



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:45 AM UTC

PDB ID : 5DA5 / pdb_00005da5
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

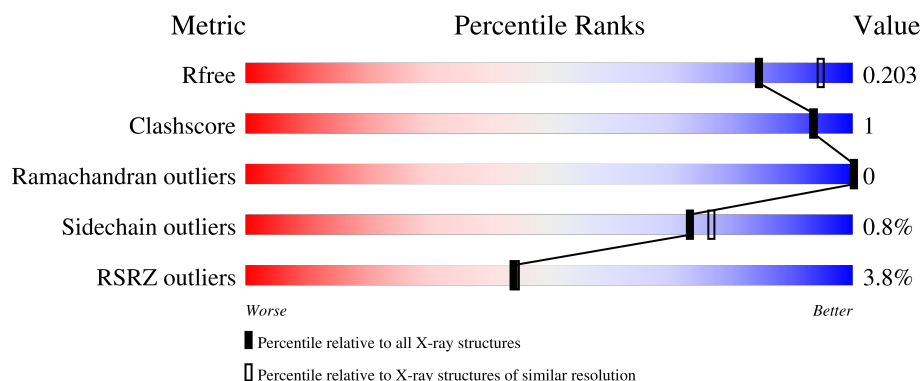
1 Overall quality at a glance

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.



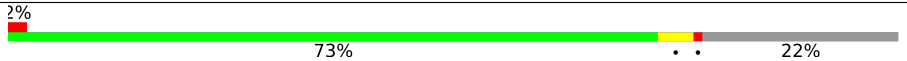
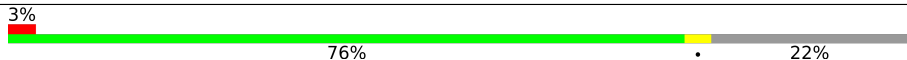
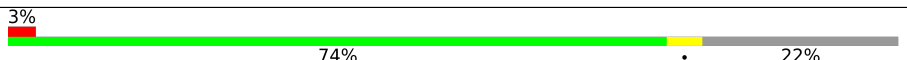
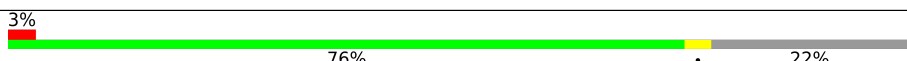
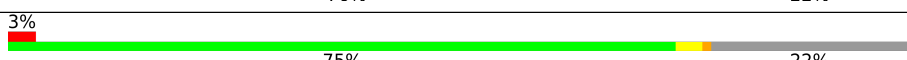
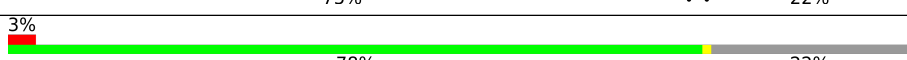
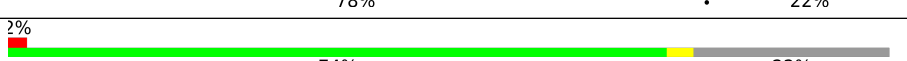
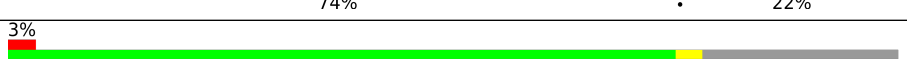
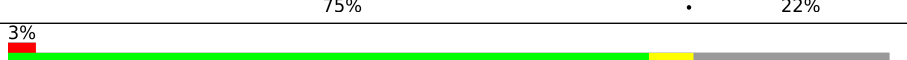
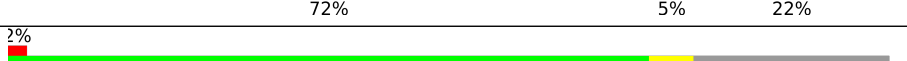
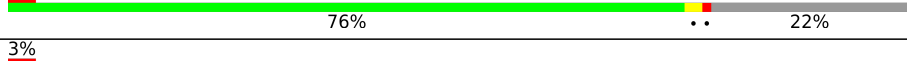
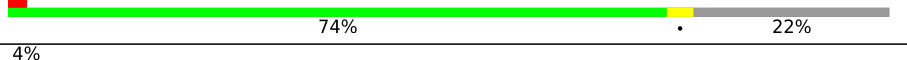
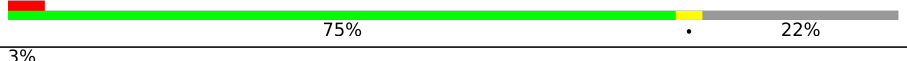
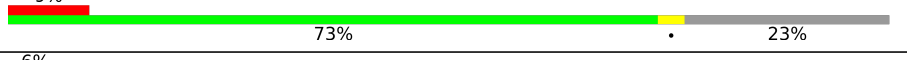
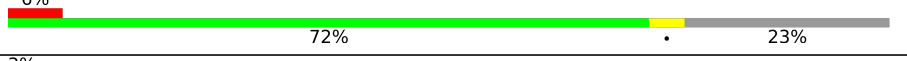
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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

Mol	Chain	Length	Quality of chain
1	A	116	
1	B	116	
1	C	116	
1	D	116	
1	E	116	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	116	
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	

2 Entry composition [i](#)

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			

Continued on next page...

Continued from previous page...

