Full wwPDB X-ray Structure Validation Report ⓘ

May 3, 2016 – 01:12 AM EDT

PDB ID	:	3IA0
Title	:	Ethanolamine Utilization Microcompartment Shell Subunit, EutS-G39V mutant
Authors	:	Tanaka, S.; Sawaya, M.R.; Yeates, T.O.
Deposited on	:	2009-07-13
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

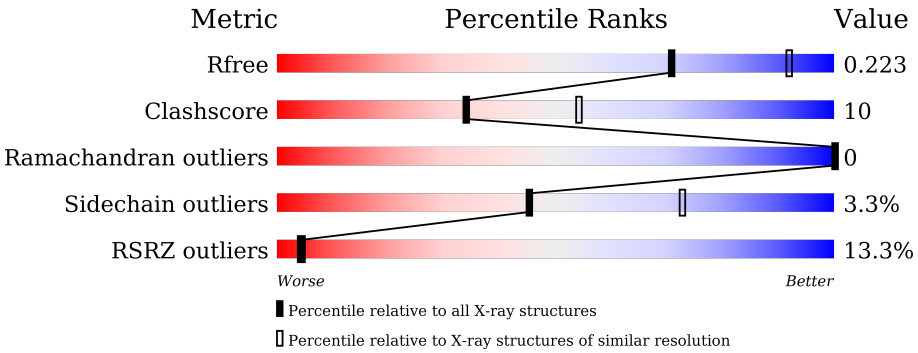
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027457
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	119	9% 67% 25% • 7%
1	B	119	14% 69% 24% • 7%
1	C	119	14% 71% 22% • 7%
1	D	119	13% 71% 22% • 7%
1	E	119	16% 67% 25% • 7%
1	F	119	17% 71% 21% • 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	119	13% 64% 29% • 7%
1	H	119	15% 71% 21% • 7%
1	I	119	9% 74% 18% • 7%
1	J	119	13% 68% 24% • 7%
1	K	119	12% 69% 24% 7%
1	L	119	7% 66% 27% • 7%
1	M	119	11% 66% 26% • 7%
1	N	119	16% 72% 20% • 7%
1	O	119	11% 70% 23% • 7%
1	P	119	11% 71% 21% • 7%
1	Q	119	13% 66% 26% • 7%
1	R	119	8% 69% 24% • 7%
1	S	119	18% 69% 24% • 7%
1	T	119	7% 71% 21% • 7%
1	U	119	11% 72% 20% • 7%
1	V	119	6% 68% 24% • 7%
1	W	119	8% 67% 25% • 7%
1	X	119	14% 71% 21% • 7%
1	Y	119	14% 70% 23% • 7%
1	Z	119	18% 71% 22% • 7%
1	a	119	15% 91% • 7%
1	b	119	13% 91% • 7%
1	c	119	10% 91% • 7%
1	d	119	13% 91% • 7%
1	e	119	11% 91% • 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	f	119	20% 91% • 7%
1	g	119	14% 91% • 7%
1	h	119	11% 91% • 7%
1	i	119	10% 92% • 7%
1	j	119	8% 92% • 7%
1	k	119	9% 91% • 7%
1	l	119	8% 91% • 7%
1	m	119	13% 92% • 7%
1	n	119	11% 91% • 7%
1	o	119	11% 91% • 7%
1	p	119	13% 91% • 7%
1	q	119	13% 91% • 7%
1	r	119	18% 92% • 7%
1	s	119	24% 91% • 7%
1	t	119	12% 91% • 7%
1	u	119	9% 91% • 7%
1	v	119	13% 92% • 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 39312 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ethanolamine utilization protein eutS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	B	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	C	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	D	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	E	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	F	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	G	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	H	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	I	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	J	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	K	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	L	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	M	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	N	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	O	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	P	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	R	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	S	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	T	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	U	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	V	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	W	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	X	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	Y	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	Z	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	a	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	b	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	c	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	d	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	e	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	f	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	g	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	h	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	i	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	j	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	k	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	l	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	m	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	n	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	o	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	p	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	q	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	r	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	s	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	t	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	u	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			
1	v	111	Total	C	N	O	S	0	0	0
			819	524	136	155	4			

There are 432 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	VAL	GLY	ENGINEERED	UNP P63746
A	112	LEU	-	EXPRESSION TAG	UNP P63746
A	113	GLU	-	EXPRESSION TAG	UNP P63746
A	114	HIS	-	EXPRESSION TAG	UNP P63746
A	115	HIS	-	EXPRESSION TAG	UNP P63746
A	116	HIS	-	EXPRESSION TAG	UNP P63746
A	117	HIS	-	EXPRESSION TAG	UNP P63746
A	118	HIS	-	EXPRESSION TAG	UNP P63746
A	119	HIS	-	EXPRESSION TAG	UNP P63746
B	39	VAL	GLY	ENGINEERED	UNP P63746
B	112	LEU	-	EXPRESSION TAG	UNP P63746
B	113	GLU	-	EXPRESSION TAG	UNP P63746
B	114	HIS	-	EXPRESSION TAG	UNP P63746
B	115	HIS	-	EXPRESSION TAG	UNP P63746
B	116	HIS	-	EXPRESSION TAG	UNP P63746
B	117	HIS	-	EXPRESSION TAG	UNP P63746
B	118	HIS	-	EXPRESSION TAG	UNP P63746

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	119	HIS	-	EXPRESSION TAG	UNP P63746
C	39	VAL	GLY	ENGINEERED	UNP P63746
C	112	LEU	-	EXPRESSION TAG	UNP P63746
C	113	GLU	-	EXPRESSION TAG	UNP P63746
C	114	HIS	-	EXPRESSION TAG	UNP P63746
C	115	HIS	-	EXPRESSION TAG	UNP P63746
C	116	HIS	-	EXPRESSION TAG	UNP P63746
C	117	HIS	-	EXPRESSION TAG	UNP P63746
C	118	HIS	-	EXPRESSION TAG	UNP P63746
C	119	HIS	-	EXPRESSION TAG	UNP P63746
D	39	VAL	GLY	ENGINEERED	UNP P63746
D	112	LEU	-	EXPRESSION TAG	UNP P63746
D	113	GLU	-	EXPRESSION TAG	UNP P63746
D	114	HIS	-	EXPRESSION TAG	UNP P63746
D	115	HIS	-	EXPRESSION TAG	UNP P63746
D	116	HIS	-	EXPRESSION TAG	UNP P63746
D	117	HIS	-	EXPRESSION TAG	UNP P63746
D	118	HIS	-	EXPRESSION TAG	UNP P63746
D	119	HIS	-	EXPRESSION TAG	UNP P63746
E	39	VAL	GLY	ENGINEERED	UNP P63746
E	112	LEU	-	EXPRESSION TAG	UNP P63746
E	113	GLU	-	EXPRESSION TAG	UNP P63746
E	114	HIS	-	EXPRESSION TAG	UNP P63746
E	115	HIS	-	EXPRESSION TAG	UNP P63746
E	116	HIS	-	EXPRESSION TAG	UNP P63746
E	117	HIS	-	EXPRESSION TAG	UNP P63746
E	118	HIS	-	EXPRESSION TAG	UNP P63746
E	119	HIS	-	EXPRESSION TAG	UNP P63746
F	39	VAL	GLY	ENGINEERED	UNP P63746
F	112	LEU	-	EXPRESSION TAG	UNP P63746
F	113	GLU	-	EXPRESSION TAG	UNP P63746
F	114	HIS	-	EXPRESSION TAG	UNP P63746
F	115	HIS	-	EXPRESSION TAG	UNP P63746
F	116	HIS	-	EXPRESSION TAG	UNP P63746
F	117	HIS	-	EXPRESSION TAG	UNP P63746
F	118	HIS	-	EXPRESSION TAG	UNP P63746
F	119	HIS	-	EXPRESSION TAG	UNP P63746
G	39	VAL	GLY	ENGINEERED	UNP P63746
G	112	LEU	-	EXPRESSION TAG	UNP P63746
G	113	GLU	-	EXPRESSION TAG	UNP P63746
G	114	HIS	-	EXPRESSION TAG	UNP P63746
G	115	HIS	-	EXPRESSION TAG	UNP P63746

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	116	HIS	-	EXPRESSION TAG	UNP P63746
G	117	HIS	-	EXPRESSION TAG	UNP P63746
G	118	HIS	-	EXPRESSION TAG	UNP P63746
G	119	HIS	-	EXPRESSION TAG	UNP P63746
H	39	VAL	GLY	ENGINEERED	UNP P63746
H	112	LEU	-	EXPRESSION TAG	UNP P63746
H	113	GLU	-	EXPRESSION TAG	UNP P63746
H	114	HIS	-	EXPRESSION TAG	UNP P63746
H	115	HIS	-	EXPRESSION TAG	UNP P63746
H	116	HIS	-	EXPRESSION TAG	UNP P63746
H	117	HIS	-	EXPRESSION TAG	UNP P63746
H	118	HIS	-	EXPRESSION TAG	UNP P63746
H	119	HIS	-	EXPRESSION TAG	UNP P63746
I	39	VAL	GLY	ENGINEERED	UNP P63746
I	112	LEU	-	EXPRESSION TAG	UNP P63746
I	113	GLU	-	EXPRESSION TAG	UNP P63746
I	114	HIS	-	EXPRESSION TAG	UNP P63746
I	115	HIS	-	EXPRESSION TAG	UNP P63746
I	116	HIS	-	EXPRESSION TAG	UNP P63746
I	117	HIS	-	EXPRESSION TAG	UNP P63746
I	118	HIS	-	EXPRESSION TAG	UNP P63746
I	119	HIS	-	EXPRESSION TAG	UNP P63746
J	39	VAL	GLY	ENGINEERED	UNP P63746
J	112	LEU	-	EXPRESSION TAG	UNP P63746
J	113	GLU	-	EXPRESSION TAG	UNP P63746
J	114	HIS	-	EXPRESSION TAG	UNP P63746
J	115	HIS	-	EXPRESSION TAG	UNP P63746
J	116	HIS	-	EXPRESSION TAG	UNP P63746
J	117	HIS	-	EXPRESSION TAG	UNP P63746
J	118	HIS	-	EXPRESSION TAG	UNP P63746
J	119	HIS	-	EXPRESSION TAG	UNP P63746
K	39	VAL	GLY	ENGINEERED	UNP P63746
K	112	LEU	-	EXPRESSION TAG	UNP P63746
K	113	GLU	-	EXPRESSION TAG	UNP P63746
K	114	HIS	-	EXPRESSION TAG	UNP P63746
K	115	HIS	-	EXPRESSION TAG	UNP P63746
K	116	HIS	-	EXPRESSION TAG	UNP P63746
K	117	HIS	-	EXPRESSION TAG	UNP P63746
K	118	HIS	-	EXPRESSION TAG	UNP P63746
K	119	HIS	-	EXPRESSION TAG	UNP P63746
L	39	VAL	GLY	ENGINEERED	UNP P63746
L	112	LEU	-	EXPRESSION TAG	UNP P63746

