0.12	-3.68	58,58,58,58	0
2	CA	a	203	1/1	0.88	0.09	-3.87	72,72,72,72	0
2	CA	O	201	1/1	0.91	0.10	-4.13	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CA	B	201	1/1	0.84	0.09	-4.68	72,72,72,72	0
2	CA	J	201	1/1	0.89	0.12	-	78,78,78,78	0
2	CA	Z	203	1/1	0.61	0.15	-	98,98,98,98	0
2	CA	U	202	1/1	0.73	0.18	-	90,90,90,90	0
2	CA	C	203	1/1	0.75	0.15	-	78,78,78,78	0
2	CA	B	202	1/1	0.88	0.34	-	65,65,65,65	0
2	CA	G	204	1/1	0.77	0.14	-	77,77,77,77	0
2	CA	B	203	1/1	0.90	0.09	-	68,68,68,68	0
2	CA	N	202	1/1	0.91	0.12	-	77,77,77,77	0
2	CA	W	202	1/1	0.73	0.17	-	83,83,83,83	0
2	CA	d	201	1/1	0.80	0.18	-	87,87,87,87	0
2	CA	D	204	1/1	0.73	0.11	-	69,69,69,69	0
2	CA	G	203	1/1	0.93	0.07	-	84,84,84,84	0
2	CA	F	201	1/1	0.78	0.17	-	83,83,83,83	0
2	CA	W	201	1/1	0.90	0.21	-	80,80,80,80	0
2	CA	a	202	1/1	0.82	0.10	-	69,69,69,69	0
2	CA	F	202	1/1	0.82	0.13	-	70,70,70,70	0
2	CA	N	204	1/1	0.88	0.14	-	74,74,74,74	0
2	CA	P	203	1/1	0.77	0.34	-	71,71,71,71	0
2	CA	C	202	1/1	0.76	0.20	-	78,78,78,78	0
2	CA	K	201	1/1	0.86	0.09	-	88,88,88,88	0
2	CA	P	204	1/1	0.85	0.21	-	78,78,78,78	0
2	CA	b	201	1/1	0.83	0.13	-	89,89,89,89	0
2	CA	E	201	1/1	0.89	0.07	-	66,66,66,66	0
2	CA	M	202	1/1	0.70	0.19	-	84,84,84,84	0
2	CA	L	201	1/1	0.87	0.16	-	86,86,86,86	0
2	CA	c	201	1/1	0.88	0.11	-	73,73,73,73	0
2	CA	J	202	1/1	0.85	0.11	-	74,74,74,74	0
2	CA	P	202	1/1	0.74	0.18	-	80,80,80,80	0
2	CA	N	203	1/1	0.93	0.11	-	71,71,71,71	0
2	CA	T	201	1/1	0.82	0.14	-	80,80,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.