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

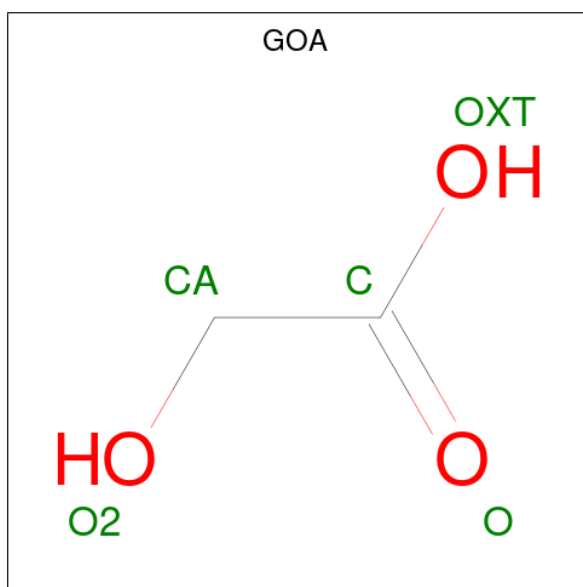
Continued from previous page...

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

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 3 is GLYCOLIC ACID (CCD ID: GOA) (formula: C₂H₄O₃).



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		

Continued on next page...

Continued from previous page...

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	a	3	Total 3	Ca 3	0	0
4	c	1	Total 1	Ca 1	0	0

- Molecule 5 is water.

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

Continued on next page...

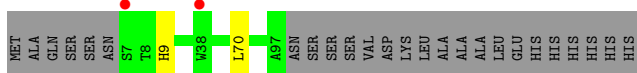
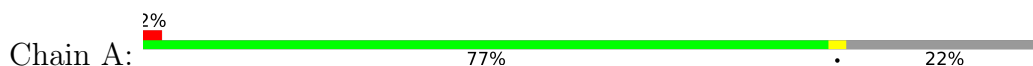
Continued from previous page...

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

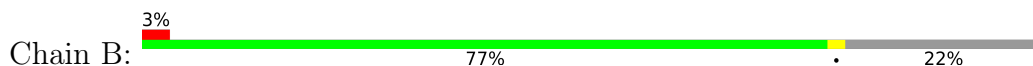
3 Residue-property plots [i](#)

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

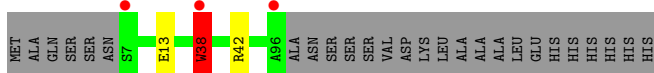
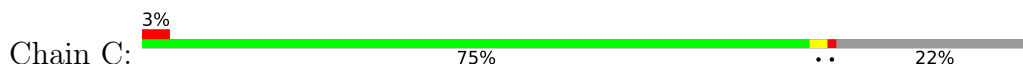
- Molecule 1: Rru_A0973



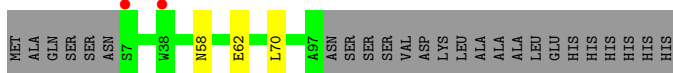
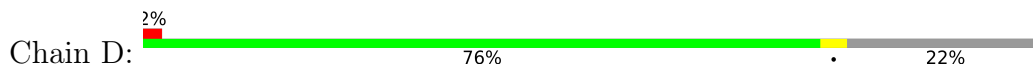
- Molecule 1: Rru_A0973



- Molecule 1: Rru_A0973



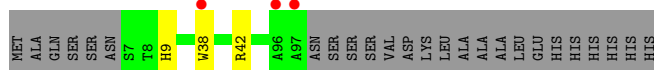
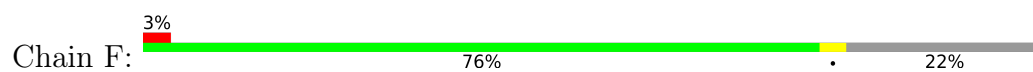
- Molecule 1: Rru_A0973



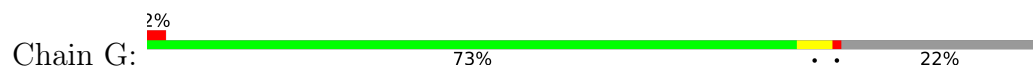
- Molecule 1: Rru_A0973



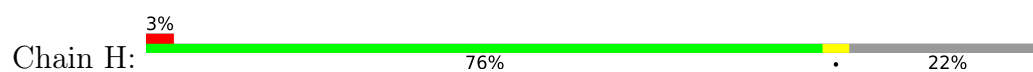
- Molecule 1: Rru_A0973



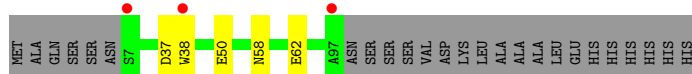
• Molecule 1: Rru_A0973



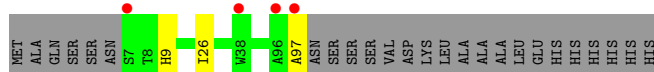
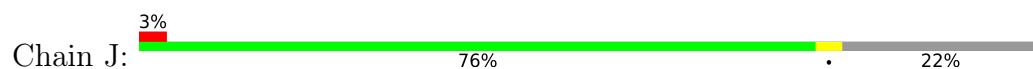
• Molecule 1: Rru_A0973



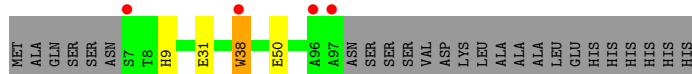
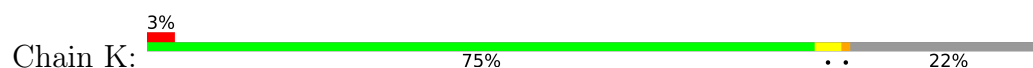
• Molecule 1: Rru_A0973



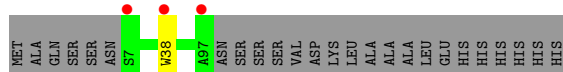
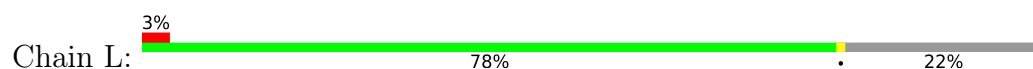
• Molecule 1: Rru_A0973