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	113	GLU	-	EXPRESSION TAG	UNP P63746
L	114	HIS	-	EXPRESSION TAG	UNP P63746
L	115	HIS	-	EXPRESSION TAG	UNP P63746
L	116	HIS	-	EXPRESSION TAG	UNP P63746
L	117	HIS	-	EXPRESSION TAG	UNP P63746
L	118	HIS	-	EXPRESSION TAG	UNP P63746
L	119	HIS	-	EXPRESSION TAG	UNP P63746
M	39	VAL	GLY	ENGINEERED	UNP P63746
M	112	LEU	-	EXPRESSION TAG	UNP P63746
M	113	GLU	-	EXPRESSION TAG	UNP P63746
M	114	HIS	-	EXPRESSION TAG	UNP P63746
M	115	HIS	-	EXPRESSION TAG	UNP P63746
M	116	HIS	-	EXPRESSION TAG	UNP P63746
M	117	HIS	-	EXPRESSION TAG	UNP P63746
M	118	HIS	-	EXPRESSION TAG	UNP P63746
M	119	HIS	-	EXPRESSION TAG	UNP P63746
N	39	VAL	GLY	ENGINEERED	UNP P63746
N	112	LEU	-	EXPRESSION TAG	UNP P63746
N	113	GLU	-	EXPRESSION TAG	UNP P63746
N	114	HIS	-	EXPRESSION TAG	UNP P63746
N	115	HIS	-	EXPRESSION TAG	UNP P63746
N	116	HIS	-	EXPRESSION TAG	UNP P63746
N	117	HIS	-	EXPRESSION TAG	UNP P63746
N	118	HIS	-	EXPRESSION TAG	UNP P63746
N	119	HIS	-	EXPRESSION TAG	UNP P63746
O	39	VAL	GLY	ENGINEERED	UNP P63746
O	112	LEU	-	EXPRESSION TAG	UNP P63746
O	113	GLU	-	EXPRESSION TAG	UNP P63746
O	114	HIS	-	EXPRESSION TAG	UNP P63746
O	115	HIS	-	EXPRESSION TAG	UNP P63746
O	116	HIS	-	EXPRESSION TAG	UNP P63746
O	117	HIS	-	EXPRESSION TAG	UNP P63746
O	118	HIS	-	EXPRESSION TAG	UNP P63746
O	119	HIS	-	EXPRESSION TAG	UNP P63746
P	39	VAL	GLY	ENGINEERED	UNP P63746
P	112	LEU	-	EXPRESSION TAG	UNP P63746
P	113	GLU	-	EXPRESSION TAG	UNP P63746
P	114	HIS	-	EXPRESSION TAG	UNP P63746
P	115	HIS	-	EXPRESSION TAG	UNP P63746
P	116	HIS	-	EXPRESSION TAG	UNP P63746
P	117	HIS	-	EXPRESSION TAG	UNP P63746
P	118	HIS	-	EXPRESSION TAG	UNP P63746

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
P	119	HIS	-	EXPRESSION TAG	UNP P63746
Q	39	VAL	GLY	ENGINEERED	UNP P63746
Q	112	LEU	-	EXPRESSION TAG	UNP P63746
Q	113	GLU	-	EXPRESSION TAG	UNP P63746
Q	114	HIS	-	EXPRESSION TAG	UNP P63746
Q	115	HIS	-	EXPRESSION TAG	UNP P63746
Q	116	HIS	-	EXPRESSION TAG	UNP P63746
Q	117	HIS	-	EXPRESSION TAG	UNP P63746
Q	118	HIS	-	EXPRESSION TAG	UNP P63746
Q	119	HIS	-	EXPRESSION TAG	UNP P63746
R	39	VAL	GLY	ENGINEERED	UNP P63746
R	112	LEU	-	EXPRESSION TAG	UNP P63746
R	113	GLU	-	EXPRESSION TAG	UNP P63746
R	114	HIS	-	EXPRESSION TAG	UNP P63746
R	115	HIS	-	EXPRESSION TAG	UNP P63746
R	116	HIS	-	EXPRESSION TAG	UNP P63746
R	117	HIS	-	EXPRESSION TAG	UNP P63746
R	118	HIS	-	EXPRESSION TAG	UNP P63746
R	119	HIS	-	EXPRESSION TAG	UNP P63746
S	39	VAL	GLY	ENGINEERED	UNP P63746
S	112	LEU	-	EXPRESSION TAG	UNP P63746
S	113	GLU	-	EXPRESSION TAG	UNP P63746
S	114	HIS	-	EXPRESSION TAG	UNP P63746
S	115	HIS	-	EXPRESSION TAG	UNP P63746
S	116	HIS	-	EXPRESSION TAG	UNP P63746
S	117	HIS	-	EXPRESSION TAG	UNP P63746
S	118	HIS	-	EXPRESSION TAG	UNP P63746
S	119	HIS	-	EXPRESSION TAG	UNP P63746
T	39	VAL	GLY	ENGINEERED	UNP P63746
T	112	LEU	-	EXPRESSION TAG	UNP P63746
T	113	GLU	-	EXPRESSION TAG	UNP P63746
T	114	HIS	-	EXPRESSION TAG	UNP P63746
T	115	HIS	-	EXPRESSION TAG	UNP P63746
T	116	HIS	-	EXPRESSION TAG	UNP P63746
T	117	HIS	-	EXPRESSION TAG	UNP P63746
T	118	HIS	-	EXPRESSION TAG	UNP P63746
T	119	HIS	-	EXPRESSION TAG	UNP P63746
U	39	VAL	GLY	ENGINEERED	UNP P63746
U	112	LEU	-	EXPRESSION TAG	UNP P63746
U	113	GLU	-	EXPRESSION TAG	UNP P63746
U	114	HIS	-	EXPRESSION TAG	UNP P63746
U	115	HIS	-	EXPRESSION TAG	UNP P63746

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
U	116	HIS	-	EXPRESSION TAG	UNP P63746
U	117	HIS	-	EXPRESSION TAG	UNP P63746
U	118	HIS	-	EXPRESSION TAG	UNP P63746
U	119	HIS	-	EXPRESSION TAG	UNP P63746
V	39	VAL	GLY	ENGINEERED	UNP P63746
V	112	LEU	-	EXPRESSION TAG	UNP P63746
V	113	GLU	-	EXPRESSION TAG	UNP P63746
V	114	HIS	-	EXPRESSION TAG	UNP P63746
V	115	HIS	-	EXPRESSION TAG	UNP P63746
V	116	HIS	-	EXPRESSION TAG	UNP P63746
V	117	HIS	-	EXPRESSION TAG	UNP P63746
V	118	HIS	-	EXPRESSION TAG	UNP P63746
V	119	HIS	-	EXPRESSION TAG	UNP P63746
W	39	VAL	GLY	ENGINEERED	UNP P63746
W	112	LEU	-	EXPRESSION TAG	UNP P63746
W	113	GLU	-	EXPRESSION TAG	UNP P63746
W	114	HIS	-	EXPRESSION TAG	UNP P63746
W	115	HIS	-	EXPRESSION TAG	UNP P63746
W	116	HIS	-	EXPRESSION TAG	UNP P63746
W	117	HIS	-	EXPRESSION TAG	UNP P63746
W	118	HIS	-	EXPRESSION TAG	UNP P63746
W	119	HIS	-	EXPRESSION TAG	UNP P63746
X	39	VAL	GLY	ENGINEERED	UNP P63746
X	112	LEU	-	EXPRESSION TAG	UNP P63746
X	113	GLU	-	EXPRESSION TAG	UNP P63746
X	114	HIS	-	EXPRESSION TAG	UNP P63746
X	115	HIS	-	EXPRESSION TAG	UNP P63746
X	116	HIS	-	EXPRESSION TAG	UNP P63746
X	117	HIS	-	EXPRESSION TAG	UNP P63746
X	118	HIS	-	EXPRESSION TAG	UNP P63746
X	119	HIS	-	EXPRESSION TAG	UNP P63746
Y	39	VAL	GLY	ENGINEERED	UNP P63746
Y	112	LEU	-	EXPRESSION TAG	UNP P63746
Y	113	GLU	-	EXPRESSION TAG	UNP P63746
Y	114	HIS	-	EXPRESSION TAG	UNP P63746
Y	115	HIS	-	EXPRESSION TAG	UNP P63746
Y	116	HIS	-	EXPRESSION TAG	UNP P63746
Y	117	HIS	-	EXPRESSION TAG	UNP P63746
Y	118	HIS	-	EXPRESSION TAG	UNP P63746
Y	119	HIS	-	EXPRESSION TAG	UNP P63746
Z	39	VAL	GLY	ENGINEERED	UNP P63746
Z	112	LEU	-	EXPRESSION TAG	UNP P63746

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Z	113	GLU	-	EXPRESSION TAG	UNP P63746
Z	114	HIS	-	EXPRESSION TAG	UNP P63746
Z	115	HIS	-	EXPRESSION TAG	UNP P63746
Z	116	HIS	-	EXPRESSION TAG	UNP P63746
Z	117	HIS	-	EXPRESSION TAG	UNP P63746
Z	118	HIS	-	EXPRESSION TAG	UNP P63746
Z	119	HIS	-	EXPRESSION TAG	UNP P63746
a	39	VAL	GLY	ENGINEERED	UNP P63746
a	112	LEU	-	EXPRESSION TAG	UNP P63746
a	113	GLU	-	EXPRESSION TAG	UNP P63746
a	114	HIS	-	EXPRESSION TAG	UNP P63746
a	115	HIS	-	EXPRESSION TAG	UNP P63746
a	116	HIS	-	EXPRESSION TAG	UNP P63746
a	117	HIS	-	EXPRESSION TAG	UNP P63746
a	118	HIS	-	EXPRESSION TAG	UNP P63746
a	119	HIS	-	EXPRESSION TAG	UNP P63746
b	39	VAL	GLY	ENGINEERED	UNP P63746
b	112	LEU	-	EXPRESSION TAG	UNP P63746
b	113	GLU	-	EXPRESSION TAG	UNP P63746
b	114	HIS	-	EXPRESSION TAG	UNP P63746
b	115	HIS	-	EXPRESSION TAG	UNP P63746
b	116	HIS	-	EXPRESSION TAG	UNP P63746
b	117	HIS	-	EXPRESSION TAG	UNP P63746
b	118	HIS	-	EXPRESSION TAG	UNP P63746
b	119	HIS	-	EXPRESSION TAG	UNP P63746
c	39	VAL	GLY	ENGINEERED	UNP P63746
c	112	LEU	-	EXPRESSION TAG	UNP P63746
c	113	GLU	-	EXPRESSION TAG	UNP P63746
c	114	HIS	-	EXPRESSION TAG	UNP P63746
c	115	HIS	-	EXPRESSION TAG	UNP P63746
c	116	HIS	-	EXPRESSION TAG	UNP P63746
c	117	HIS	-	EXPRESSION TAG	UNP P63746
c	118	HIS	-	EXPRESSION TAG	UNP P63746
c	119	HIS	-	EXPRESSION TAG	UNP P63746
d	39	VAL	GLY	ENGINEERED	UNP P63746
d	112	LEU	-	EXPRESSION TAG	UNP P63746
d	113	GLU	-	EXPRESSION TAG	UNP P63746
d	114	HIS	-	EXPRESSION TAG	UNP P63746
d	115	HIS	-	EXPRESSION TAG	UNP P63746
d	116	HIS	-	EXPRESSION TAG	UNP P63746
d	117	HIS	-	EXPRESSION TAG	UNP P63746
d	118	HIS	-	EXPRESSION TAG	UNP P63746

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
d	119	HIS	-	EXPRESSION TAG	UNP P63746
e	39	VAL	GLY	ENGINEERED	UNP P63746
e	112	LEU	-	EXPRESSION TAG	UNP P63746
e	113	GLU	-	EXPRESSION TAG	UNP P63746
e	114	HIS	-	EXPRESSION TAG	UNP P63746
e	115	HIS	-	EXPRESSION TAG	UNP P63746
e	116	HIS	-	EXPRESSION TAG	UNP P63746
e	117	HIS	-	EXPRESSION TAG	UNP P63746
e	118	HIS	-	EXPRESSION TAG	UNP P63746
e	119	HIS	-	EXPRESSION TAG	UNP P63746
f	39	VAL	GLY	ENGINEERED	UNP P63746
f	112	LEU	-	EXPRESSION TAG	UNP P63746
f	113	GLU	-	EXPRESSION TAG	UNP P63746
f	114	HIS	-	EXPRESSION TAG	UNP P63746
f	115	HIS	-	EXPRESSION TAG	UNP P63746
f	116	HIS	-	EXPRESSION TAG	UNP P63746
f	117	HIS	-	EXPRESSION TAG	UNP P63746
f	118	HIS	-	EXPRESSION TAG	UNP P63746
f	119	HIS	-	EXPRESSION TAG	UNP P63746
g	39	VAL	GLY	ENGINEERED	UNP P63746
g	112	LEU	-	EXPRESSION TAG	UNP P63746
g	113	GLU	-	EXPRESSION TAG	UNP P63746
g	114	HIS	-	EXPRESSION TAG	UNP P63746
g	115	HIS	-	EXPRESSION TAG	UNP P63746
g	116	HIS	-	EXPRESSION TAG	UNP P63746
g	117	HIS	-	EXPRESSION TAG	UNP P63746
g	118	HIS	-	EXPRESSION TAG	UNP P63746
g	119	HIS	-	EXPRESSION TAG	UNP P63746
h	39	VAL	GLY	ENGINEERED	UNP P63746
h	112	LEU	-	EXPRESSION TAG	UNP P63746
h	113	GLU	-	EXPRESSION TAG	UNP P63746
h	114	HIS	-	EXPRESSION TAG	UNP P63746
h	115	HIS	-	EXPRESSION TAG	UNP P63746
h	116	HIS	-	EXPRESSION TAG	UNP P63746
h	117	HIS	-	EXPRESSION TAG	UNP P63746
h	118	HIS	-	EXPRESSION TAG	UNP P63746
h	119	HIS	-	EXPRESSION TAG	UNP P63746
i	39	VAL	GLY	ENGINEERED	UNP P63746
i	112	LEU	-	EXPRESSION TAG	UNP P63746
i	113	GLU	-	EXPRESSION TAG	UNP P63746
i	114	HIS	-	EXPRESSION TAG	UNP P63746
i	115	HIS	-	EXPRESSION TAG	UNP P63746

