Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2016 – 09:43 PM EDT

PDB ID	:	5DA5
Title	:	Crystal structure of Rhodospirillum rubrum Rru_A0973
Authors	:	He, D.; Vanden Hehier, S.; Georgiev, A.; Altenbach, K.; Tarrant, E.; Mackay, C.L.; Waldron, K.J.; Clarke, D.J.; Marles-Wright, J.
Deposited on	:	2015-08-19
Resolution	:	2.06 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:

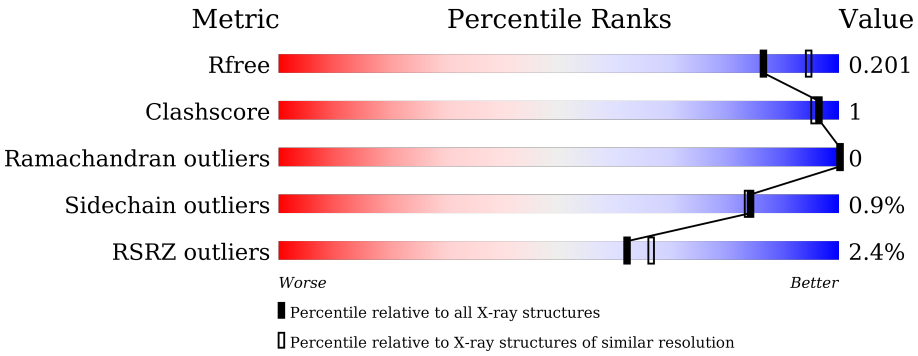
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.06 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	1799 (2.08-2.04)
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (2.08-2.04)

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 <=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	2% 76% • 22%
1	B	116	4% 77% •• 22%
1	C	116	72% 5% • 22%
1	D	116	% 73% • • 22%
1	E	116	73% • • 22%
1	F	116	2% 75% • • 22%

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Mol	Chain	Length	Quality of chain
1	G	116	74% 22%
1	H	116	2% 77% 22%
1	I	116	2% 74% 22%
1	J	116	3% 76% 22%
1	K	116	2% 74% 22%
1	L	116	77% 22%
1	M	116	% 74% 22%
1	N	116	73% 5% 22%
1	O	116	% 72% 5% 22%
1	P	116	2% 72% 6% 22%
1	Q	116	4% 77% 22%
1	R	116	3% 76% 22%
1	S	116	74% 23%
1	T	116	2% 75% 22%
1	U	116	3% 72% 6% 22%
1	V	116	3% 72% 5% 22%
1	W	116	2% 75% 22%
1	X	116	3% 72% 23%
1	Y	116	4% 73% 23%
1	Z	116	3% 73% 23%
1	a	116	5% 78% 22%
1	b	116	3% 76% 24%
1	c	116	72% 28%
1	d	116	2% 78% 22%

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	FE	A	201	-	-	-	X
2	FE	Z	201	-	-	-	X
3	GOA	A	202	-	-	-	X
3	GOA	D	202	-	-	-	X
3	GOA	G	202	-	-	-	X
3	GOA	K	204	-	-	-	X
3	GOA	L	202	-	-	-	X
3	GOA	P	202	-	-	-	X
3	GOA	Q	203	-	-	-	X
3	GOA	X	202	-	-	-	X
3	GOA	Z	202	-	-	-	X
3	GOA	a	205	-	-	-	X
4	CA	N	205	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 44491 atoms, of which 21269 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	1	0
			1471	469	720	132	148	2			
1	B	91	Total	C	H	N	O	S	0	0	0
			1455	464	709	132	148	2			
1	C	90	Total	C	H	N	O	S	0	0	0
			1445	461	704	131	147	2			
1	D	91	Total	C	H	N	O	S	0	0	0
			1455	464	709	132	148	2			
1	E	90	Total	C	H	N	O	S	0	0	0
			1445	461	704	131	147	2			
1	F	91	Total	C	H	N	O	S	0	0	0
			1455	464	709	132	148	2			
1	G	91	Total	C	H	N	O	S	0	0	0
			1455	464	709	132	148	2			
1	H	91	Total	C	H	N	O	S	0	2	0
			1487	474	731	132	148	2			
1	I	91	Total	C	H	N	O	S	0	0	0
			1455	464	709	132	148	2			
1	J	91	Total	C	H	N	O	S	0	2	0
			1487	474	731	132	148	2			
1	K	91	Total	C	H	N	O	S	0	1	0
			1468	468	718	132	148	2			
1	L	91	Total	C	H	N	O	S	0	1	0
			1472	469	721	132	148	2			
1	M	90	Total	C	H	N	O	S	0	0	0
			1445	461	704	131	147	2			
1	N	91	Total	C	H	N	O	S	0	0	0
			1455	464	709	132	148	2			
1	O	90	Total	C	H	N	O	S	0	1	0
			1456	465	711	131	147	2			
1	P	90	Total	C	H	N	O	S	0	1	0
			1461	466	716	131	146	2			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	90	Total	C	H	N	O	S	0	0	0
			1445	461	704	131	147	2			
1	R	90	Total	C	H	N	O	S	0	0	0
			1445	461	704	131	147	2			
1	S	89	Total	C	H	N	O	S	0	0	0
			1435	458	699	130	146	2			
1	T	91	Total	C	H	N	O	S	0	0	0
			1455	464	709	132	148	2			
1	U	91	Total	C	H	N	O	S	0	0	0
			1455	464	709	132	148	2			
1	V	90	Total	C	H	N	O	S	0	0	0
			1445	461	704	131	147	2			
1	W	90	Total	C	H	N	O	S	0	0	0
			1445	461	704	131	147	2			
1	X	89	Total	C	H	N	O	S	0	0	0
			1435	458	699	130	146	2			
1	Y	89	Total	C	H	N	O	S	0	0	0
			1435	458	699	130	146	2			
1	Z	89	Total	C	H	N	O	S	0	0	0
			1435	458	699	130	146	2			
1	a	91	Total	C	H	N	O	S	0	0	0
			1455	464	709	132	148	2			
1	b	88	Total	C	H	N	O	S	0	0	0
			1424	455	694	129	144	2			
1	c	84	Total	C	H	N	O	S	0	0	0
			1366	436	665	125	138	2			
1	d	91	Total	C	H	N	O	S	0	0	0
			1455	464	709	132	148	2			

There are 600 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
A	107	ALA	-	expression tag	UNP Q2RVS1

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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	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
C	107	ALA	-	expression tag	UNP Q2RVS1
C	108	ALA	-	expression tag	UNP Q2RVS1
C	109	LEU	-	expression tag	UNP Q2RVS1

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
G	114	HIS	-	expression tag	UNP Q2RVS1
G	115	HIS	-	expression tag	UNP Q2RVS1
G	116	HIS	-	expression tag	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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
I	116	HIS	-	expression tag	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	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
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	97	ALA	-	expression tag	UNP Q2RVS1