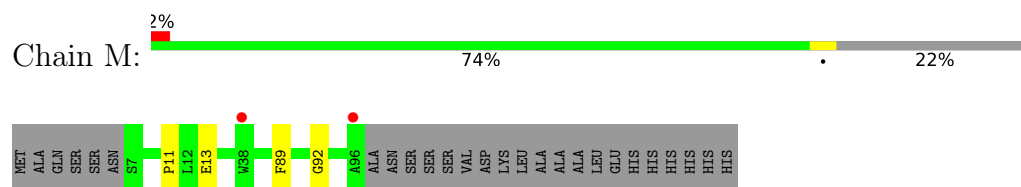
• Molecule 1: Rru_A0973



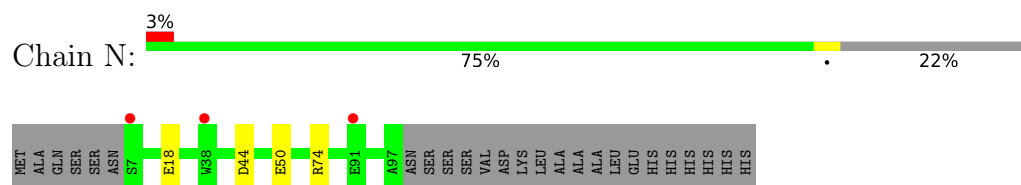
• Molecule 1: Rru_A0973



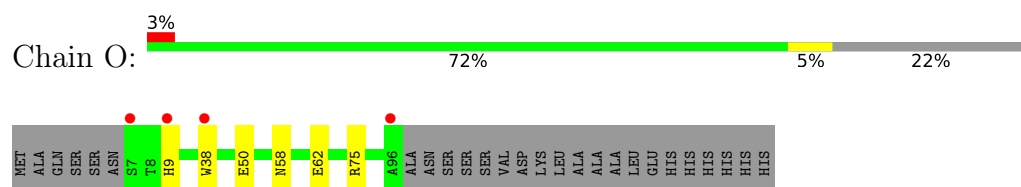
- Molecule 1: Rru_A0973



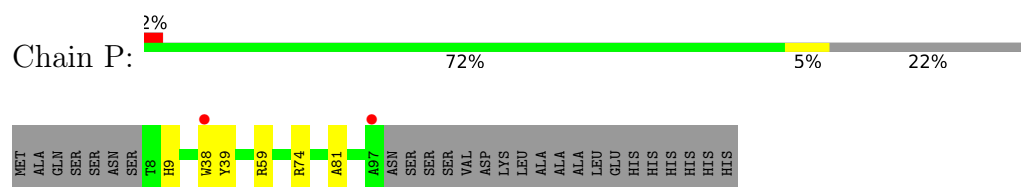
- Molecule 1: Rru_A0973



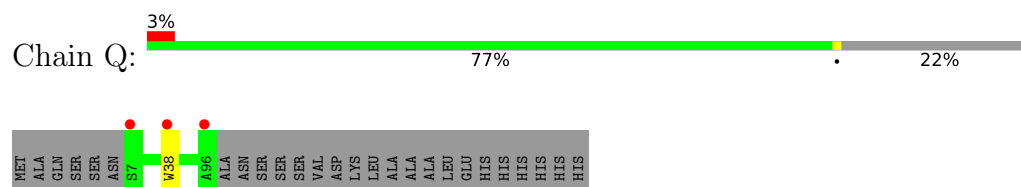
- Molecule 1: Rru_A0973



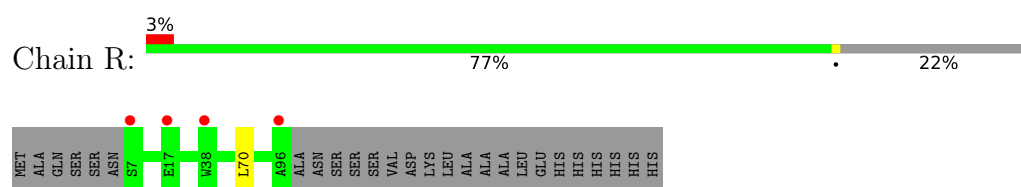
- Molecule 1: Rru_A0973



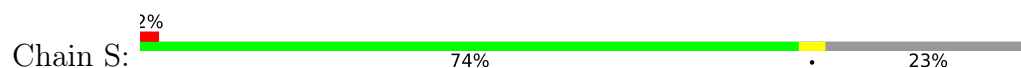
- Molecule 1: Rru_A0973

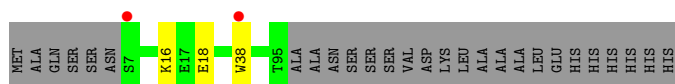


- Molecule 1: Rru_A0973

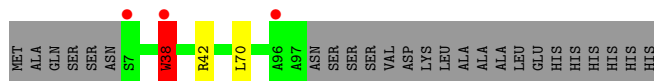
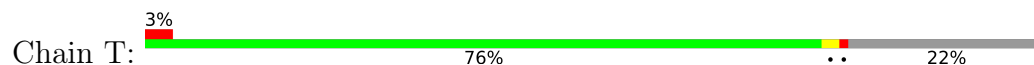


- Molecule 1: Rru_A0973

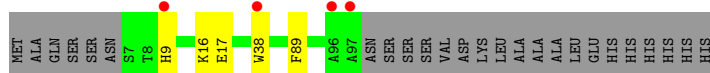




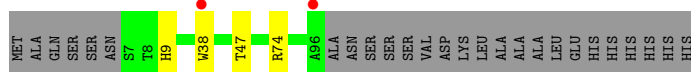
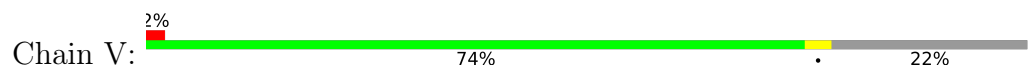
● Molecule 1: Rru_A0973