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
i	116	HIS	-	EXPRESSION TAG	UNP P63746
i	117	HIS	-	EXPRESSION TAG	UNP P63746
i	118	HIS	-	EXPRESSION TAG	UNP P63746
i	119	HIS	-	EXPRESSION TAG	UNP P63746
j	39	VAL	GLY	ENGINEERED	UNP P63746
j	112	LEU	-	EXPRESSION TAG	UNP P63746
j	113	GLU	-	EXPRESSION TAG	UNP P63746
j	114	HIS	-	EXPRESSION TAG	UNP P63746
j	115	HIS	-	EXPRESSION TAG	UNP P63746
j	116	HIS	-	EXPRESSION TAG	UNP P63746
j	117	HIS	-	EXPRESSION TAG	UNP P63746
j	118	HIS	-	EXPRESSION TAG	UNP P63746
j	119	HIS	-	EXPRESSION TAG	UNP P63746
k	39	VAL	GLY	ENGINEERED	UNP P63746
k	112	LEU	-	EXPRESSION TAG	UNP P63746
k	113	GLU	-	EXPRESSION TAG	UNP P63746
k	114	HIS	-	EXPRESSION TAG	UNP P63746
k	115	HIS	-	EXPRESSION TAG	UNP P63746
k	116	HIS	-	EXPRESSION TAG	UNP P63746
k	117	HIS	-	EXPRESSION TAG	UNP P63746
k	118	HIS	-	EXPRESSION TAG	UNP P63746
k	119	HIS	-	EXPRESSION TAG	UNP P63746
l	39	VAL	GLY	ENGINEERED	UNP P63746
l	112	LEU	-	EXPRESSION TAG	UNP P63746
l	113	GLU	-	EXPRESSION TAG	UNP P63746
l	114	HIS	-	EXPRESSION TAG	UNP P63746
l	115	HIS	-	EXPRESSION TAG	UNP P63746
l	116	HIS	-	EXPRESSION TAG	UNP P63746
l	117	HIS	-	EXPRESSION TAG	UNP P63746
l	118	HIS	-	EXPRESSION TAG	UNP P63746
l	119	HIS	-	EXPRESSION TAG	UNP P63746
m	39	VAL	GLY	ENGINEERED	UNP P63746
m	112	LEU	-	EXPRESSION TAG	UNP P63746
m	113	GLU	-	EXPRESSION TAG	UNP P63746
m	114	HIS	-	EXPRESSION TAG	UNP P63746
m	115	HIS	-	EXPRESSION TAG	UNP P63746
m	116	HIS	-	EXPRESSION TAG	UNP P63746
m	117	HIS	-	EXPRESSION TAG	UNP P63746
m	118	HIS	-	EXPRESSION TAG	UNP P63746
m	119	HIS	-	EXPRESSION TAG	UNP P63746
n	39	VAL	GLY	ENGINEERED	UNP P63746
n	112	LEU	-	EXPRESSION TAG	UNP P63746

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
n	113	GLU	-	EXPRESSION TAG	UNP P63746
n	114	HIS	-	EXPRESSION TAG	UNP P63746
n	115	HIS	-	EXPRESSION TAG	UNP P63746
n	116	HIS	-	EXPRESSION TAG	UNP P63746
n	117	HIS	-	EXPRESSION TAG	UNP P63746
n	118	HIS	-	EXPRESSION TAG	UNP P63746
n	119	HIS	-	EXPRESSION TAG	UNP P63746
o	39	VAL	GLY	ENGINEERED	UNP P63746
o	112	LEU	-	EXPRESSION TAG	UNP P63746
o	113	GLU	-	EXPRESSION TAG	UNP P63746
o	114	HIS	-	EXPRESSION TAG	UNP P63746
o	115	HIS	-	EXPRESSION TAG	UNP P63746
o	116	HIS	-	EXPRESSION TAG	UNP P63746
o	117	HIS	-	EXPRESSION TAG	UNP P63746
o	118	HIS	-	EXPRESSION TAG	UNP P63746
o	119	HIS	-	EXPRESSION TAG	UNP P63746
p	39	VAL	GLY	ENGINEERED	UNP P63746
p	112	LEU	-	EXPRESSION TAG	UNP P63746
p	113	GLU	-	EXPRESSION TAG	UNP P63746
p	114	HIS	-	EXPRESSION TAG	UNP P63746
p	115	HIS	-	EXPRESSION TAG	UNP P63746
p	116	HIS	-	EXPRESSION TAG	UNP P63746
p	117	HIS	-	EXPRESSION TAG	UNP P63746
p	118	HIS	-	EXPRESSION TAG	UNP P63746
p	119	HIS	-	EXPRESSION TAG	UNP P63746
q	39	VAL	GLY	ENGINEERED	UNP P63746
q	112	LEU	-	EXPRESSION TAG	UNP P63746
q	113	GLU	-	EXPRESSION TAG	UNP P63746
q	114	HIS	-	EXPRESSION TAG	UNP P63746
q	115	HIS	-	EXPRESSION TAG	UNP P63746
q	116	HIS	-	EXPRESSION TAG	UNP P63746
q	117	HIS	-	EXPRESSION TAG	UNP P63746
q	118	HIS	-	EXPRESSION TAG	UNP P63746
q	119	HIS	-	EXPRESSION TAG	UNP P63746
r	39	VAL	GLY	ENGINEERED	UNP P63746
r	112	LEU	-	EXPRESSION TAG	UNP P63746
r	113	GLU	-	EXPRESSION TAG	UNP P63746
r	114	HIS	-	EXPRESSION TAG	UNP P63746
r	115	HIS	-	EXPRESSION TAG	UNP P63746
r	116	HIS	-	EXPRESSION TAG	UNP P63746
r	117	HIS	-	EXPRESSION TAG	UNP P63746
r	118	HIS	-	EXPRESSION TAG	UNP P63746

Continued on next page...

Continued from previous page...

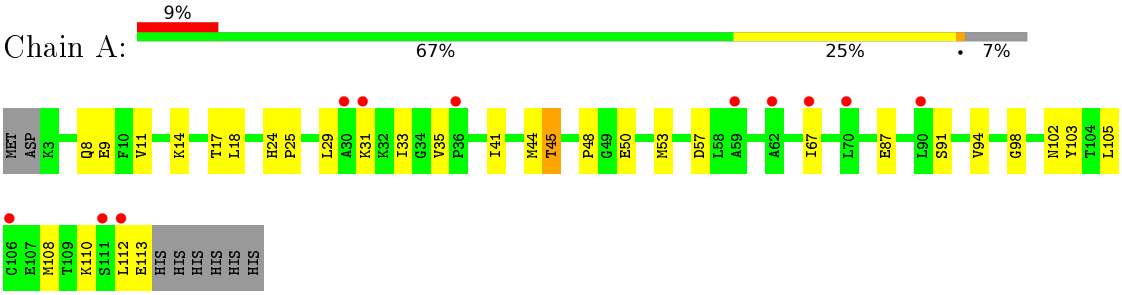
Chain	Residue	Modelled	Actual	Comment	Reference
r	119	HIS	-	EXPRESSION TAG	UNP P63746
s	39	VAL	GLY	ENGINEERED	UNP P63746
s	112	LEU	-	EXPRESSION TAG	UNP P63746
s	113	GLU	-	EXPRESSION TAG	UNP P63746
s	114	HIS	-	EXPRESSION TAG	UNP P63746
s	115	HIS	-	EXPRESSION TAG	UNP P63746
s	116	HIS	-	EXPRESSION TAG	UNP P63746
s	117	HIS	-	EXPRESSION TAG	UNP P63746
s	118	HIS	-	EXPRESSION TAG	UNP P63746
s	119	HIS	-	EXPRESSION TAG	UNP P63746
t	39	VAL	GLY	ENGINEERED	UNP P63746
t	112	LEU	-	EXPRESSION TAG	UNP P63746
t	113	GLU	-	EXPRESSION TAG	UNP P63746
t	114	HIS	-	EXPRESSION TAG	UNP P63746
t	115	HIS	-	EXPRESSION TAG	UNP P63746
t	116	HIS	-	EXPRESSION TAG	UNP P63746
t	117	HIS	-	EXPRESSION TAG	UNP P63746
t	118	HIS	-	EXPRESSION TAG	UNP P63746
t	119	HIS	-	EXPRESSION TAG	UNP P63746
u	39	VAL	GLY	ENGINEERED	UNP P63746
u	112	LEU	-	EXPRESSION TAG	UNP P63746
u	113	GLU	-	EXPRESSION TAG	UNP P63746
u	114	HIS	-	EXPRESSION TAG	UNP P63746
u	115	HIS	-	EXPRESSION TAG	UNP P63746
u	116	HIS	-	EXPRESSION TAG	UNP P63746
u	117	HIS	-	EXPRESSION TAG	UNP P63746
u	118	HIS	-	EXPRESSION TAG	UNP P63746
u	119	HIS	-	EXPRESSION TAG	UNP P63746
v	39	VAL	GLY	ENGINEERED	UNP P63746
v	112	LEU	-	EXPRESSION TAG	UNP P63746
v	113	GLU	-	EXPRESSION TAG	UNP P63746
v	114	HIS	-	EXPRESSION TAG	UNP P63746
v	115	HIS	-	EXPRESSION TAG	UNP P63746
v	116	HIS	-	EXPRESSION TAG	UNP P63746
v	117	HIS	-	EXPRESSION TAG	UNP P63746
v	118	HIS	-	EXPRESSION TAG	UNP P63746
v	119	HIS	-	EXPRESSION TAG	UNP P63746

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.

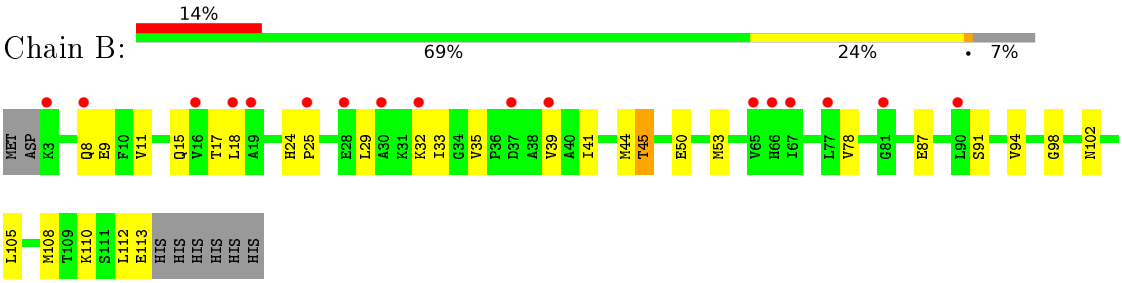
- Molecule 1: Ethanolamine utilization protein eutS

Chain A:



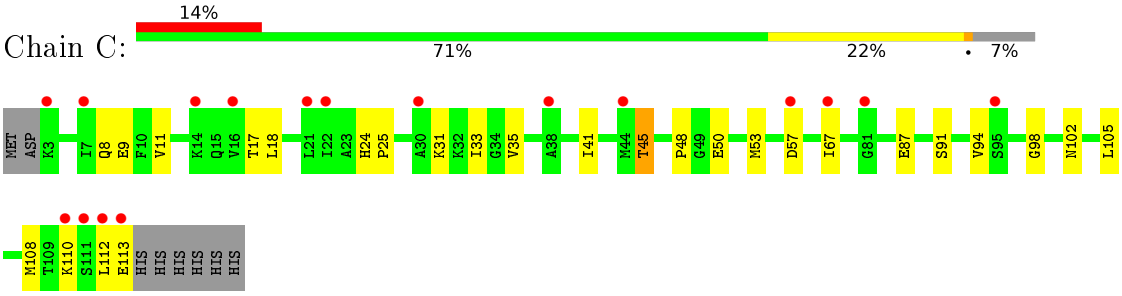
- Molecule 1: Ethanolamine utilization protein eutS