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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	97	ALA	-	expression tag	UNP Q2RVS1
N	98	ASN	-	expression tag	UNP Q2RVS1
N	99	SER	-	expression tag	UNP Q2RVS1

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
b	114	HIS	-	expression tag	UNP Q2RVS1
b	115	HIS	-	expression tag	UNP Q2RVS1
b	116	HIS	-	expression tag	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
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	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

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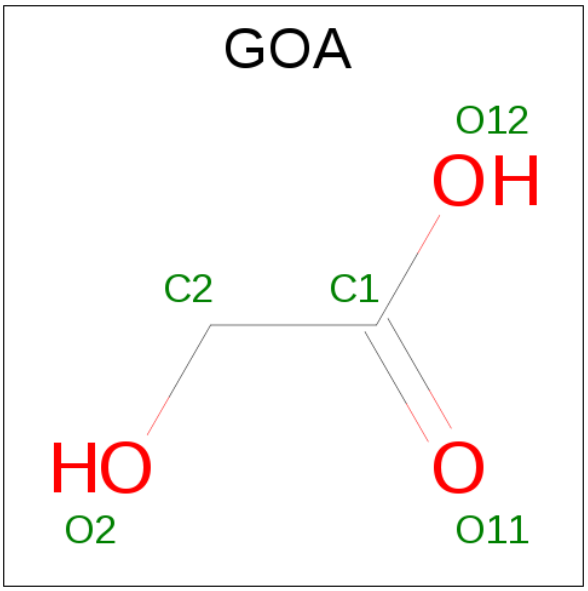
Chain	Residue	Modelled	Actual	Comment	Reference
d	116	HIS	-	expression tag	UNP Q2RVS1

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	2	Total Fe 2 2	0	0
2	G	2	Total Fe 2 2	0	0
2	Q	2	Total Fe 2 2	0	0
2	D	2	Total Fe 2 2	0	0
2	K	2	Total Fe 2 2	0	0
2	a	2	Total Fe 2 2	0	0
2	B	2	Total Fe 2 2	0	0
2	V	2	Total Fe 2 2	0	0
2	Z	2	Total Fe 2 2	0	0
2	A	2	Total Fe 2 2	0	0
2	N	2	Total Fe 2 2	0	0
2	U	2	Total Fe 2 2	0	0
2	X	2	Total Fe 2 2	0	0
2	L	2	Total Fe 2 2	0	0
2	F	2	Total Fe 2 2	0	0

- Molecule 3 is GLYCOLIC ACID (three-letter code: GOA) (formula: $C_2H_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			8	2	3	3		
3	B	1	Total	C	H	O	0	0
			8	2	3	3		
3	C	1	Total	C	H	O	0	0
			8	2	3	3		
3	D	1	Total	C	H	O	0	0
			8	2	3	3		
3	F	1	Total	C	H	O	0	0
			8	2	3	3		
3	G	1	Total	C	H	O	0	0
			8	2	3	3		
3	K	1	Total	C	H	O	0	0
			8	2	3	3		
3	L	1	Total	C	H	O	0	0
			8	2	3	3		
3	N	1	Total	C	H	O	0	0
			8	2	3	3		
3	P	1	Total	C	H	O	0	0
			8	2	3	3		
3	Q	1	Total	C	H	O	0	0
			8	2	3	3		
3	U	1	Total	C	H	O	0	0
			8	2	3	3		
3	V	1	Total	C	H	O	0	0
			8	2	3	3		
3	X	1	Total	C	H	O	0	0
			8	2	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Z	1	Total C H O 8 2 3 3	0	0
3	a	1	Total C H O 8 2 3 3	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	1	Total Ca 1 1	0	0
4	G	1	Total Ca 1 1	0	0
4	J	1	Total Ca 1 1	0	0
4	Q	1	Total Ca 1 1	0	0
4	D	3	Total Ca 3 3	0	0
4	K	1	Total Ca 1 1	0	0
4	a	3	Total Ca 3 3	0	0
4	B	1	Total Ca 1 1	0	0
4	I	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0
4	V	2	Total Ca 2 2	0	0
4	c	1	Total Ca 1 1	0	0
4	Z	1	Total Ca 1 1	0	0
4	A	1	Total Ca 1 1	0	0
4	N	2	Total Ca 2 2	0	0
4	U	1	Total Ca 1 1	0	0
4	X	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	3	Total Ca 3 3	0	0
4	F	2	Total Ca 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	34	Total O 34 34	0	0
5	B	24	Total O 24 24	0	0
5	C	38	Total O 38 38	0	0
5	D	35	Total O 35 35	0	0
5	E	46	Total O 46 46	0	0
5	F	32	Total O 32 32	0	0
5	G	35	Total O 35 35	0	0
5	H	30	Total O 30 30	0	0
5	I	43	Total O 43 43	0	0
5	J	40	Total O 40 40	0	0
5	K	30	Total O 30 30	0	0
5	L	32	Total O 32 32	0	0
5	M	34	Total O 34 34	0	0
5	N	34	Total O 34 34	0	0
5	O	17	Total O 17 17	0	0
5	P	23	Total O 23 23	0	0
5	Q	25	Total O 25 25	0	0

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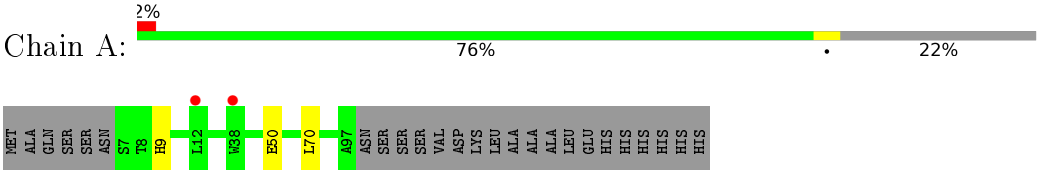
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	R	17	Total O 17 17	0	0
5	S	23	Total O 23 23	0	0
5	T	26	Total O 26 26	0	0
5	U	29	Total O 29 29	0	0
5	V	18	Total O 18 18	0	0
5	W	19	Total O 19 19	0	0
5	X	20	Total O 20 20	0	0
5	Y	5	Total O 5 5	0	0
5	Z	9	Total O 9 9	0	0
5	a	23	Total O 23 23	0	0
5	b	17	Total O 17 17	0	0
5	c	27	Total O 27 27	0	0
5	d	23	Total O 23 23	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