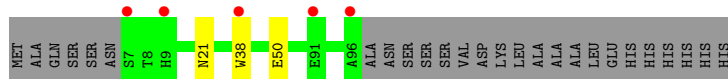
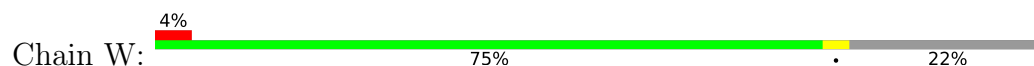
● Molecule 1: Rru_A0973



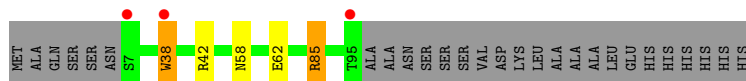
● Molecule 1: Rru_A0973



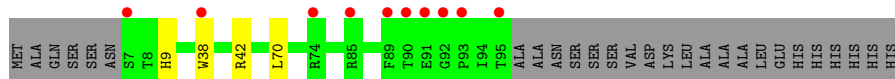
● Molecule 1: Rru_A0973



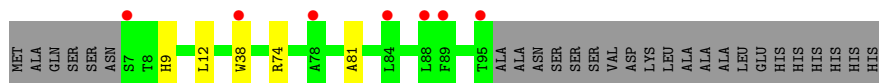
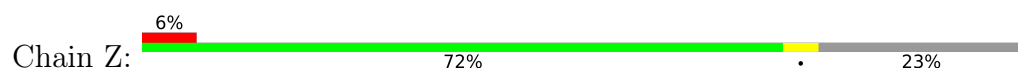
● Molecule 1: Rru_A0973



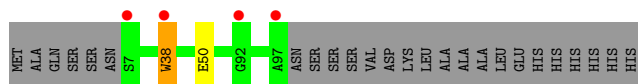
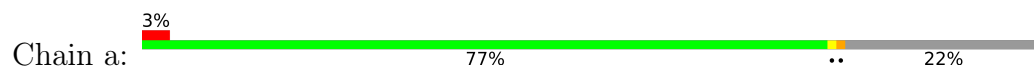
● Molecule 1: Rru_A0973



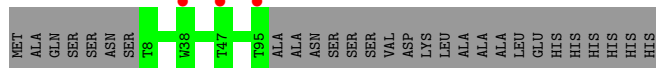
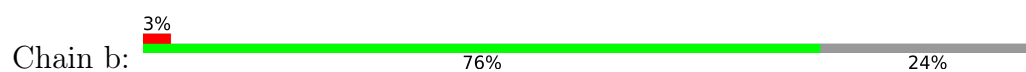
● Molecule 1: Rru_A0973



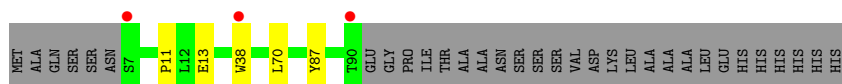
• Molecule 1: Rru_A0973



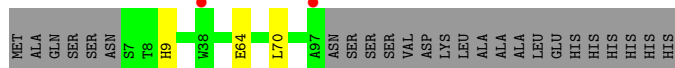
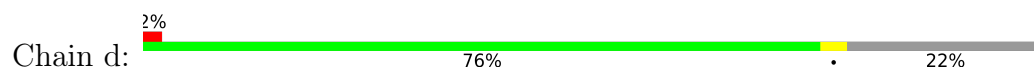
• Molecule 1: Rru_A0973



• Molecule 1: Rru_A0973



• Molecule 1: Rru_A0973



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, 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
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.171 , 0.206 0.167 , 0.203	Depositor DCC
R_{free} test set	9843 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 38.0	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	0.96	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.*

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, FE, GOA

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	0.81	0/770	0.81	0/1048
1	B	0.76	0/762	0.78	0/1037
1	C	0.83	0/757	0.87	1/1030 (0.1%)
1	D	0.80	0/762	0.85	0/1037
1	E	0.83	0/757	0.86	1/1030 (0.1%)
1	F	0.83	0/762	0.82	0/1037
1	G	0.88	0/762	0.94	1/1037 (0.1%)
1	H	0.77	0/778	0.83	0/1059
1	I	0.84	0/762	0.82	0/1037
1	J	0.78	0/778	0.83	0/1059
1	K	0.80	0/769	0.84	1/1047 (0.1%)
1	L	0.82	0/770	0.84	0/1048
1	M	0.83	0/757	0.87	2/1030 (0.2%)
1	N	0.84	0/762	0.82	0/1037
1	O	0.73	0/764	0.85	0/1040
1	P	0.73	0/764	0.79	0/1040
1	Q	0.74	0/757	0.85	0/1030
1	R	0.75	0/757	0.82	0/1030
1	S	0.80	0/752	0.85	1/1023 (0.1%)
1	T	0.75	0/762	0.83	1/1037 (0.1%)
1	U	0.76	0/762	0.79	0/1037
1	V	0.79	0/757	0.78	0/1030
1	W	0.72	0/757	0.84	1/1030 (0.1%)
1	X	0.69	0/752	0.86	1/1023 (0.1%)
1	Y	0.68	0/752	0.78	0/1023
1	Z	0.66	0/752	0.82	1/1023 (0.1%)
1	a	0.70	0/762	0.85	1/1037 (0.1%)
1	b	0.69	0/746	0.83	0/1015
1	c	0.75	0/716	0.80	0/973
1	d	0.74	0/762	0.80	0/1037
All	All	0.77	0/22782	0.83	12/31001 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	38	TRP	CA-CB-CG	8.09	128.97	113.60
1	C	38	TRP	CA-CB-CG	7.42	127.71	113.60
1	a	38	TRP	CA-CB-CG	7.14	127.16	113.60
1	X	38	TRP	CA-CB-CG	6.57	126.08	113.60
1	W	38	TRP	CA-CB-CG	6.16	125.30	113.60
1	E	38	TRP	CA-CB-CG	5.98	124.97	113.60
1	T	38	TRP	CA-CB-CG	5.86	124.73	113.60
1	K	38	TRP	CA-CB-CG	5.79	124.61	113.60
1	M	92	GLY	CA-C-N	5.39	125.70	119.93
1	M	92	GLY	C-N-CA	5.39	125.70	119.93
1	Z	12	LEU	N-CA-C	5.23	117.73	111.71
1	S	38	TRP	CA-CB-CG	5.07	123.23	113.60