Chain B:



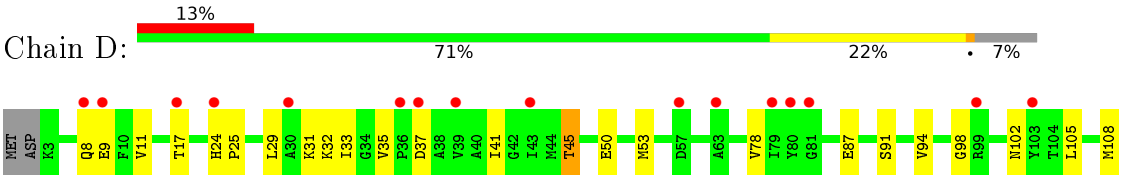
- Molecule 1: Ethanolamine utilization protein eutS

Chain C:



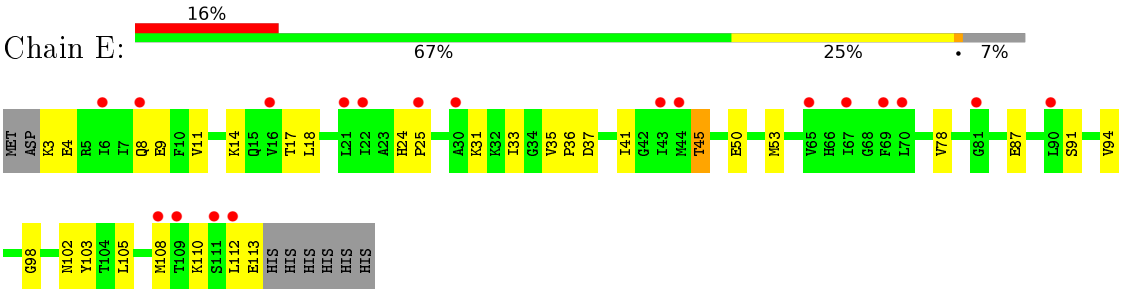
- Molecule 1: Ethanolamine utilization protein eutS

Chain D:



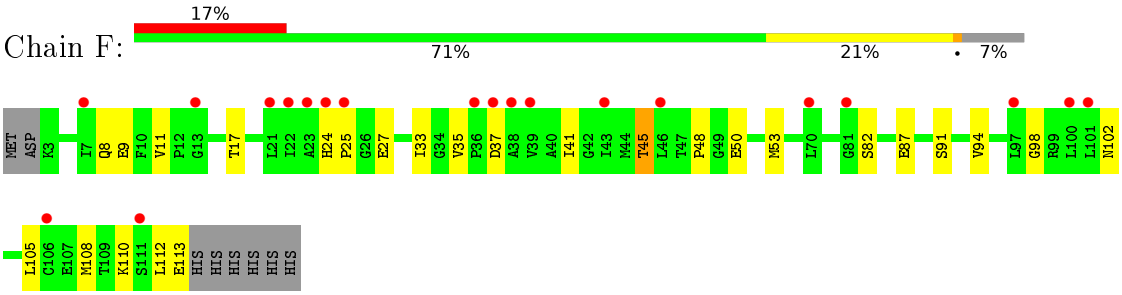
• Molecule 1: Ethanolamine utilization protein eutS

Chain E:



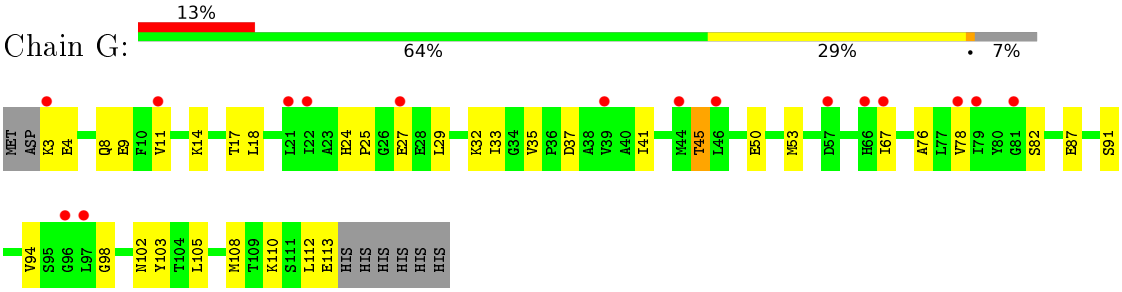
• Molecule 1: Ethanolamine utilization protein eutS

Chain F:



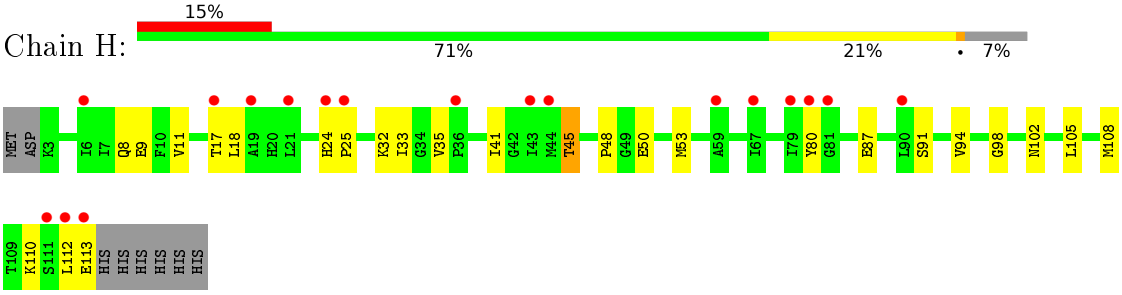
• Molecule 1: Ethanolamine utilization protein eutS

Chain G:



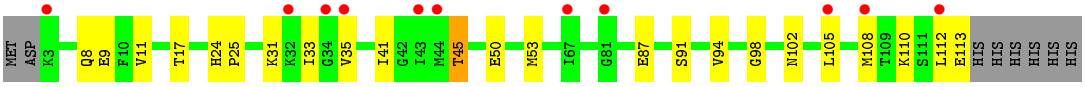
• Molecule 1: Ethanolamine utilization protein eutS

Chain H:

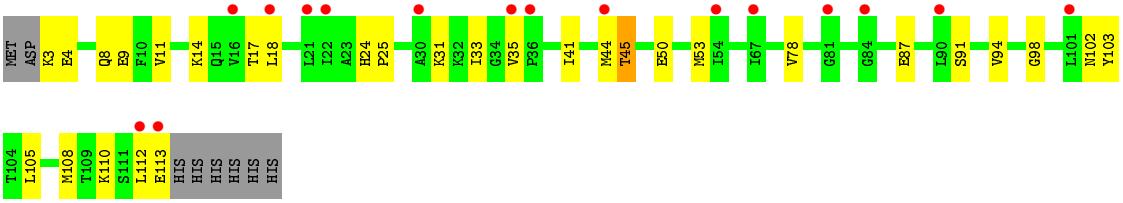


• Molecule 1: Ethanolamine utilization protein eutS

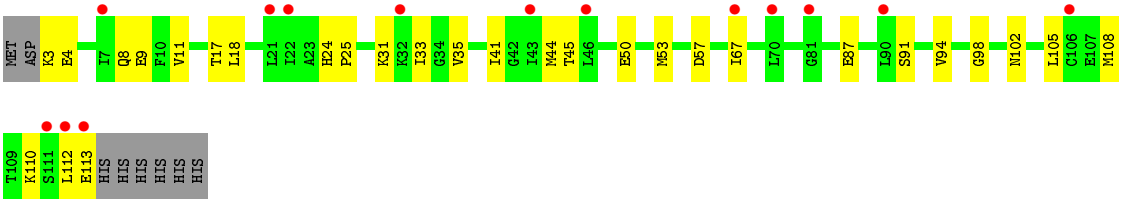
Chain I:



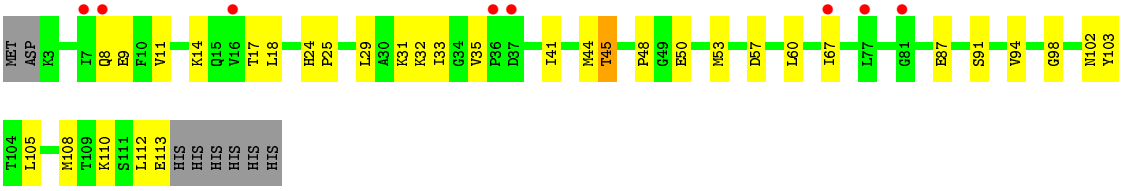
• Molecule 1: Ethanolamine utilization protein eutS



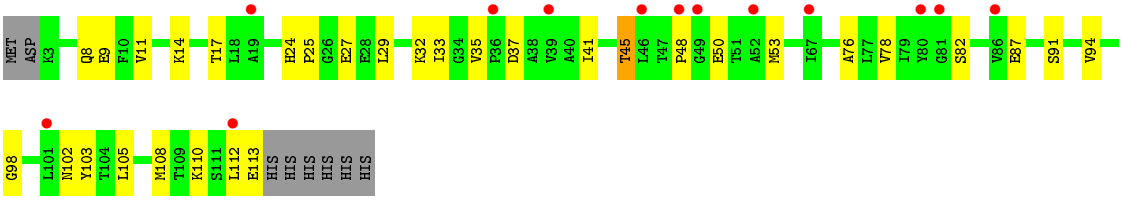
• Molecule 1: Ethanolamine utilization protein eutS



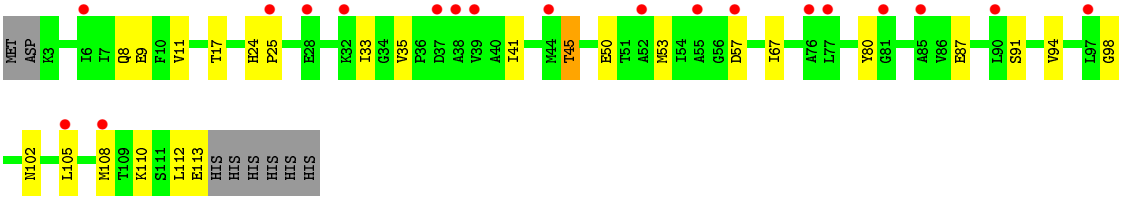
• Molecule 1: Ethanolamine utilization protein eutS



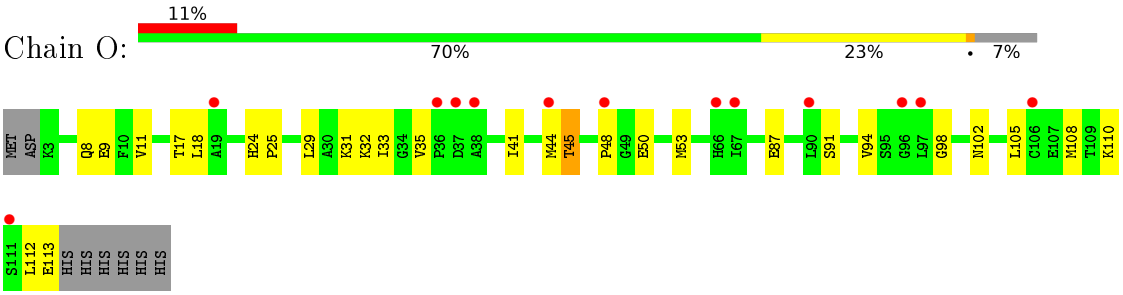
• Molecule 1: Ethanolamine utilization protein eutS