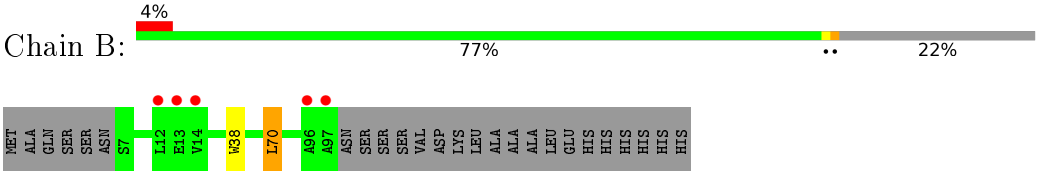
- Molecule 1: Rru_A0973

Chain A:



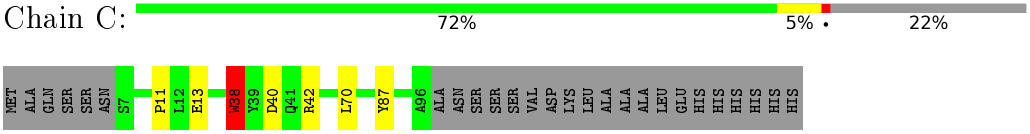
- Molecule 1: Rru_A0973

Chain B:



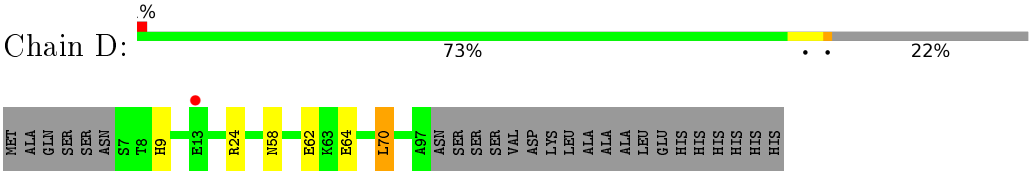
- Molecule 1: Rru_A0973

Chain C:



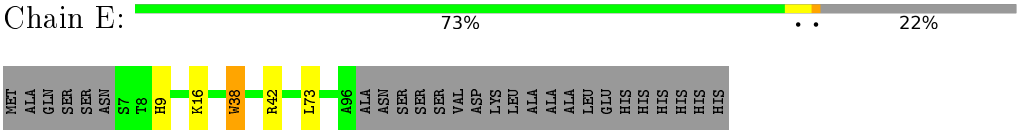
- Molecule 1: Rru_A0973

Chain D:



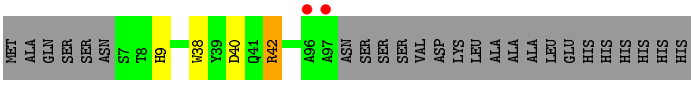
- Molecule 1: Rru_A0973

Chain E:



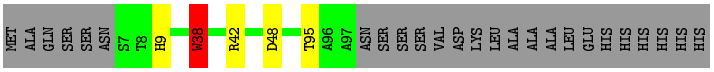
- Molecule 1: Rru_A0973

Chain F:



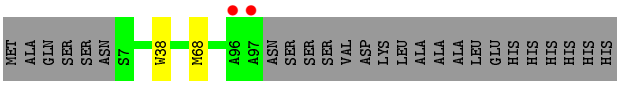
• Molecule 1: Rru_A0973

Chain G:



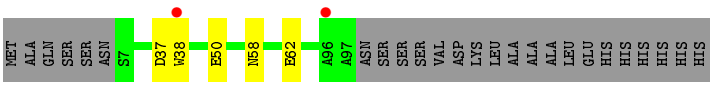
• Molecule 1: Rru_A0973

Chain H:



• Molecule 1: Rru_A0973

Chain I:

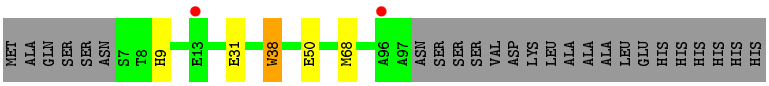


• Molecule 1: Rru_A0973

Chain J:

• Molecule 1: Rru_A0973

Chain K:

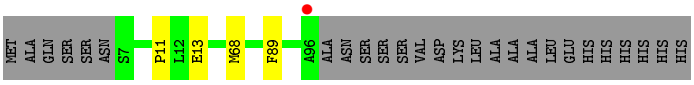


• Molecule 1: Rru_A0973

Chain L:

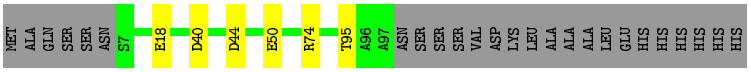
• Molecule 1: Rru_A0973

Chain M:



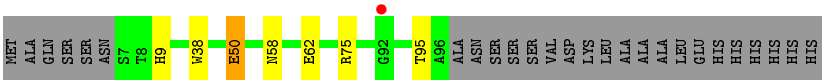
• Molecule 1: Rru_A0973

Chain N:



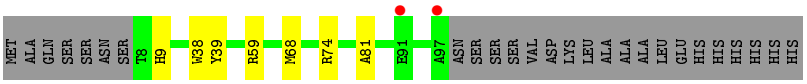
• Molecule 1: Rru_A0973

Chain O:



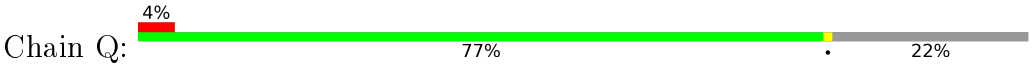
• Molecule 1: Rru_A0973

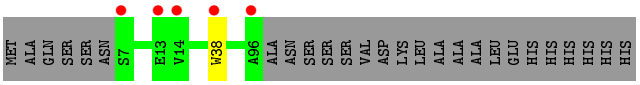
Chain P:



• Molecule 1: Rru_A0973

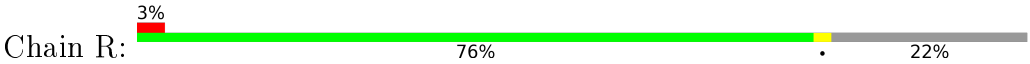
Chain Q:

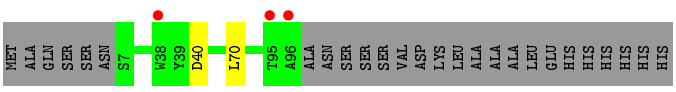




• Molecule 1: Rru_A0973

Chain R:



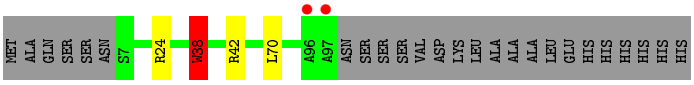


• Molecule 1: Rru_A0973

Chain S:

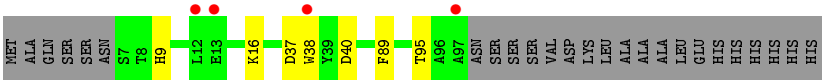
• Molecule 1: Rru_A0973

Chain T:



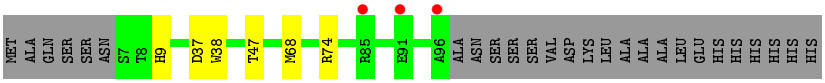
• Molecule 1: Rru_A0973

Chain U:



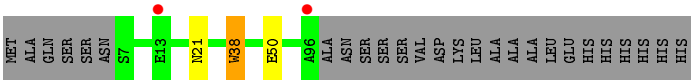
• Molecule 1: Rru_A0973

Chain V:



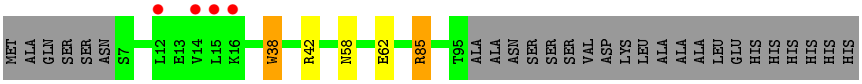
• Molecule 1: Rru_A0973

Chain W:



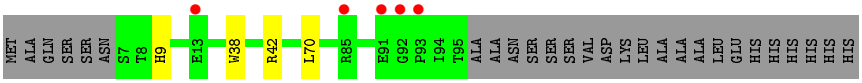
• Molecule 1: Rru_A0973

Chain X:



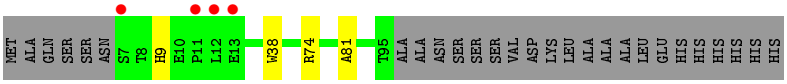
• Molecule 1: Rru_A0973

Chain Y:



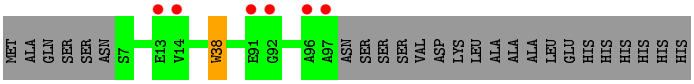
• Molecule 1: Rru_A0973

Chain Z:



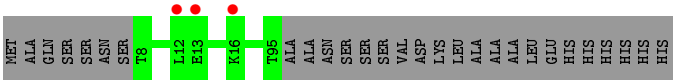
• Molecule 1: Rru_A0973

Chain a:



• Molecule 1: Rru_A0973

Chain b:



• Molecule 1: Rru_A0973

Chain c:

• Molecule 1: Rru_A0973

Chain d:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.18Å 120.53Å 140.25Å 90.00° 95.36° 90.00°	Depositor
Resolution (Å)	49.63 – 2.06 49.63 – 2.06	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.63-2.06) 99.2 (49.63-2.06)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.171 , 0.206 0.165 , 0.201	Depositor DCC
R_{free} test set	9851 reflections (4.98%)	DCC
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 45.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	44491	wwPDB-VP
Average B, all atoms (Å^2)	36.0	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.64	0/770	0.66	0/1048
1	B	0.61	0/762	0.67	1/1037 (0.1%)
1	C	0.68	0/757	0.71	1/1030 (0.1%)
1	D	0.67	0/762	0.74	1/1037 (0.1%)
1	E	0.67	0/757	0.75	1/1030 (0.1%)
1	F	0.68	0/762	0.71	1/1037 (0.1%)
1	G	0.67	0/762	0.76	1/1037 (0.1%)
1	H	0.63	0/778	0.65	0/1059
1	I	0.67	0/762	0.71	0/1037
1	J	0.64	0/778	0.68	0/1059
1	K	0.66	0/769	0.69	1/1047 (0.1%)
1	L	0.69	0/770	0.70	0/1048
1	M	0.64	0/757	0.70	0/1030
1	N	0.64	0/762	0.68	0/1037
1	O	0.61	1/764 (0.1%)	0.65	0/1040
1	P	0.56	0/764	0.61	0/1040
1	Q	0.60	0/757	0.70	0/1030
1	R	0.59	0/757	0.62	0/1030
1	S	0.63	0/752	0.67	1/1023 (0.1%)
1	T	0.57	0/762	0.66	2/1037 (0.2%)
1	U	0.61	0/762	0.69	1/1037 (0.1%)
1	V	0.61	0/757	0.65	1/1030 (0.1%)
1	W	0.60	0/757	0.67	1/1030 (0.1%)
1	X	0.59	0/752	0.68	1/1023 (0.1%)
1	Y	0.56	0/752	0.63	0/1023
1	Z	0.53	0/752	0.60	0/1023
1	a	0.59	0/762	0.67	1/1037 (0.1%)
1	b	0.57	0/746	0.66	0/1015
1	c	0.58	0/716	0.71	1/973 (0.1%)
1	d	0.60	0/762	0.66	1/1037 (0.1%)
All	All	0.62	1/22782 (0.0%)	0.68	17/31001 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	50	GLU	CG-CD	5.70	1.60	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	38	TRP	CA-CB-CG	8.03	128.97	113.70
1	C	38	TRP	CA-CB-CG	7.37	127.71	113.70
1	a	38	TRP	CA-CB-CG	7.08	127.16	113.70
1	D	24	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	X	38	TRP	CA-CB-CG	6.52	126.08	113.70
1	W	38	TRP	CA-CB-CG	6.11	125.30	113.70
1	E	38	TRP	CA-CB-CG	5.93	124.97	113.70
1	T	38	TRP	CA-CB-CG	5.80	124.73	113.70
1	K	38	TRP	CA-CB-CG	5.74	124.61	113.70
1	c	70	LEU	CB-CG-CD2	-5.70	101.32	111.00
1	U	37	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	70	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	T	24	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	V	37	ASP	CB-CG-OD1	5.08	122.88	118.30
1	d	42	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	F	42	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	S	38	TRP	CA-CB-CG	5.02	123.23	113.70