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	5	0
1	B	746	709	709	5	0
1	C	741	704	704	1	0
1	D	746	709	709	1	0
1	E	741	704	704	5	0
1	F	746	709	709	3	0
1	G	746	709	709	7	0
1	H	756	731	731	4	0
1	I	746	709	709	4	0
1	J	756	731	731	3	0
1	K	750	718	718	3	0
1	L	751	721	720	1	0
1	M	741	704	704	2	0
1	N	746	709	709	5	0
1	O	745	711	713	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	745	716	715	4	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	4	0
1	Y	736	699	699	4	0
1	Z	736	699	699	4	0
1	a	746	709	709	1	0
1	b	730	694	694	0	0
1	c	701	665	665	4	0
1	d	746	709	709	3	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	0	1	0
3	B	5	3	0	0	0
3	C	5	3	0	0	0
3	D	5	3	0	0	0
3	F	5	3	0	0	0
3	G	5	3	0	0	0
3	K	5	3	0	0	0
3	L	5	3	0	0	0
3	N	5	3	0	0	0
3	P	5	3	0	0	0
3	Q	5	3	0	0	0
3	U	5	3	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	V	5	3	0	1	0
3	X	5	3	0	0	0
3	Z	5	3	0	0	0
3	a	5	3	0	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	1	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	2	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	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	21221	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	2.01	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
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:O	5:A:301:HOH:O	2.15	0.64
1:U:38:TRP:CE2	1:V:9:HIS:NE2	2.73	0.57
1:E:16:LYS:NZ	5:E:305:HOH:O	2.38	0.56
1:F:38:TRP:HE3	1:F:42:ARG:NH2	2.04	0.56
1:E:16:LYS:NZ	5:E:302:HOH:O	2.35	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
1:G:95:THR:HG22	1:H:68:MET:HE1	1.89	0.54
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:G:95:THR:HG22	1:H:68:MET:CE	2.39	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:HD21	1:B:70:LEU:HD21	1.93	0.50
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	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	1.98	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:U:9:HIS:NE2	1:V:38:TRP:CE2	2.85	0.44
1:c:38:TRP:CE2	1:d:9:HIS:NE2	2.85	0.44
1:E:9:HIS:NE2	1:F:38:TRP:CE2	2.86	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:X:85:ARG:HD3	1:X:85:ARG:C	2.43	0.43
1:c:87:TYR:CE2	1:d:64:GLU:HG3	2.54	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
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
1:U:9:HIS:HE2	1:V:38:TRP:NE1	2.19	0.40
1:G:95:THR:HA	1:H:68:MET:HE3	2.04	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	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	42	38
1	D	79/100 (79%)	78 (99%)	1 (1%)	61	62
1	E	79/100 (79%)	77 (98%)	2 (2%)	42	38
1	F	79/100 (79%)	79 (100%)	0	100	100
1	G	79/100 (79%)	77 (98%)	2 (2%)	42	38
1	H	81/100 (81%)	79 (98%)	2 (2%)	42	38
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%)	61	62
1	L	80/100 (80%)	80 (100%)	0	100	100
1	M	79/100 (79%)	79 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	79/100 (79%)	79 (100%)	0	100	100
1	O	80/100 (80%)	79 (99%)	1 (1%)	61	62
1	P	79/100 (79%)	79 (100%)	0	100	100
1	Q	79/100 (79%)	78 (99%)	1 (1%)	61	62
1	R	79/100 (79%)	78 (99%)	1 (1%)	61	62
1	S	79/100 (79%)	79 (100%)	0	100	100
1	T	79/100 (79%)	77 (98%)	2 (2%)	42	38
1	U	79/100 (79%)	77 (98%)	2 (2%)	42	38
1	V	79/100 (79%)	79 (100%)	0	100	100
1	W	79/100 (79%)	79 (100%)	0	100	100
1	X	79/100 (79%)	78 (99%)	1 (1%)	61	62
1	Y	79/100 (79%)	78 (99%)	1 (1%)	61	62
1	Z	79/100 (79%)	79 (100%)	0	100	100
1	a	79/100 (79%)	78 (99%)	1 (1%)	61	62
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%)	2353 (99%)	20 (1%)	73	77