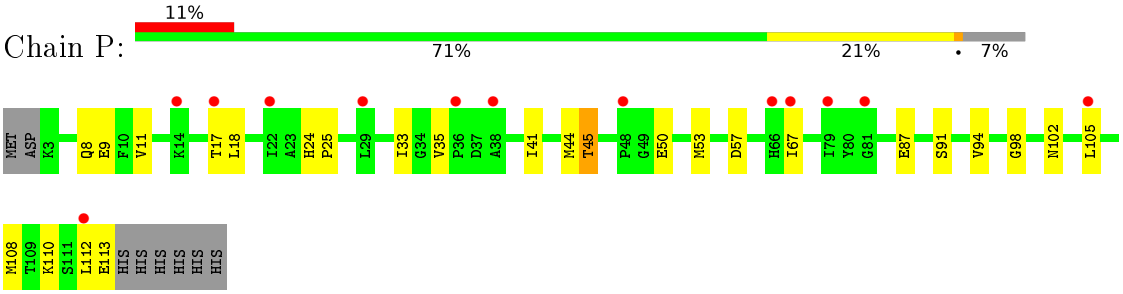
• Molecule 1: Ethanolamine utilization protein eutS



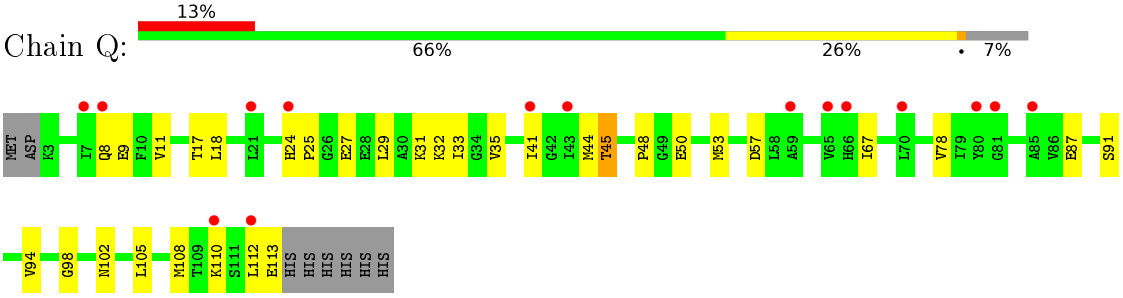
• Molecule 1: Ethanolamine utilization protein eutS



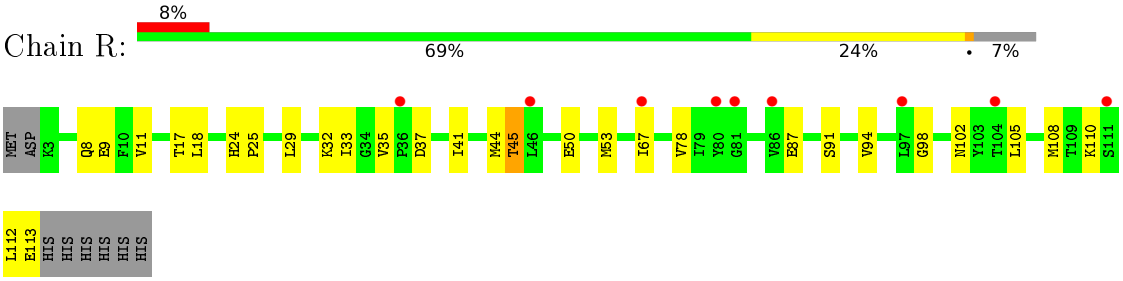
• Molecule 1: Ethanolamine utilization protein eutS



• Molecule 1: Ethanolamine utilization protein eutS

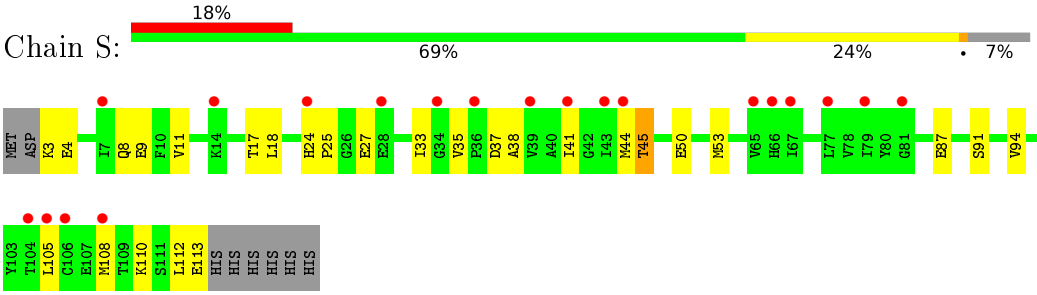


• Molecule 1: Ethanolamine utilization protein eutS



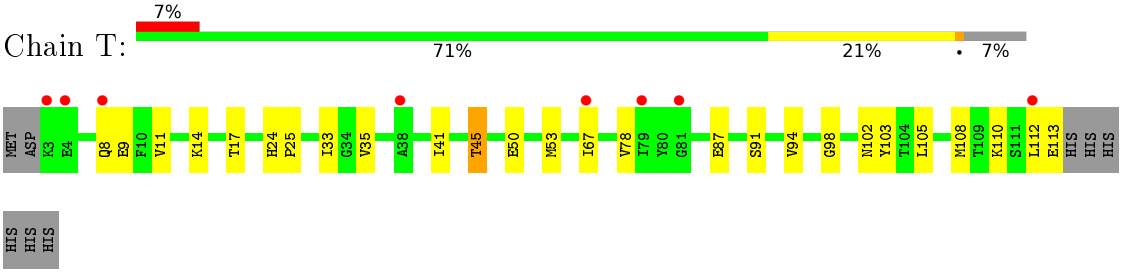
• Molecule 1: Ethanolamine utilization protein eutS

Chain S:



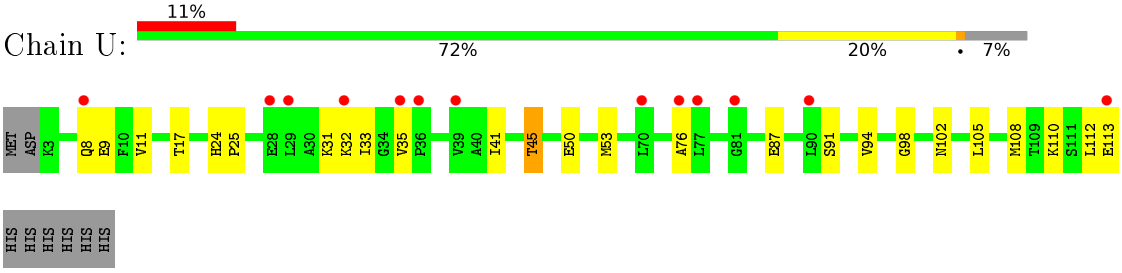
• Molecule 1: Ethanolamine utilization protein eutS

Chain T:



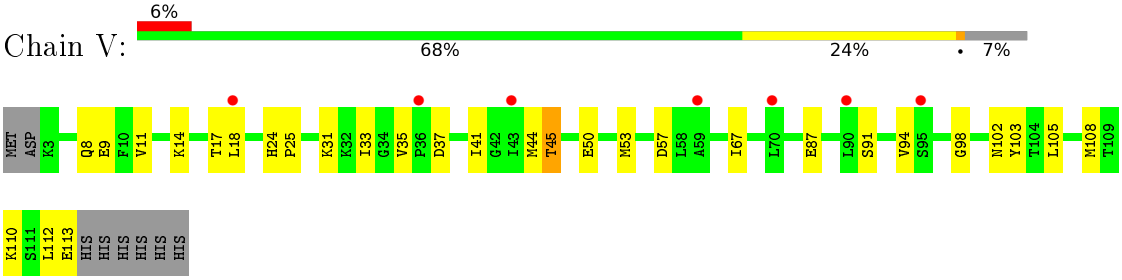
• Molecule 1: Ethanolamine utilization protein eutS

Chain U:



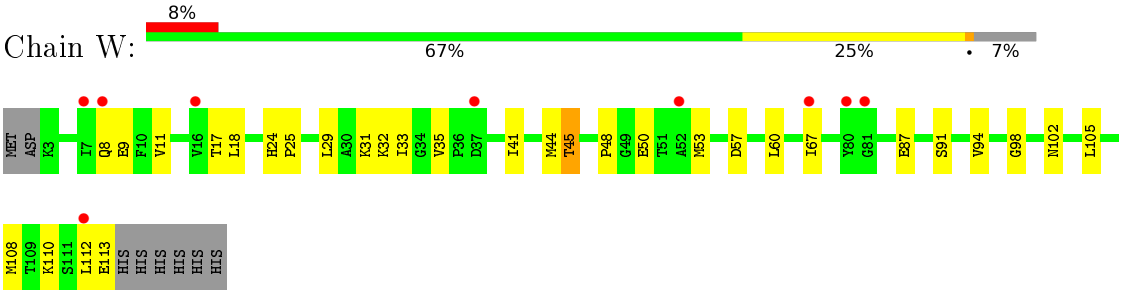
• Molecule 1: Ethanolamine utilization protein eutS

Chain V:



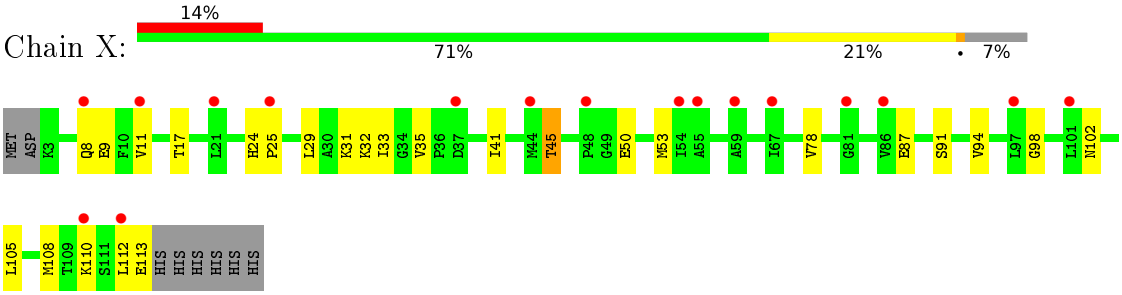
• Molecule 1: Ethanolamine utilization protein eutS

Chain W:



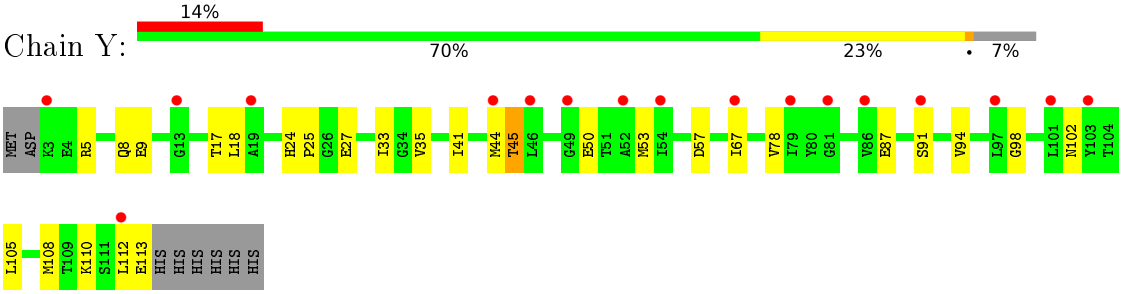
• Molecule 1: Ethanolamine utilization protein eutS

Chain X:



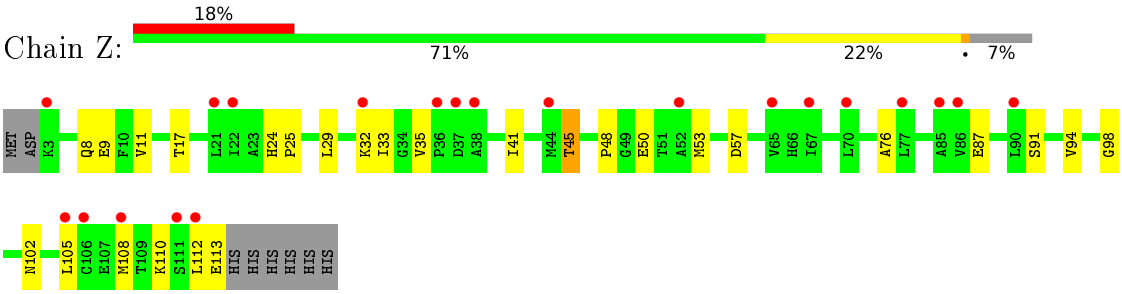
• Molecule 1: Ethanolamine utilization protein eutS