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	751	720	720	6	0
1	B	746	709	709	5	0
1	C	741	704	704	5	0
1	D	746	709	709	4	0
1	E	741	704	704	4	0
1	F	746	709	709	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	746	709	709	6	0
1	H	756	731	731	3	0
1	I	746	709	709	4	0
1	J	756	731	731	3	0
1	K	750	718	718	4	0
1	L	751	721	720	2	0
1	M	741	704	704	3	0
1	N	746	709	709	6	0
1	O	745	711	713	5	0
1	P	745	716	715	5	0
1	Q	741	704	704	0	0
1	R	741	704	704	0	0
1	S	736	699	699	1	0
1	T	746	709	709	1	0
1	U	746	709	709	4	0
1	V	741	704	704	5	0
1	W	741	704	704	2	0
1	X	736	699	699	3	0
1	Y	736	699	699	4	0
1	Z	736	699	699	4	0
1	a	746	709	709	0	0
1	b	730	694	694	0	0
1	c	701	665	665	0	0
1	d	746	709	709	0	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	D	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	N	2	0	0	0	0
2	P	2	0	0	0	0
2	Q	2	0	0	0	0
2	U	2	0	0	0	0
2	V	2	0	0	0	0
2	X	2	0	0	0	0
2	Z	2	0	0	0	0
2	a	2	0	0	0	0
3	A	5	3	3	1	0
3	B	5	3	3	0	0
3	C	5	3	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	5	3	3	0	0
3	F	5	3	3	0	0
3	G	5	3	3	0	0
3	K	5	3	3	0	0
3	L	5	3	3	0	0
3	N	5	3	3	0	0
3	P	5	3	3	0	0
3	Q	5	3	3	0	0
3	U	5	3	3	0	0
3	V	5	3	3	1	0
3	X	5	3	3	0	0
3	Z	5	3	3	0	0
3	a	5	3	3	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	3	0	0	0	0
4	F	2	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	3	0	0	0	0
4	N	2	0	0	0	0
4	P	1	0	0	0	0
4	Q	1	0	0	0	0
4	U	1	0	0	0	0
4	V	2	0	0	0	0
4	X	1	0	0	0	0
4	Z	1	0	0	0	0
4	a	3	0	0	0	0
4	c	1	0	0	0	0
5	A	34	0	0	2	0
5	B	24	0	0	0	0
5	C	38	0	0	0	0
5	D	35	0	0	0	0
5	E	46	0	0	1	0
5	F	32	0	0	0	0
5	G	35	0	0	1	0
5	H	30	0	0	0	0
5	I	43	0	0	1	0
5	J	40	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	30	0	0	2	0
5	L	32	0	0	0	0
5	M	34	0	0	0	0
5	N	34	0	0	3	0
5	O	17	0	0	0	0
5	P	23	0	0	0	0
5	Q	25	0	0	0	0
5	R	17	0	0	0	0
5	S	23	0	0	0	0
5	T	26	0	0	0	0
5	U	29	0	0	0	0
5	V	18	0	0	1	0
5	W	19	0	0	1	0
5	X	20	0	0	0	0
5	Y	5	0	0	0	0
5	Z	9	0	0	0	0
5	a	23	0	0	0	0
5	b	17	0	0	0	0
5	c	27	0	0	0	0
5	d	23	0	0	0	0
All	All	23222	21269	21269	63	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 (63) 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:W:50:GLU:OE1	5:W:301:HOH:O	2.00	0.79
1:A:50:GLU:OE1	5:A:301:HOH:O	26.15	0.79
1:K:50:GLU:OE1	5:K:301:HOH:O	2.02	0.77
1:N:50:GLU:OE1	5:N:301:HOH:O	2.04	0.75
1:G:95:THR:HG22	1:H:68:MET:HE1	1.70	0.73
3:V:202:GOA:O2	5:V:301:HOH:O	2.07	0.72
1:K:31:GLU:OE2	5:K:302:HOH:O	2.13	0.67
3:A:202:GOA:O11	5:A:301:HOH:O	2.15	0.64
1:E:16:LYS:NZ	5:E:302:HOH:O	2.35	0.58
1:U:38:TRP:CE2	1:V:9:HIS:NE2	2.73	0.57
1:F:38:TRP:HE3	1:F:42:ARG:NH2	2.04	0.56
1:N:18:GLU:OE1	5:N:302:HOH:O	2.18	0.55
1:A:9:HIS:CE1	1:B:38:TRP:NE1	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:48:ASP:OD2	5:G:301:HOH:O	2.18	0.54
1:T:38:TRP:CE3	1:T:42:ARG:NH2	2.77	0.54
1:A:9:HIS:HE1	1:B:38:TRP:NE1	2.07	0.53
1:X:85:ARG:O	1:X:85:ARG:HD3	2.08	0.52
1:N:44:ASP:O	5:N:303:HOH:O	2.19	0.51
1:I:50:GLU:HG3	5:I:324:HOH:O	2.10	0.51
1:O:38:TRP:CE2	1:P:9:HIS:NE2	2.80	0.50
1:A:70:LEU:HD21	1:B:70:LEU:HD21	1.93	0.50
1:G:95:THR:HG22	1:H:68:MET:CE	2.39	0.49
1:A:9:HIS:CE1	1:B:38:TRP:CD1	3.01	0.49
1:Y:9:HIS:NE2	1:Z:38:TRP:CE2	2.82	0.48
1:I:38:TRP:CE2	1:J:9:HIS:NE2	2.81	0.48
1:C:11:PRO:HB2	1:C:13:GLU:HG2	2.46	0.47
1:M:68:MET:HE1	1:N:95:THR:HG22	1.96	0.47
1:O:58:ASN:O	1:O:62:GLU:HG2	2.13	0.47
1:P:39:TYR:HB3	1:P:59:ARG:HB2	1.97	0.47
1:V:47:THR:OG1	1:W:21:ASN:ND2	2.47	0.47
1:A:9:HIS:CE1	1:B:38:TRP:CE2	3.03	0.47
1:Z:74:ARG:HG3	1:Z:81:ALA:HA	1.96	0.46
1:Y:38:TRP:CE2	1:Z:9:HIS:NE2	2.83	0.46
1:G:38:TRP:CE3	1:G:42:ARG:NH2	2.83	0.46
1:C:70:LEU:HD21	1:D:70:LEU:HD21	2.37	0.45
1:G:9:HIS:NE2	1:H:38:TRP:CE2	2.84	0.45
1:E:38:TRP:CE3	1:E:42:ARG:NH2	2.85	0.45