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	13	GLU
1	C	38	TRP
1	D	70	LEU
1	E	13	GLU
1	E	73	LEU
1	G	17	GLU
1	G	38	TRP
1	H	70[A]	LEU
1	H	70[B]	LEU
1	K	38	TRP
1	O	50	GLU
1	Q	38	TRP
1	R	70	LEU
1	T	38	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	70	LEU
1	U	16	LYS
1	U	17	GLU
1	X	85	ARG
1	Y	70	LEU
1	a	38	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	H	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 oligosaccharides 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	F	202	2	4,4,4	0.71	0	4,4,4	2.61	1 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOA	C	201	-	4,4,4	0.90	0	4,4,4	2.73	1 (25%)
3	GOA	G	202	2	4,4,4	1.20	0	4,4,4	1.70	1 (25%)
3	GOA	Q	203	2	4,4,4	0.75	0	4,4,4	3.35	2 (50%)
3	GOA	a	205	2	4,4,4	1.18	0	4,4,4	2.19	1 (25%)
3	GOA	K	204	2	4,4,4	0.86	0	4,4,4	2.69	1 (25%)
3	GOA	N	202	2	4,4,4	0.82	0	4,4,4	2.32	2 (50%)
3	GOA	U	204	2	4,4,4	1.22	0	4,4,4	1.79	1 (25%)
3	GOA	P	202	2	4,4,4	1.03	0	4,4,4	1.82	2 (50%)
3	GOA	V	202	2	4,4,4	0.93	0	4,4,4	2.02	1 (25%)
3	GOA	B	204	2	4,4,4	0.78	0	4,4,4	3.33	3 (75%)
3	GOA	A	202	2	4,4,4	1.17	0	4,4,4	2.18	1 (25%)
3	GOA	D	202	2	4,4,4	1.08	0	4,4,4	2.05	1 (25%)
3	GOA	L	202	2	4,4,4	0.96	0	4,4,4	2.02	2 (50%)
3	GOA	X	202	2	4,4,4	0.79	0	4,4,4	3.03	1 (25%)
3	GOA	Z	202	2	4,4,4	0.77	0	4,4,4	3.40	3 (75%)

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	F	202	2	-	0/2/2/2	-
3	GOA	C	201	-	-	0/2/2/2	-
3	GOA	G	202	2	-	0/2/2/2	-
3	GOA	Q	203	2	-	0/2/2/2	-
3	GOA	a	205	2	-	2/2/2/2	-
3	GOA	K	204	2	-	2/2/2/2	-
3	GOA	N	202	2	-	0/2/2/2	-
3	GOA	U	204	2	-	0/2/2/2	-
3	GOA	P	202	2	-	0/2/2/2	-
3	GOA	V	202	2	-	0/2/2/2	-
3	GOA	B	204	2	-	0/2/2/2	-
3	GOA	A	202	2	-	0/2/2/2	-
3	GOA	D	202	2	-	2/2/2/2	-
3	GOA	L	202	2	-	0/2/2/2	-
3	GOA	X	202	2	-	0/2/2/2	-
3	GOA	Z	202	2	-	0/2/2/2	-

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	203	GOA	OXT-C-CA	5.92	122.66	111.90
3	B	204	GOA	OXT-C-CA	5.64	122.15	111.90
3	X	202	GOA	OXT-C-CA	5.52	121.92	111.90
3	Z	202	GOA	OXT-C-CA	5.41	121.72	111.90
3	C	201	GOA	OXT-C-CA	5.01	121.00	111.90
3	F	202	GOA	OXT-C-CA	4.81	120.64	111.90
3	K	204	GOA	OXT-C-CA	4.78	120.59	111.90
3	A	202	GOA	OXT-C-CA	4.00	119.17	111.90
3	a	205	GOA	OXT-C-CA	3.94	119.05	111.90
3	D	202	GOA	OXT-C-CA	3.82	118.85	111.90
3	N	202	GOA	OXT-C-CA	3.80	118.81	111.90
3	V	202	GOA	OXT-C-CA	3.59	118.43	111.90
3	U	204	GOA	OXT-C-CA	3.35	117.99	111.90
3	G	202	GOA	OXT-C-CA	3.10	117.53	111.90
3	Z	202	GOA	O-C-CA	-2.92	115.02	123.48
3	Q	203	GOA	O-C-CA	-2.91	115.07	123.48
3	Z	202	GOA	O2-CA-C	-2.90	105.18	112.37
3	L	202	GOA	O2-CA-C	-2.87	105.26	112.37
3	B	204	GOA	O-C-CA	-2.79	115.40	123.48
3	L	202	GOA	OXT-C-CA	2.67	116.76	111.90
3	P	202	GOA	OXT-C-CA	2.54	116.52	111.90
3	P	202	GOA	O2-CA-C	-2.45	106.30	112.37
3	B	204	GOA	O2-CA-C	-2.15	107.05	112.37
3	N	202	GOA	O2-CA-C	-2.08	107.22	112.37