Chain Y:



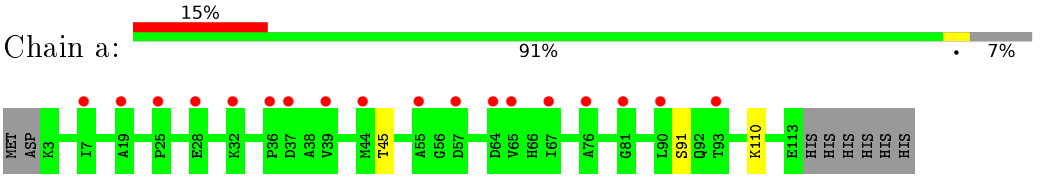
• Molecule 1: Ethanolamine utilization protein eutS

Chain Z:



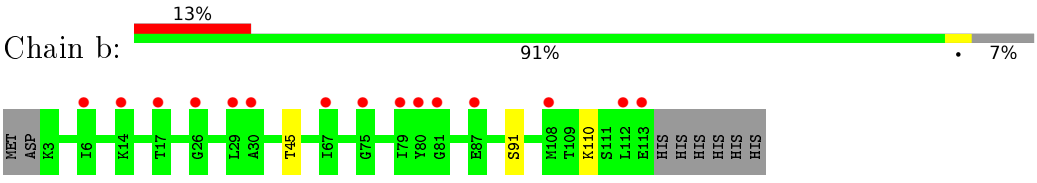
• Molecule 1: Ethanolamine utilization protein eutS

Chain a:



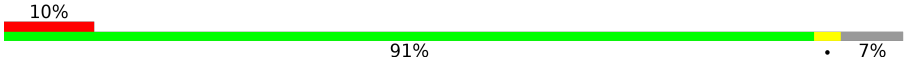
• Molecule 1: Ethanolamine utilization protein eutS

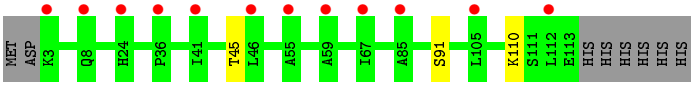
Chain b:



• Molecule 1: Ethanolamine utilization protein eutS

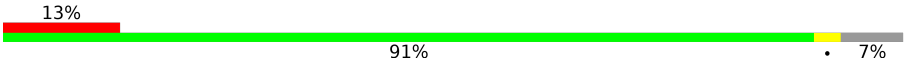
Chain c:

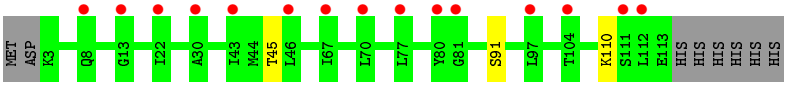




• Molecule 1: Ethanolamine utilization protein eutS

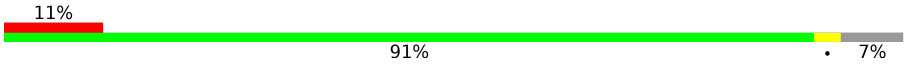
Chain d:

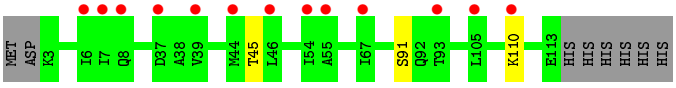




• Molecule 1: Ethanolamine utilization protein eutS

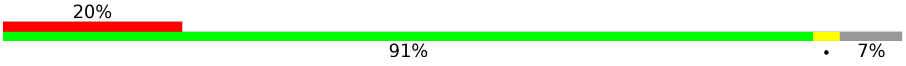
Chain e:

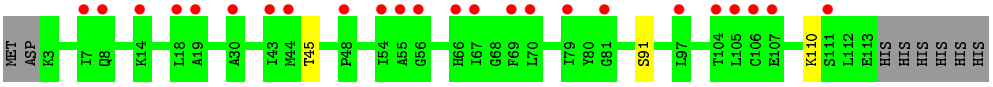




• Molecule 1: Ethanolamine utilization protein eutS

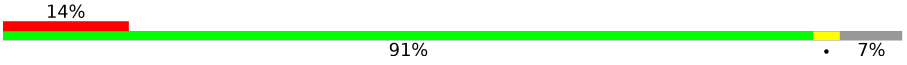
Chain f:

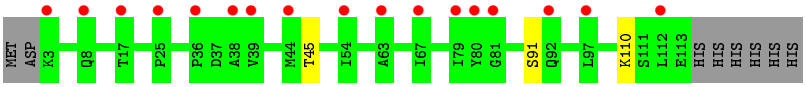




• Molecule 1: Ethanolamine utilization protein eutS

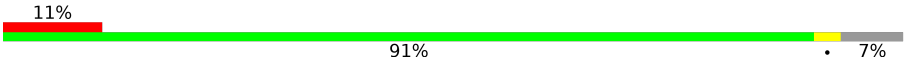
Chain g:

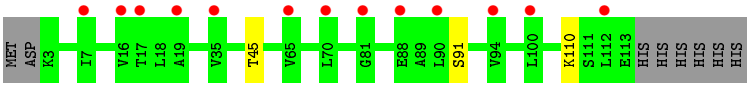




• Molecule 1: Ethanolamine utilization protein eutS

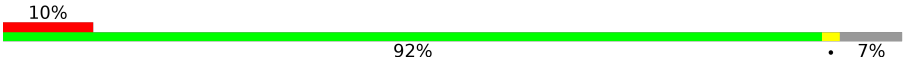
Chain h:

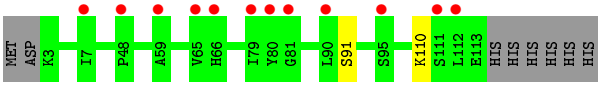




• Molecule 1: Ethanolamine utilization protein eutS

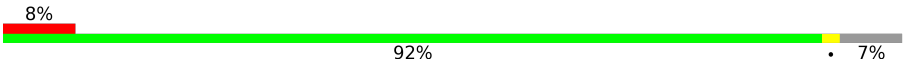
Chain i:

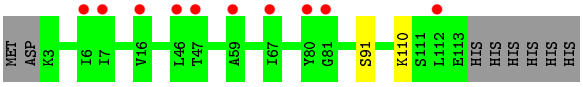




• Molecule 1: Ethanolamine utilization protein eutS

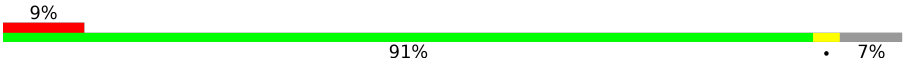
Chain j:

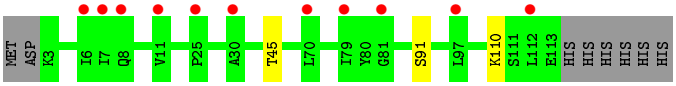




• Molecule 1: Ethanolamine utilization protein eutS

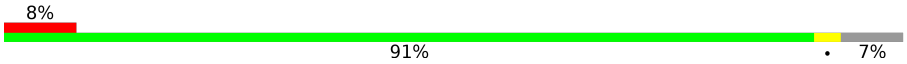
Chain k:

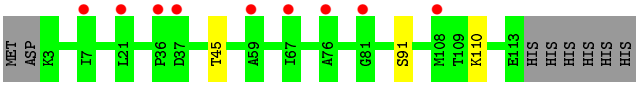




• Molecule 1: Ethanolamine utilization protein eutS

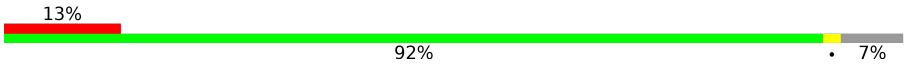
Chain l:

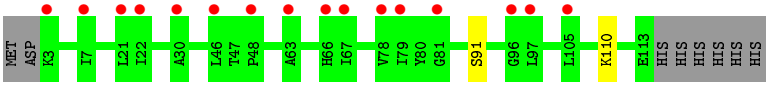




• Molecule 1: Ethanolamine utilization protein eutS

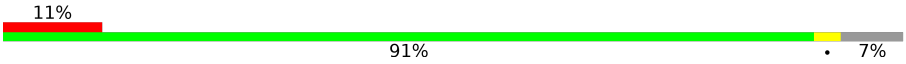
Chain m:

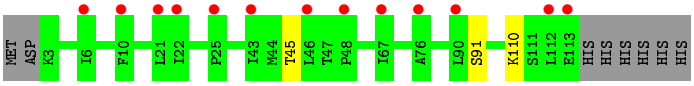




• Molecule 1: Ethanolamine utilization protein eutS

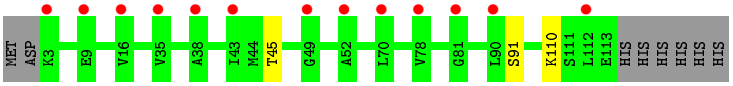
Chain n:





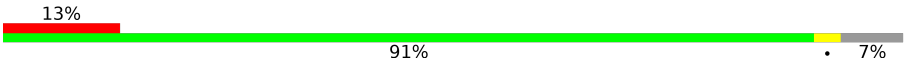
• Molecule 1: Ethanolamine utilization protein eutS

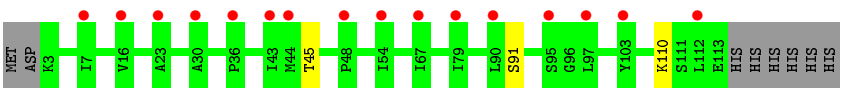
Chain o:



• Molecule 1: Ethanolamine utilization protein eutS

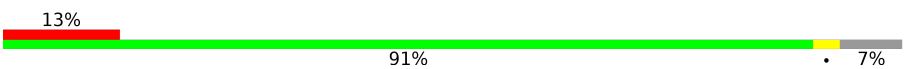
Chain p:

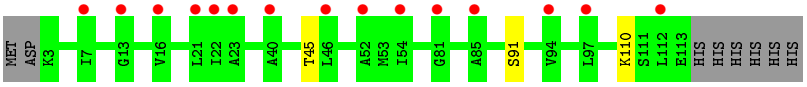




• Molecule 1: Ethanolamine utilization protein eutS

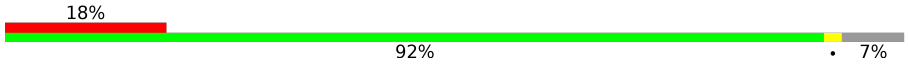
Chain q:

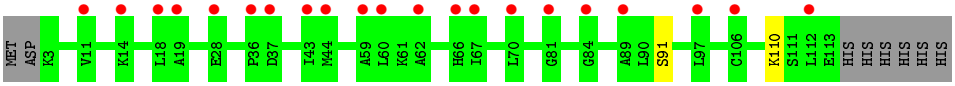




• Molecule 1: Ethanolamine utilization protein eutS

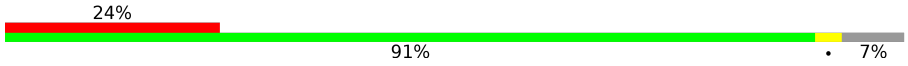
Chain r:

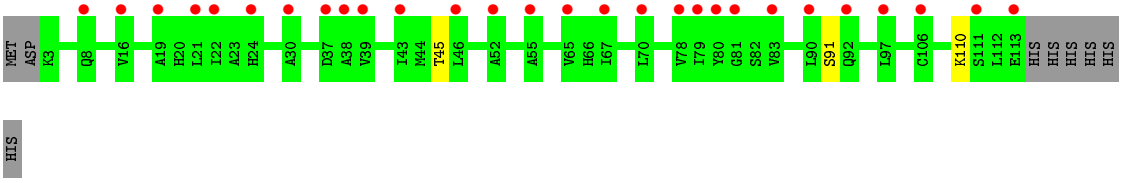




• Molecule 1: Ethanolamine utilization protein eutS

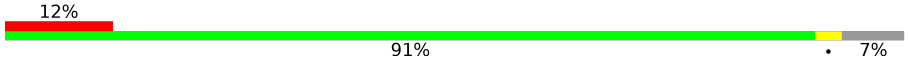
Chain s:

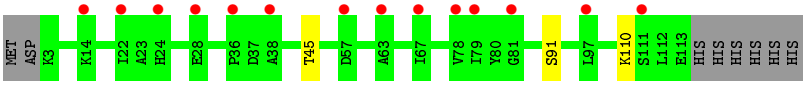




• Molecule 1: Ethanolamine utilization protein eutS

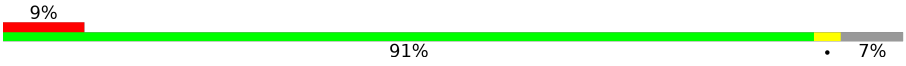
Chain t:

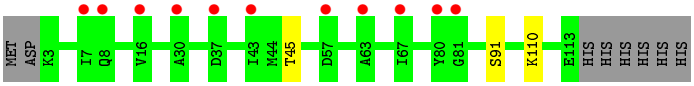




• Molecule 1: Ethanolamine utilization protein eutS

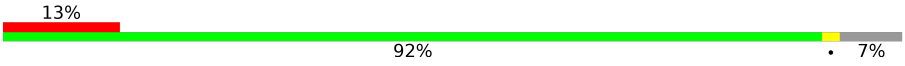
Chain u:

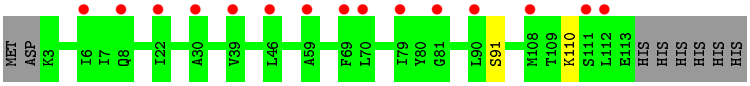




• Molecule 1: Ethanolamine utilization protein eutS

Chain v:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	73.58Å 151.39Å 127.46Å 90.00° 90.39° 90.00°	Depositor
Resolution (Å)	58.88 – 2.50 58.88 – 2.49	Depositor EDS
% Data completeness (in resolution range)	80.2 (58.88-2.50) 88.7 (58.88-2.49)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4_4)	Depositor
R, R_{free}	0.217 , 0.239 0.225 , 0.223	Depositor DCC
R_{free} test set	8716 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	48.2	Xtriage
Anisotropy	0.760	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.408 for h,-k,-l 0.408 for -h,-k,l 0.388 for -h,k,-l	Xtriage
Reported twinning fraction	0.463 for -h,-k,l	Depositor
Outliers	0 of 173036 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	39312	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.88% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.31	0/830	0.51	0/1123
1	B	0.30	0/830	0.51	0/1123
1	C	0.32	0/830	0.51	0/1123
1	D	0.30	0/830	0.51	0/1123
1	E	0.30	0/830	0.51	0/1123
1	F	0.31	0/830	0.51	0/1123
1	G	0.32	0/830	0.51	0/1123
1	H	0.31	0/830	0.50	0/1123
1	I	0.31	0/830	0.51	0/1123
1	J	0.31	0/830	0.51	0/1123
1	K	0.31	0/830	0.51	0/1123
1	L	0.32	0/830	0.51	0/1123
1	M	0.33	0/830	0.51	0/1123
1	N	0.32	0/830	0.51	0/1123
1	O	0.30	0/830	0.51	0/1123
1	P	0.31	0/830	0.51	0/1123
1	Q	0.32	0/830	0.51	0/1123
1	R	0.31	0/830	0.51	0/1123
1	S	0.31	0/830	0.51	0/1123
1	T	0.30	0/830	0.50	0/1123
1	U	0.31	0/830	0.51	0/1123
1	V	0.31	0/830	0.51	0/1123
1	W	0.32	0/830	0.50	0/1123
1	X	0.30	0/830	0.50	0/1123
1	Y	0.31	0/830	0.51	0/1123
1	Z	0.31	0/830	0.51	0/1123
1	a	0.30	0/830	0.51	0/1123
1	b	0.32	0/830	0.51	0/1123
1	c	0.31	0/830	0.51	0/1123
1	d	0.30	0/830	0.50	0/1123
1	e	0.30	0/830	0.51	0/1123
1	f	0.31	0/830	0.51	0/1123
1	g	0.30	0/830	0.50	0/1123
1	h	0.30	0/830	0.51	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	i	0.30	0/830	0.50	0/1123
1	j	0.31	0/830	0.50	0/1123
1	k	0.31	0/830	0.51	0/1123
1	l	0.31	0/830	0.51	0/1123
1	m	0.31	0/830	0.51	0/1123
1	n	0.30	0/830	0.50	0/1123
1	o	0.32	0/830	0.51	0/1123
1	p	0.31	0/830	0.51	0/1123
1	q	0.31	0/830	0.51	0/1123
1	r	0.30	0/830	0.51	0/1123
1	s	0.29	0/830	0.51	0/1123
1	t	0.31	0/830	0.51	0/1123
1	u	0.31	0/830	0.51	0/1123
1	v	0.31	0/830	0.51	0/1123
All	All	0.31	0/39840	0.51	0/53904

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	819	0	851	50	0
1	B	819	0	851	42	0
1	C	819	0	851	52	0
1	D	819	0	851	66	0
1	E	819	0	851	60	0
1	F	819	0	851	51	0
1	G	819	0	851	65	0
1	H	819	0	851	38	0
1	I	819	0	851	35	0
1	J	819	0	851	42	0
1	K	819	0	851	47	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	819	0	851	84	0
1	M	819	0	851	62	0
1	N	819	0	851	38	0
1	O	819	0	851	39	0
1	P	819	0	851	46	0
1	Q	819	0	851	61	0
1	R	819	0	851	51	0
1	S	819	0	851	51	0
1	T	819	0	851	36	0
1	U	819	0	851	47	0
1	V	819	0	851	57	0
1	W	819	0	851	40	0
1	X	819	0	851	43	0
1	Y	819	0	851	36	0
1	Z	819	0	851	37	0
1	a	819	0	851	0	0
1	b	819	0	851	0	0
1	c	819	0	851	0	0
1	d	819	0	851	0	0
1	e	819	0	851	0	0
1	f	819	0	851	0	0
1	g	819	0	851	0	0
1	h	819	0	851	0	0
1	i	819	0	851	0	0
1	j	819	0	851	0	0
1	k	819	0	851	0	0
1	l	819	0	851	0	0
1	m	819	0	851	0	0
1	n	819	0	851	0	0
1	o	819	0	851	0	0
1	p	819	0	851	0	0
1	q	819	0	851	0	0
1	r	819	0	851	0	0
1	s	819	0	851	0	0
1	t	819	0	851	0	0
1	u	819	0	851	0	0
1	v	819	0	851	0	0
All	All	39312	0	40848	806	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 10.