1:C:38:TRP:CD2	1:C:42:ARG:NH2	2.86	0.44
1:O:95:THR:HG22	1:P:68:MET:HE1	1.98	0.44
1:U:9:HIS:NE2	1:V:38:TRP:CE2	2.85	0.44
1:C:38:TRP:CE2	1:D:9:HIS:NE2	3.40	0.44
1:E:9:HIS:NE2	1:F:38:TRP:CE2	2.86	0.43
1:K:68:MET:HE1	1:L:95:THR:HG22	2.00	0.43
1:X:38:TRP:CE3	1:X:42:ARG:NH2	2.87	0.43
1:X:58:ASN:O	1:X:62:GLU:HG2	2.18	0.43
1:U:95:THR:HG22	1:V:68:MET:HE1	2.01	0.43
1:C:87:TYR:CE2	1:D:64:GLU:HG3	2.82	0.43
1:I:37:ASP:HB2	1:J:26:ILE:HG21	2.02	0.42
1:G:38:TRP:CD2	1:G:42:ARG:NH2	2.88	0.42
1:N:50:GLU:OE2	1:O:75:ARG:NH1	2.53	0.42
1:U:89:PHE:CE1	1:V:74:ARG:HD2	2.55	0.41
1:D:58:ASN:O	1:D:62:GLU:HG2	2.21	0.41
1:J:97:ALA:HB2	5:J:328:HOH:O	2.19	0.41
1:O:9:HIS:NE2	1:P:38:TRP:CE2	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:74:ARG:HG3	1:P:81:ALA:HA	2.03	0.41
1:K:9:HIS:NE2	1:L:38:TRP:CE2	2.89	0.41
1:E:38:TRP:CZ2	1:F:9:HIS:CE1	3.09	0.41
1:I:58:ASN:O	1:I:62:GLU:HG2	2.21	0.41
1:M:89:PHE:CE1	1:N:74:ARG:HD2	2.55	0.41
1:Y:38:TRP:HE3	1:Y:42:ARG:NH2	2.19	0.40
1:Y:38:TRP:CZ2	1:Z:9:HIS:NE2	2.89	0.40
1:M:11:PRO:HB2	1:M:13:GLU:HG2	2.02	0.40
1:S:16:LYS:NZ	1:S:18:GLU:OE2	2.44	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	90/116 (78%)	90 (100%)	0	0	100	100
1	B	89/116 (77%)	89 (100%)	0	0	100	100
1	C	88/116 (76%)	87 (99%)	1 (1%)	0	100	100
1	D	89/116 (77%)	89 (100%)	0	0	100	100
1	E	88/116 (76%)	87 (99%)	1 (1%)	0	100	100
1	F	89/116 (77%)	89 (100%)	0	0	100	100
1	G	89/116 (77%)	89 (100%)	0	0	100	100
1	H	91/116 (78%)	91 (100%)	0	0	100	100
1	I	89/116 (77%)	88 (99%)	1 (1%)	0	100	100
1	J	91/116 (78%)	91 (100%)	0	0	100	100
1	K	90/116 (78%)	90 (100%)	0	0	100	100
1	L	90/116 (78%)	90 (100%)	0	0	100	100
1	M	88/116 (76%)	87 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	89/116 (77%)	89 (100%)	0	0	100	100
1	O	89/116 (77%)	88 (99%)	1 (1%)	0	100	100
1	P	89/116 (77%)	89 (100%)	0	0	100	100
1	Q	88/116 (76%)	88 (100%)	0	0	100	100
1	R	88/116 (76%)	88 (100%)	0	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	88/116 (76%)	87 (99%)	1 (1%)	0	100	100
1	W	88/116 (76%)	87 (99%)	1 (1%)	0	100	100
1	X	87/116 (75%)	87 (100%)	0	0	100	100
1	Y	87/116 (75%)	87 (100%)	0	0	100	100
1	Z	87/116 (75%)	86 (99%)	1 (1%)	0	100	100
1	a	89/116 (77%)	89 (100%)	0	0	100	100
1	b	86/116 (74%)	86 (100%)	0	0	100	100
1	c	82/116 (71%)	82 (100%)	0	0	100	100
1	d	89/116 (77%)	89 (100%)	0	0	100	100
All	All	2652/3480 (76%)	2643 (100%)	9 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	80/100 (80%)	80 (100%)	0	100	100
1	B	79/100 (79%)	79 (100%)	0	100	100
1	C	79/100 (79%)	77 (98%)	2 (2%)	55	49
1	D	79/100 (79%)	78 (99%)	1 (1%)	76	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	79/100 (79%)	78 (99%)	1 (1%)	76	74
1	F	79/100 (79%)	78 (99%)	1 (1%)	76	74
1	G	79/100 (79%)	78 (99%)	1 (1%)	76	74
1	H	81/100 (81%)	81 (100%)	0	100	100
1	I	79/100 (79%)	79 (100%)	0	100	100
1	J	81/100 (81%)	81 (100%)	0	100	100
1	K	80/100 (80%)	79 (99%)	1 (1%)	76	74
1	L	80/100 (80%)	80 (100%)	0	100	100
1	M	79/100 (79%)	79 (100%)	0	100	100
1	N	79/100 (79%)	78 (99%)	1 (1%)	76	74
1	O	80/100 (80%)	79 (99%)	1 (1%)	76	74
1	P	79/100 (79%)	79 (100%)	0	100	100
1	Q	79/100 (79%)	78 (99%)	1 (1%)	76	74
1	R	79/100 (79%)	77 (98%)	2 (2%)	55	49
1	S	79/100 (79%)	78 (99%)	1 (1%)	76	74
1	T	79/100 (79%)	77 (98%)	2 (2%)	55	49
1	U	79/100 (79%)	77 (98%)	2 (2%)	55	49
1	V	79/100 (79%)	79 (100%)	0	100	100
1	W	79/100 (79%)	78 (99%)	1 (1%)	76	74
1	X	79/100 (79%)	78 (99%)	1 (1%)	76	74
1	Y	79/100 (79%)	78 (99%)	1 (1%)	76	74
1	Z	79/100 (79%)	79 (100%)	0	100	100
1	a	79/100 (79%)	78 (99%)	1 (1%)	76	74
1	b	78/100 (78%)	78 (100%)	0	100	100
1	c	75/100 (75%)	75 (100%)	0	100	100
1	d	79/100 (79%)	79 (100%)	0	100	100
All	All	2373/3000 (79%)	2352 (99%)	21 (1%)	84	84