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	202	GOA	OXT-C-CA-O2
3	a	205	GOA	OXT-C-CA-O2
3	D	202	GOA	O-C-CA-O2
3	K	204	GOA	O-C-CA-O2
3	K	204	GOA	OXT-C-CA-O2
3	a	205	GOA	O-C-CA-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	91/116 (78%)	-0.45	2 (2%) 62 64	18, 30, 59, 65	1 (1%)
1	B	91/116 (78%)	-0.41	3 (3%) 49 49	20, 31, 60, 73	0
1	C	90/116 (77%)	-0.53	3 (3%) 49 49	21, 28, 54, 68	0
1	D	91/116 (78%)	-0.51	2 (2%) 62 64	20, 27, 54, 64	0
1	E	90/116 (77%)	-0.51	3 (3%) 49 49	21, 27, 51, 65	0
1	F	91/116 (78%)	-0.51	3 (3%) 49 49	20, 28, 55, 72	0
1	G	91/116 (78%)	-0.52	2 (2%) 62 64	19, 30, 53, 65	0
1	H	91/116 (78%)	-0.45	4 (4%) 39 39	16, 27, 57, 71	2 (2%)
1	I	91/116 (78%)	-0.42	3 (3%) 49 49	22, 28, 57, 68	0
1	J	91/116 (78%)	-0.48	4 (4%) 39 39	13, 29, 56, 67	2 (2%)
1	K	91/116 (78%)	-0.49	4 (4%) 39 39	16, 29, 58, 70	1 (1%)
1	L	91/116 (78%)	-0.48	3 (3%) 49 49	14, 30, 53, 79	1 (1%)
1	M	90/116 (77%)	-0.51	2 (2%) 62 64	20, 27, 56, 71	0
1	N	91/116 (78%)	-0.47	3 (3%) 49 49	20, 30, 49, 61	0
1	O	90/116 (77%)	-0.24	4 (4%) 39 39	20, 33, 66, 70	1 (1%)
1	P	90/116 (77%)	-0.26	2 (2%) 62 64	16, 35, 58, 63	1 (1%)
1	Q	90/116 (77%)	-0.26	3 (3%) 49 49	25, 34, 62, 84	0
1	R	90/116 (77%)	-0.17	4 (4%) 39 39	25, 37, 66, 81	0
1	S	89/116 (76%)	-0.39	2 (2%) 62 64	24, 33, 60, 64	0
1	T	91/116 (78%)	-0.45	3 (3%) 49 49	21, 31, 56, 65	0
1	U	91/116 (78%)	-0.23	4 (4%) 39 39	23, 33, 61, 73	0
1	V	90/116 (77%)	-0.20	2 (2%) 62 64	23, 37, 63, 72	0
1	W	90/116 (77%)	-0.03	5 (5%) 30 30	26, 37, 68, 83	0
1	X	89/116 (76%)	0.20	3 (3%) 48 48	30, 42, 66, 77	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	89/116 (76%)	0.79	10 (11%) 10 10	38, 49, 73, 82	0
1	Z	89/116 (76%)	0.69	7 (7%) 18 19	34, 51, 75, 88	0
1	a	91/116 (78%)	-0.17	4 (4%) 39 39	24, 35, 69, 81	0
1	b	88/116 (75%)	-0.02	3 (3%) 48 48	29, 39, 60, 75	0
1	c	84/116 (72%)	-0.46	3 (3%) 46 47	23, 31, 54, 65	0
1	d	91/116 (78%)	-0.41	2 (2%) 62 64	21, 32, 58, 74	0
All	All	2703/3480 (77%)	-0.28	102 (3%) 44 44	13, 33, 63, 88	9 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	38	TRP	4.1
1	V	96	ALA	4.1
1	W	96	ALA	4.0
1	U	97	ALA	3.9
1	C	96	ALA	3.7
1	Q	96	ALA	3.7
1	R	38	TRP	3.6
1	A	38	TRP	3.6
1	O	38	TRP	3.5
1	X	38	TRP	3.5
1	B	97	ALA	3.5
1	Y	95	THR	3.5
1	Q	38	TRP	3.4
1	F	96	ALA	3.4
1	c	7	SER	3.4
1	a	97	ALA	3.4
1	K	96	ALA	3.3
1	F	38	TRP	3.3
1	I	38	TRP	3.3
1	R	96	ALA	3.3
1	W	38	TRP	3.2
1	O	96	ALA	3.2
1	Z	89	PHE	3.2
1	U	38	TRP	3.2
1	Y	91	GLU	3.2
1	E	96	ALA	3.2
1	R	7	SER	3.1
1	M	96	ALA	3.1
1	Z	88	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	38	TRP	3.0
1	J	38	TRP	3.0
1	b	38	TRP	3.0
1	X	7	SER	3.0
1	Y	92	GLY	3.0
1	Q	7	SER	3.0
1	Z	38	TRP	3.0
1	X	95	THR	2.9
1	F	97	ALA	2.9
1	Y	93	PRO	2.9
1	d	97	ALA	2.9
1	W	9	HIS	2.9
1	Z	7	SER	2.9
1	Y	90	THR	2.8
1	T	38	TRP	2.8
1	H	96	ALA	2.8
1	K	38	TRP	2.8
1	S	38	TRP	2.8
1	O	7	SER	2.7
1	H	7	SER	2.7
1	E	38	TRP	2.7
1	V	38	TRP	2.7
1	J	97	ALA	2.7
1	M	38	TRP	2.7
1	Y	85	ARG	2.6
1	N	38	TRP	2.6
1	H	97	ALA	2.6
1	B	96	ALA	2.6
1	K	7	SER	2.6
1	J	96	ALA	2.5
1	P	97	ALA	2.5
1	D	7	SER	2.5
1	E	7	SER	2.5
1	G	38	TRP	2.5
1	P	38	TRP	2.5
1	Y	89	PHE	2.5
1	a	92	GLY	2.5
1	Z	95	THR	2.5
1	J	7	SER	2.5
1	K	97	ALA	2.5
1	Z	78	ALA	2.5
1	a	38	TRP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	7	SER	2.4
1	Y	7	SER	2.4
1	c	90	THR	2.4
1	T	96	ALA	2.4
1	G	7	SER	2.4
1	S	7	SER	2.4
1	W	7	SER	2.4
1	I	7	SER	2.4
1	b	95	THR	2.4
1	N	91	GLU	2.4
1	H	38	TRP	2.4
1	U	96	ALA	2.3
1	U	9	HIS	2.3
1	L	97	ALA	2.3
1	A	7	SER	2.3
1	Z	84	LEU	2.3
1	c	38	TRP	2.3
1	B	9	HIS	2.2
1	W	91	GLU	2.2
1	D	38	TRP	2.2
1	d	38	TRP	2.2
1	C	7	SER	2.2
1	a	7	SER	2.2
1	L	7	SER	2.2
1	O	9	HIS	2.1
1	T	7	SER	2.1
1	R	17	GLU	2.1
1	L	38	TRP	2.1
1	I	97	ALA	2.1
1	Y	74	ARG	2.0
1	b	47	THR	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

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. 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	B-factors(Å ²)	Q<0.9
3	GOA	C	201	5/5	0.61	0.18	50,60,61,65	0
4	CA	D	203	1/1	0.80	0.15	85,85,85,85	0
4	CA	L	204	1/1	0.80	0.18	87,87,87,87	0
4	CA	a	203	1/1	0.80	0.13	88,88,88,88	0
4	CA	c	201	1/1	0.80	0.13	77,77,77,77	0
4	CA	D	206	1/1	0.82	0.13	75,75,75,75	0
4	CA	N	205	1/1	0.82	0.15	84,84,84,84	0
4	CA	V	203	1/1	0.83	0.16	81,81,81,81	0
4	CA	L	203	1/1	0.85	0.10	84,84,84,84	0
3	GOA	Q	203	5/5	0.87	0.17	32,43,52,63	0
4	CA	a	202	1/1	0.87	0.10	78,78,78,78	0
3	GOA	P	202	5/5	0.89	0.15	29,39,47,54	0
3	GOA	Z	202	5/5	0.89	0.16	43,48,52,58	0
3	GOA	a	205	5/5	0.89	0.14	27,42,48,57	0
3	GOA	G	202	5/5	0.90	0.14	30,43,49,58	0
3	GOA	K	204	5/5	0.90	0.14	31,41,51,62	0
4	CA	C	202	1/1	0.90	0.08	76,76,76,76	0
3	GOA	B	204	5/5	0.90	0.14	28,40,45,52	0
3	GOA	F	202	5/5	0.90	0.14	30,43,48,51	0
3	GOA	X	202	5/5	0.90	0.13	42,48,59,59	0
3	GOA	D	202	5/5	0.91	0.13	30,34,41,50	0
3	GOA	N	202	5/5	0.92	0.12	30,44,49,58	0
3	GOA	U	204	5/5	0.92	0.12	30,37,44,53	0
3	GOA	V	202	5/5	0.92	0.14	31,40,48,54	0
3	GOA	L	202	5/5	0.92	0.13	27,40,45,54	0
4	CA	F	203	1/1	0.95	0.11	68,68,68,68	0
3	GOA	A	202	5/5	0.95	0.11	26,38,44,53	0
4	CA	I	201	1/1	0.96	0.12	57,57,57,57	0
4	CA	X	203	1/1	0.97	0.05	54,54,54,54	0
2	FE	X	201	1/1	0.97	0.08	34,34,34,34	0
2	FE	V	201	1/1	0.98	0.06	24,24,24,24	0
4	CA	N	203	1/1	0.98	0.04	46,46,46,46	0
2	FE	X	204	1/1	0.98	0.06	35,35,35,35	0
4	CA	P	203	1/1	0.98	0.06	48,48,48,48	0
4	CA	Q	204	1/1	0.98	0.05	41,41,41,41	0
2	FE	Z	201	1/1	0.98	0.07	36,36,36,36	0
2	FE	Z	204	1/1	0.98	0.06	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	G	203	1/1	0.98	0.06	39,39,39,39	0
4	CA	A	203	1/1	0.98	0.04	42,42,42,42	0
4	CA	a	206	1/1	0.98	0.04	45,45,45,45	0
4	CA	B	202	1/1	0.98	0.06	38,38,38,38	0
4	CA	F	205	1/1	0.99	0.04	37,37,37,37	0
2	FE	F	204	1/1	0.99	0.05	21,21,21,21	0
2	FE	G	201	1/1	0.99	0.05	23,23,23,23	0
4	CA	J	201	1/1	0.99	0.04	45,45,45,45	0
4	CA	K	202	1/1	0.99	0.07	44,44,44,44	0
2	FE	a	201	1/1	0.99	0.05	23,23,23,23	0
2	FE	a	204	1/1	0.99	0.06	23,23,23,23	0
4	CA	L	205	1/1	0.99	0.04	41,41,41,41	0
2	FE	K	201	1/1	0.99	0.04	24,24,24,24	0
2	FE	N	201	1/1	0.99	0.08	26,26,26,26	0
2	FE	P	201	1/1	0.99	0.07	23,23,23,23	0
2	FE	P	204	1/1	0.99	0.06	27,27,27,27	0
4	CA	U	202	1/1	0.99	0.03	42,42,42,42	0
2	FE	U	203	1/1	0.99	0.08	18,18,18,18	0
4	CA	V	204	1/1	0.99	0.04	46,46,46,46	0
2	FE	A	201	1/1	0.99	0.07	23,23,23,23	0
4	CA	Z	203	1/1	0.99	0.04	46,46,46,46	0
2	FE	V	205	1/1	0.99	0.07	22,22,22,22	0
4	CA	D	204	1/1	0.99	0.03	40,40,40,40	0
2	FE	D	205	1/1	0.99	0.07	20,20,20,20	0
2	FE	F	201	1/1	0.99	0.08	21,21,21,21	0
2	FE	B	201	1/1	1.00	0.05	21,21,21,21	0
2	FE	N	204	1/1	1.00	0.07	26,26,26,26	0
2	FE	B	203	1/1	1.00	0.05	20,20,20,20	0
2	FE	D	201	1/1	1.00	0.05	20,20,20,20	0
2	FE	Q	201	1/1	1.00	0.07	28,28,28,28	0
2	FE	Q	202	1/1	1.00	0.08	25,25,25,25	0
2	FE	U	201	1/1	1.00	0.07	21,21,21,21	0
2	FE	G	204	1/1	1.00	0.07	20,20,20,20	0
2	FE	A	204	1/1	1.00	0.06	21,21,21,21	0
2	FE	K	203	1/1	1.00	0.05	23,23,23,23	0
2	FE	L	201	1/1	1.00	0.06	21,21,21,21	0
2	FE	L	206	1/1	1.00	0.06	23,23,23,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.