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	38	TRP
1	C	40	ASP

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Mol	Chain	Res	Type
1	D	70	LEU
1	E	73	LEU
1	F	40	ASP
1	G	38	TRP
1	K	38	TRP
1	N	40	ASP
1	O	50	GLU
1	Q	38	TRP
1	R	40	ASP
1	R	70	LEU
1	S	38	TRP
1	T	38	TRP
1	T	70	LEU
1	U	16	LYS
1	U	40	ASP
1	W	38	TRP
1	X	85	ARG
1	Y	70	LEU
1	a	38	TRP

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

Mol	Chain	Res	Type
1	A	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, 58 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOA	A	202	2	1,4,4	0.15	0	1,4,4	0.16	0
3	GOA	B	204	2	1,4,4	0.20	0	1,4,4	1.73	0
3	GOA	C	201	-	1,4,4	0.25	0	1,4,4	0.49	0
3	GOA	D	202	2	1,4,4	0.55	0	1,4,4	0.11	0
3	GOA	F	202	2	1,4,4	0.23	0	1,4,4	0.36	0
3	GOA	G	202	2	1,4,4	0.48	0	1,4,4	0.55	0
3	GOA	K	204	2	1,4,4	0.36	0	1,4,4	0.98	0
3	GOA	L	202	2	1,4,4	0.15	0	1,4,4	2.41	1 (100%)
3	GOA	N	202	2	1,4,4	0.36	0	1,4,4	1.67	0
3	GOA	P	202	2	1,4,4	0.72	0	1,4,4	2.02	1 (100%)
3	GOA	Q	203	2	1,4,4	0.47	0	1,4,4	0.74	0
3	GOA	U	204	2	1,4,4	0.40	0	1,4,4	0.31	0
3	GOA	V	202	2	1,4,4	0.17	0	1,4,4	0.76	0
3	GOA	X	202	2	1,4,4	0.16	0	1,4,4	0.71	0
3	GOA	Z	202	2	1,4,4	0.18	0	1,4,4	2.44	1 (100%)
3	GOA	a	205	2	1,4,4	0.47	0	1,4,4	0.40	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOA	A	202	2	-	0/0/2/2	0/0/0/0
3	GOA	B	204	2	-	0/0/2/2	0/0/0/0
3	GOA	C	201	-	-	0/0/2/2	0/0/0/0
3	GOA	D	202	2	-	0/0/2/2	0/0/0/0
3	GOA	F	202	2	-	0/0/2/2	0/0/0/0
3	GOA	G	202	2	-	0/0/2/2	0/0/0/0
3	GOA	K	204	2	-	0/0/2/2	0/0/0/0
3	GOA	L	202	2	-	0/0/2/2	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOA	N	202	2	-	0/0/2/2	0/0/0/0
3	GOA	P	202	2	-	0/0/2/2	0/0/0/0
3	GOA	Q	203	2	-	0/0/2/2	0/0/0/0
3	GOA	U	204	2	-	0/0/2/2	0/0/0/0
3	GOA	V	202	2	-	0/0/2/2	0/0/0/0
3	GOA	X	202	2	-	0/0/2/2	0/0/0/0
3	GOA	Z	202	2	-	0/0/2/2	0/0/0/0
3	GOA	a	205	2	-	0/0/2/2	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Z	202	GOA	O2-C2-C1	-2.44	105.18	111.65
3	L	202	GOA	O2-C2-C1	-2.41	105.26	111.65
3	P	202	GOA	O2-C2-C1	-2.02	106.30	111.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	202	GOA	1	0
3	V	202	GOA	1	0

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^{th} 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%)	-0.26	2 (2%) 65 69	20, 27, 52, 61	0
1	B	91/116 (78%)	0.01	5 (5%) 29 31	19, 28, 55, 68	0
1	C	90/116 (77%)	-0.23	0 100 100	19, 25, 51, 63	0
1	D	91/116 (78%)	-0.23	1 (1%) 82 85	18, 25, 48, 60	0
1	E	90/116 (77%)	-0.31	0 100 100	19, 25, 48, 64	0
1	F	91/116 (78%)	-0.12	2 (2%) 65 69	18, 25, 50, 68	0
1	G	91/116 (78%)	-0.24	0 100 100	19, 26, 50, 57	0
1	H	91/116 (78%)	-0.04	2 (2%) 65 69	18, 25, 55, 68	0
1	I	91/116 (78%)	-0.23	2 (2%) 65 69	19, 26, 52, 62	0
1	J	91/116 (78%)	-0.34	3 (3%) 50 55	20, 26, 49, 59	0
1	K	91/116 (78%)	-0.27	2 (2%) 65 69	19, 26, 53, 66	0
1	L	91/116 (78%)	-0.33	0 100 100	20, 27, 50, 70	0
1	M	90/116 (77%)	-0.26	1 (1%) 82 85	20, 25, 50, 66	0
1	N	91/116 (78%)	-0.32	0 100 100	19, 27, 45, 57	0
1	O	90/116 (77%)	-0.23	1 (1%) 82 85	20, 30, 61, 67	0
1	P	90/116 (77%)	-0.09	2 (2%) 65 69	22, 33, 56, 62	0
1	Q	90/116 (77%)	-0.20	5 (5%) 28 31	23, 31, 59, 77	0
1	R	90/116 (77%)	-0.04	3 (3%) 50 55	22, 34, 61, 74	0
1	S	89/116 (76%)	-0.32	0 100 100	23, 30, 52, 59	0
1	T	91/116 (78%)	-0.31	2 (2%) 65 69	20, 29, 51, 61	0
1	U	91/116 (78%)	-0.03	4 (4%) 38 42	22, 31, 59, 68	0
1	V	90/116 (77%)	-0.03	3 (3%) 50 55	20, 34, 58, 67	0
1	W	90/116 (77%)	0.00	2 (2%) 65 69	24, 34, 64, 76	0
1	X	89/116 (76%)	0.14	4 (4%) 37 41	27, 38, 60, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	Y	89/116 (76%)	0.15	5 (5%) 28 31	34, 45, 66, 74	0
1	Z	89/116 (76%)	0.14	4 (4%) 37 41	30, 46, 67, 81	0
1	a	91/116 (78%)	-0.02	6 (6%) 22 23	21, 32, 62, 76	0
1	b	88/116 (75%)	-0.13	3 (3%) 49 54	26, 36, 55, 71	0
1	c	84/116 (72%)	-0.32	0 100 100	21, 28, 49, 62	0
1	d	91/116 (78%)	-0.25	2 (2%) 65 69	19, 29, 52, 72	0
All	All	2703/3480 (77%)	-0.16	66 (2%) 62 66	18, 30, 58, 81	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	96	ALA	6.0
1	K	96	ALA	5.5
1	R	96	ALA	4.8
1	H	96	ALA	4.7
1	b	12	LEU	4.5
1	B	13	GLU	4.2
1	Y	93	PRO	4.2
1	T	96	ALA	4.1
1	Q	96	ALA	3.9
1	F	97	ALA	3.8
1	B	12	LEU	3.7
1	X	12	LEU	3.6
1	B	96	ALA	3.5
1	a	92	GLY	3.5
1	B	97	ALA	3.2
1	d	96	ALA	3.1
1	Y	91	GLU	2.9
1	b	13	GLU	2.9
1	Y	92	GLY	2.9
1	U	97	ALA	2.9
1	a	97	ALA	2.8
1	Z	12	LEU	2.8
1	Z	7	SER	2.8
1	a	96	ALA	2.7
1	D	13	GLU	2.6
1	P	91	GLU	2.6
1	W	96	ALA	2.6
1	R	38	TRP	2.5
1	X	14	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	a	91	GLU	2.5
1	P	97	ALA	2.5
1	M	96	ALA	2.5
1	Y	13	GLU	2.4
1	U	13	GLU	2.4
1	Q	13	GLU	2.4
1	H	97	ALA	2.4
1	R	95	THR	2.4
1	J	7	SER	2.3
1	V	96	ALA	2.3
1	V	91	GLU	2.3
1	U	12	LEU	2.3
1	b	16	LYS	2.3
1	Z	13	GLU	2.3
1	V	85	ARG	2.3
1	J	96	ALA	2.3
1	I	38	TRP	2.3
1	a	13	GLU	2.2
1	Q	38	TRP	2.2
1	Y	85	ARG	2.2
1	A	12	LEU	2.2
1	U	38	TRP	2.2
1	B	14	VAL	2.2
1	X	16	LYS	2.2
1	A	38	TRP	2.1
1	Z	11	PRO	2.1
1	W	13	GLU	2.1
1	Q	7	SER	2.1
1	I	96	ALA	2.1
1	d	85	ARG	2.1
1	O	92	GLY	2.1
1	J	38	TRP	2.1
1	X	15	LEU	2.0
1	T	97	ALA	2.0
1	K	13	GLU	2.0
1	a	14	VAL	2.0
1	Q	14	VAL	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^{th} 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^2)	Q<0.9
3	GOA	P	202	5/5	0.92	0.19	6.91	29,39,47,54	0
3	GOA	Z	202	5/5	0.93	0.21	6.59	43,48,52,58	0
3	GOA	L	202	5/5	0.96	0.17	5.04	27,40,45,54	0
3	GOA	Q	203	5/5	0.92	0.17	4.01	32,43,52,63	0
2	FE	Z	201	1/1	0.98	0.13	3.84	36,36,36,36	0
3	GOA	G	202	5/5	0.91	0.17	3.35	30,43,49,58	0
3	GOA	K	204	5/5	0.94	0.15	3.30	31,41,51,62	0
3	GOA	a	205	5/5	0.95	0.15	3.04	27,42,48,57	0
3	GOA	X	202	5/5	0.91	0.16	2.80	42,48,59,59	0
3	GOA	A	202	5/5	0.96	0.13	2.31	26,38,44,53	0
2	FE	A	201	1/1	0.99	0.10	2.29	23,23,23,23	0
3	GOA	D	202	5/5	0.94	0.14	2.16	30,34,41,50	0
4	CA	N	205	1/1	0.76	0.18	2.11	84,84,84,84	0
3	GOA	U	204	5/5	0.94	0.14	1.87	30,37,44,53	0
3	GOA	N	202	5/5	0.96	0.12	1.56	30,44,49,58	0
3	GOA	F	202	5/5	0.95	0.16	1.52	30,43,48,51	0
3	GOA	V	202	5/5	0.94	0.15	1.45	31,40,48,54	0
3	GOA	B	204	5/5	0.94	0.14	1.38	28,40,45,52	0
2	FE	N	201	1/1	0.99	0.11	0.84	26,26,26,26	0
2	FE	Q	201	1/1	0.99	0.10	0.63	28,28,28,28	0
4	CA	a	202	1/1	0.74	0.22	0.36	78,78,78,78	0
4	CA	L	203	1/1	0.89	0.13	0.20	84,84,84,84	0
2	FE	Q	202	1/1	0.99	0.09	-0.24	25,25,25,25	0
4	CA	F	203	1/1	0.93	0.11	-0.26	68,68,68,68	0
2	FE	N	204	1/1	0.99	0.09	-0.41	26,26,26,26	0
4	CA	V	203	1/1	0.85	0.10	-0.84	81,81,81,81	0
2	FE	D	205	1/1	0.99	0.09	-0.99	20,20,20,20	0
4	CA	J	201	1/1	0.97	0.07	-1.04	45,45,45,45	0
4	CA	I	201	1/1	0.94	0.07	-1.09	57,57,57,57	0
4	CA	L	204	1/1	0.82	0.09	-1.13	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FE	Z	204	1/1	0.98	0.09	-1.18	34,34,34,34	0
4	CA	c	201	1/1	0.92	0.07	-1.19	77,77,77,77	0
2	FE	X	201	1/1	0.95	0.09	-1.55	34,34,34,34	0
2	FE	A	204	1/1	1.00	0.08	-1.80	21,21,21,21	0
2	FE	a	204	1/1	0.99	0.08	-2.09	23,23,23,23	0
2	FE	F	201	1/1	0.99	0.09	-2.16	21,21,21,21	0
2	FE	G	204	1/1	1.00	0.07	-2.17	20,20,20,20	0
4	CA	C	202	1/1	0.82	0.06	-2.25	76,76,76,76	0
2	FE	X	204	1/1	0.97	0.08	-2.40	35,35,35,35	0
2	FE	D	201	1/1	1.00	0.07	-2.47	20,20,20,20	0
2	FE	L	206	1/1	1.00	0.08	-2.62	23,23,23,23	0
2	FE	G	201	1/1	0.99	0.07	-2.73	23,23,23,23	0
2	FE	B	201	1/1	1.00	0.05	-3.23	21,21,21,21	0
2	FE	P	204	1/1	0.98	0.07	-3.39	27,27,27,27	0
2	FE	a	201	1/1	1.00	0.07	-3.45	23,23,23,23	0
2	FE	B	203	1/1	1.00	0.04	-3.98	20,20,20,20	0
2	FE	F	204	1/1	0.99	0.05	-3.99	21,21,21,21	0
2	FE	U	201	1/1	1.00	0.07	-4.13	21,21,21,21	0
2	FE	K	201	1/1	0.99	0.06	-4.67	24,24,24,24	0
2	FE	L	201	1/1	1.00	0.06	-4.77	21,21,21,21	0
2	FE	K	203	1/1	0.99	0.06	-5.14	23,23,23,23	0
2	FE	U	203	1/1	0.99	0.08	-5.22	18,18,18,18	0
2	FE	P	201	1/1	0.99	0.07	-5.51	23,23,23,23	0
2	FE	V	205	1/1	0.99	0.07	-5.86	22,22,22,22	0
2	FE	V	201	1/1	0.99	0.06	-6.17	24,24,24,24	0
4	CA	V	204	1/1	0.97	0.14	-	46,46,46,46	0
4	CA	A	203	1/1	0.97	0.12	-	42,42,42,42	0
4	CA	N	203	1/1	0.98	0.12	-	46,46,46,46	0
4	CA	D	203	1/1	0.75	0.22	-	85,85,85,85	0
4	CA	D	206	1/1	0.81	0.11	-	75,75,75,75	0
4	CA	B	202	1/1	0.99	0.09	-	38,38,38,38	0
4	CA	K	202	1/1	0.99	0.06	-	44,44,44,44	0
4	CA	U	202	1/1	0.98	0.13	-	42,42,42,42	0
4	CA	a	203	1/1	0.80	0.10	-	88,88,88,88	0
4	CA	D	204	1/1	0.99	0.14	-	40,40,40,40	0
4	CA	Z	203	1/1	0.98	0.09	-	46,46,46,46	0
4	CA	L	205	1/1	0.99	0.11	-	41,41,41,41	0
4	CA	F	205	1/1	0.99	0.12	-	37,37,37,37	0
4	CA	X	203	1/1	0.98	0.15	-	54,54,54,54	0
4	CA	Q	204	1/1	0.99	0.10	-	41,41,41,41	0
4	CA	a	206	1/1	0.98	0.10	-	45,45,45,45	0
4	CA	G	203	1/1	0.98	0.10	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	CA	P	203	1/1	0.96	0.08	-	48,48,48,48	0
3	GOA	C	201	5/5	0.83	0.15	-	50,60,61,65	0

6.5 Other polymers (i)

There are no such residues in this entry.