All (806) 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:E:35:VAL:HG21	1:E:41:ILE:HD11	1.31	1.17
1:P:35:VAL:HG21	1:P:41:ILE:HD11	1.28	1.15
1:Q:35:VAL:HG21	1:Q:41:ILE:HD11	1.28	1.14
1:T:35:VAL:HG21	1:T:41:ILE:HD11	1.29	1.14
1:C:35:VAL:HG21	1:C:41:ILE:HD11	1.27	1.13
1:N:35:VAL:HG21	1:N:41:ILE:HD11	1.29	1.13
1:D:35:VAL:HG21	1:D:41:ILE:HD11	1.31	1.13
1:L:35:VAL:HG21	1:L:41:ILE:HD11	1.29	1.13
1:M:35:VAL:HG21	1:M:41:ILE:HD11	1.28	1.13
1:U:35:VAL:HG21	1:U:41:ILE:HD11	1.29	1.13
1:H:35:VAL:HG21	1:H:41:ILE:HD11	1.30	1.12
1:I:35:VAL:HG21	1:I:41:ILE:HD11	1.28	1.12
1:O:35:VAL:HG21	1:O:41:ILE:HD11	1.30	1.12
1:A:35:VAL:HG21	1:A:41:ILE:HD11	1.32	1.11
1:D:37:ASP:HB2	1:L:31:LYS:HZ1	75.86	1.11
1:S:35:VAL:HG21	1:S:41:ILE:HD11	1.29	1.11
1:G:35:VAL:HG21	1:G:41:ILE:HD11	1.31	1.11
1:Y:35:VAL:HG21	1:Y:41:ILE:HD11	1.29	1.11
1:V:35:VAL:HG21	1:V:41:ILE:HD11	1.29	1.10
1:F:35:VAL:HG21	1:F:41:ILE:HD11	1.31	1.10
1:R:35:VAL:HG21	1:R:41:ILE:HD11	1.32	1.10
1:K:35:VAL:HG21	1:K:41:ILE:HD11	1.31	1.09
1:X:35:VAL:HG21	1:X:41:ILE:HD11	1.28	1.09
1:J:35:VAL:HG21	1:J:41:ILE:HD11	1.29	1.09
1:W:35:VAL:HG21	1:W:41:ILE:HD11	1.30	1.09
1:K:31:LYS:HE2	1:M:27:GLU:OE1	1.51	1.08
1:Z:35:VAL:HG21	1:Z:41:ILE:HD11	1.31	1.08
1:B:35:VAL:HG21	1:B:41:ILE:HD11	1.30	1.07
1:D:37:ASP:CB	1:L:31:LYS:HZ1	76.34	1.03
1:D:37:ASP:HB2	1:L:31:LYS:NZ	75.57	1.02
1:K:31:LYS:HE2	1:Y:27:GLU:OE1	110.85	1.01
1:J:31:LYS:HE2	1:Q:27:GLU:OE1	59.22	1.00
1:F:27:GLU:OE1	1:W:31:LYS:HE2	1.61	0.98
1:G:27:GLU:OE1	1:Q:31:LYS:HE3	1.65	0.95
1:D:37:ASP:CB	1:L:31:LYS:NZ	76.05	0.95
1:L:31:LYS:HZ1	1:R:37:ASP:HB2	1.33	0.94
1:D:31:LYS:HE3	1:S:27:GLU:OE1	1.68	0.94
1:D:37:ASP:H	1:L:31:LYS:HZ3	73.41	0.91
1:D:37:ASP:H	1:L:31:LYS:NZ	73.67	0.90
1:B:87:GLU:OE1	1:G:82:SER:HB2	126.76	0.87
1:A:8:GLN:NE2	1:F:8:GLN:HE22	1.74	0.85
1:C:31:LYS:HE3	1:M:27:GLU:OE1	77.39	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:GLU:OE1	1:U:31:LYS:HG3	36.98	0.85
1:Y:8:GLN:HE22	1:Z:8:GLN:NE2	1.74	0.85
1:L:31:LYS:HZ1	1:R:37:ASP:CB	1.89	0.85
1:M:8:GLN:HE22	1:N:8:GLN:NE2	1.75	0.84
1:T:8:GLN:HE22	1:U:8:GLN:NE2	1.97	0.83
1:E:31:LYS:NZ	1:V:37:ASP:H	44.66	0.82
1:D:8:GLN:HE22	1:Y:8:GLN:NE2	81.05	0.82
1:N:8:GLN:HE22	1:O:8:GLN:NE2	2.04	0.82
1:B:8:GLN:HE22	1:C:8:GLN:NE2	1.94	0.81
1:E:8:GLN:HE22	1:F:8:GLN:NE2	1.80	0.81
1:Q:8:GLN:NE2	1:V:8:GLN:HE22	78.80	0.81
1:D:8:GLN:HE22	1:E:8:GLN:NE2	1.79	0.81
1:L:31:LYS:NZ	1:R:37:ASP:HB2	1.95	0.80
1:U:8:GLN:HE22	1:V:8:GLN:NE2	1.89	0.80
1:M:8:GLN:NE2	1:R:8:GLN:HE22	1.77	0.80
1:S:8:GLN:NE2	1:X:8:GLN:HE22	1.80	0.79
1:Q:8:GLN:HE22	1:R:8:GLN:NE2	1.90	0.79
1:E:31:LYS:HZ1	1:V:37:ASP:CB	46.64	0.78
1:A:8:GLN:HE22	1:B:8:GLN:NE2	1.81	0.78
1:G:27:GLU:CD	1:Q:31:LYS:HG3	2.03	0.78
1:C:8:GLN:HE22	1:D:8:GLN:NE2	1.82	0.78
1:F:27:GLU:OE1	1:U:31:LYS:HE3	38.12	0.78
1:D:37:ASP:N	1:L:31:LYS:NZ	73.86	0.77
1:J:8:GLN:HE22	1:K:8:GLN:NE2	1.82	0.77
1:P:8:GLN:HE22	1:Q:8:GLN:NE2	1.83	0.77
1:R:8:GLN:HE22	1:S:8:GLN:NE2	75.33	0.77
1:H:8:GLN:HE22	1:I:8:GLN:NE2	1.83	0.77
1:C:31:LYS:NZ	1:M:37:ASP:OD2	79.51	0.77
1:W:8:GLN:HE22	1:X:8:GLN:NE2	1.83	0.77
1:G:8:GLN:HE22	1:H:8:GLN:NE2	1.82	0.77
1:E:8:GLN:NE2	1:J:8:GLN:HE22	74.04	0.76
1:E:31:LYS:HZ1	1:V:37:ASP:H	44.49	0.76
1:L:31:LYS:NZ	1:R:37:ASP:CB	2.47	0.76
1:O:8:GLN:HE22	1:P:8:GLN:NE2	1.88	0.75
1:G:37:ASP:OD2	1:Q:31:LYS:NZ	2.19	0.75
1:C:31:LYS:HG3	1:M:27:GLU:CD	77.95	0.75
1:L:8:GLN:HE22	1:M:8:GLN:NE2	70.83	0.75
1:K:8:GLN:HE22	1:L:8:GLN:NE2	1.86	0.75
1:S:9:GLU:HA	1:T:11:VAL:O	2.14	0.74
1:G:112:LEU:O	1:G:113:GLU:HB2	1.93	0.73
1:I:8:GLN:HE22	1:J:8:GLN:NE2	1.85	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:9:GLU:HA	1:R:11:VAL:O	1.89	0.73
1:E:31:LYS:HZ1	1:V:37:ASP:HB2	46.06	0.73
1:K:112:LEU:O	1:K:113:GLU:HB2	1.89	0.73
1:R:112:LEU:O	1:R:113:GLU:HB2	1.91	0.73
1:M:82:SER:HB2	1:S:87:GLU:OE1	96.03	0.73
1:F:8:GLN:HE22	1:G:8:GLN:NE2	73.46	0.73
1:V:8:GLN:HE22	1:W:8:GLN:NE2	1.86	0.73
1:E:37:ASP:H	1:X:31:LYS:HZ1	1.36	0.73
1:H:112:LEU:O	1:H:113:GLU:HB2	1.88	0.72
1:Y:112:LEU:O	1:Y:113:GLU:HB2	1.89	0.72
1:T:112:LEU:O	1:T:113:GLU:HB2	1.89	0.72
1:F:112:LEU:O	1:F:113:GLU:HB2	1.89	0.72
1:N:112:LEU:O	1:N:113:GLU:HB2	1.90	0.72
1:D:112:LEU:O	1:D:113:GLU:HB2	1.89	0.72
1:D:37:ASP:N	1:L:31:LYS:HZ1	74.16	0.72
1:I:94:VAL:HG12	1:I:105:LEU:HD23	1.77	0.72
1:P:112:LEU:O	1:P:113:GLU:HB2	1.89	0.72
1:V:94:VAL:HG12	1:V:105:LEU:HD23	1.72	0.72
1:Z:112:LEU:O	1:Z:113:GLU:HB2	1.90	0.72
1:L:112:LEU:O	1:L:113:GLU:HB2	1.89	0.72
1:T:8:GLN:HE22	1:U:8:GLN:CD	2.23	0.72
1:Q:112:LEU:O	1:Q:113:GLU:HB2	1.89	0.71
1:F:27:GLU:CD	1:U:31:LYS:HG3	35.90	0.71
1:C:94:VAL:HG12	1:C:105:LEU:HD23	1.77	0.71
1:E:112:LEU:O	1:E:113:GLU:HB2	1.91	0.71
1:L:31:LYS:NZ	1:R:37:ASP:H	1.88	0.71
1:S:8:GLN:HE22	1:T:8:GLN:NE2	1.88	0.71
1:W:112:LEU:O	1:W:113:GLU:HB2	1.90	0.71
1:M:112:LEU:O	1:M:113:GLU:HB2	1.90	0.71
1:F:50:GLU:HB2	1:G:45:THR:HG22	74.92	0.71
1:C:112:LEU:O	1:C:113:GLU:HB2	1.91	0.71
1:H:9:GLU:HA	1:I:11:VAL:O	2.16	0.71
1:E:31:LYS:HZ1	1:V:37:ASP:N	44.57	0.71
1:A:112:LEU:O	1:A:113:GLU:HB2	1.90	0.70
1:I:112:LEU:O	1:I:113:GLU:HB2	1.91	0.70
1:B:53:MET:HE3	1:C:33:ILE:HG12	1.73	0.70
1:X:112:LEU:O	1:X:113:GLU:HB2	1.88	0.70
1:U:112:LEU:O	1:U:113:GLU:HB2	1.91	0.70
1:J:112:LEU:O	1:J:113:GLU:HB2	1.90	0.70
1:K:8:GLN:NE2	1:P:8:GLN:HE22	69.84	0.70
1:B:112:LEU:O	1:B:113:GLU:HB2	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:94:VAL:HG12	1:X:105:LEU:HD23	1.73	0.69
1:Y:8:GLN:HE22	1:Z:8:GLN:CD	1.94	0.69
1:V:112:LEU:O	1:V:113:GLU:HB2	1.92	0.69
1:Q:94:VAL:HG12	1:Q:105:LEU:HD23	1.73	0.69
1:S:112:LEU:O	1:S:113:GLU:HB2	1.93	0.69
1:F:94:VAL:HG12	1:F:105:LEU:HD23	1.75	0.69
1:M:53:MET:HE3	1:N:33:ILE:HG12	1.83	0.69
1:O:112:LEU:O	1:O:113:GLU:HB2	1.93	0.68
1:O:50:GLU:HB2	1:P:45:THR:HG22	1.74	0.68
1:A:11:VAL:O	1:Z:9:GLU:HA	84.60	0.68
1:G:8:GLN:NE2	1:L:8:GLN:HE22	1.90	0.68
1:K:33:ILE:HG12	1:P:53:MET:HE3	42.76	0.68
1:A:94:VAL:HG12	1:A:105:LEU:HD23	1.81	0.68
1:A:8:GLN:CD	1:F:8:GLN:HE22	1.95	0.68
1:H:94:VAL:HG12	1:H:105:LEU:HD23	1.76	0.68
1:O:94:VAL:HG12	1:O:105:LEU:HD23	1.76	0.68
1:D:31:LYS:HG3	1:S:27:GLU:OE1	1.94	0.68
1:T:53:MET:HE3	1:U:33:ILE:HG12	1.75	0.68
1:S:94:VAL:HG12	1:S:105:LEU:HD23	1.81	0.68
1:T:94:VAL:HG12	1:T:105:LEU:HD23	1.76	0.68
1:R:94:VAL:HG12	1:R:105:LEU:HD23	1.75	0.68
1:E:94:VAL:HG12	1:E:105:LEU:HD23	1.78	0.67
1:C:9:GLU:HA	1:D:11:VAL:O	2.02	0.67
1:K:94:VAL:HG12	1:K:105:LEU:HD23	1.78	0.67
1:M:50:GLU:HB2	1:N:45:THR:HG22	1.76	0.67
1:M:8:GLN:HE22	1:N:8:GLN:CD	2.03	0.67
1:U:94:VAL:HG12	1:U:105:LEU:HD23	1.77	0.67
1:B:94:VAL:HG12	1:B:105:LEU:HD23	1.77	0.67
1:L:94:VAL:HG12	1:L:105:LEU:HD23	1.76	0.67
1:P:94:VAL:HG12	1:P:105:LEU:HD23	1.79	0.67
1:E:53:MET:HE3	1:F:33:ILE:HG12	1.78	0.67
1:M:94:VAL:HG12	1:M:105:LEU:HD23	1.77	0.67
1:J:53:MET:HE3	1:K:33:ILE:HG12	1.76	0.66
1:U:53:MET:HE3	1:V:33:ILE:HG12	1.76	0.66
1:L:50:GLU:HB2	1:M:45:THR:HG22	45.27	0.66
1:M:9:GLU:HA	1:N:11:VAL:O	2.22	0.66
1:G:50:GLU:HB2	1:H:45:THR:HG22	1.77	0.66
1:A:9:GLU:HA	1:B:11:VAL:O	2.31	0.65
1:C:53:MET:HE3	1:D:33:ILE:HG12	2.02	0.65
1:D:94:VAL:HG12	1:D:105:LEU:HD23	1.79	0.65
1:E:45:THR:HG22	1:J:50:GLU:HB2	53.54	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:94:VAL:HG12	1:J:105:LEU:HD23	1.78	0.65
1:Q:8:GLN:HE22	1:R:8:GLN:CD	2.05	0.65
1:H:53:MET:HE3	1:I:33:ILE:HG12	1.86	0.65
1:U:9:GLU:HA	1:V:11:VAL:O	1.97	0.65
1:S:50:GLU:HB2	1:T:45:THR:HG22	1.78	0.65
1:N:94:VAL:HG12	1:N:105:LEU:HD23	1.79	0.65
1:G:94:VAL:HG12	1:G:105:LEU:HD23	1.78	0.65
1:B:9:GLU:HA	1:C:11:VAL:O	1.97	0.64
1:D:31:LYS:HG3	1:S:27:GLU:CD	2.17	0.64
1:C:31:LYS:HG3	1:M:27:GLU:OE1	76.85	0.64
1:C:8:GLN:HE22	1:D:8:GLN:CD	2.02	0.63
1:D:37:ASP:CA	1:L:31:LYS:HZ1	75.59	0.63
1:E:31:LYS:NZ	1:V:37:ASP:CB	46.81	0.63
1:B:50:GLU:HB2	1:C:45:THR:HG22	1.93	0.62
1:K:9:GLU:HA	1:L:11:VAL:O	2.02	0.62
1:Y:50:GLU:HB2	1:Z:45:THR:HG22	1.80	0.62
1:A:50:GLU:HB2	1:B:45:THR:HG22	1.87	0.62
1:G:53:MET:HE3	1:H:33:ILE:HG12	1.81	0.62
1:R:50:GLU:HB2	1:S:45:THR:HG22	80.70	0.62
1:S:53:MET:HE3	1:T:33:ILE:HG12	1.89	0.62
1:B:87:GLU:OE1	1:G:82:SER:CB	126.47	0.62
1:F:53:MET:HE3	1:G:33:ILE:HG12	72.06	0.62
1:W:94:VAL:HG12	1:W:105:LEU:HD23	1.80	0.62
1:Z:94:VAL:HG12	1:Z:105:LEU:HD23	1.79	0.62
1:G:27:GLU:OE1	1:Q:31:LYS:HG3	1.98	0.62
1:B:8:GLN:HE22	1:C:8:GLN:CD	2.06	0.62
1:L:31:LYS:HZ1	1:R:37:ASP:N	1.96	0.62
1:G:45:THR:HG22	1:L:50:GLU:HB2	1.81	0.61
1:W:67:ILE:HB	1:X:32:LYS:HE3	1.82	0.61
1:Q:9:GLU:HG2	1:R:11:VAL:HG23	1.83	0.61
1:Q:53:MET:HE3	1:R:33:ILE:HG12	1.83	0.61
1:G:27:GLU:OE2	1:Q:31:LYS:HG3	2.00	0.61
1:K:8:GLN:HE22	1:L:8:GLN:CD	2.11	0.61
1:Q:45:THR:HG22	1:V:50:GLU:HB2	57.27	0.61
1:Y:94:VAL:HG12	1:Y:105:LEU:HD23	1.81	0.61
1:Y:53:MET:HE3	1:Z:33:ILE:HG12	1.83	0.61
1:C:9:GLU:HG2	1:D:11:VAL:HG23	2.03	0.61
1:D:50:GLU:HB2	1:Y:45:THR:HG22	92.27	0.60
1:A:45:THR:HG22	1:F:50:GLU:HB2	1.82	0.60
1:A:11:VAL:O	1:F:9:GLU:HA	2.00	0.60
1:E:8:GLN:CD	1:J:8:GLN:HE22	73.56	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:8:GLN:CD	1:R:8:GLN:HE22	2.04	0.60
1:A:33:ILE:HG12	1:F:53:MET:HE3	1.83	0.60
1:S:8:GLN:HE22	1:T:8:GLN:CD	2.18	0.60
1:V:50:GLU:HB2	1:W:45:THR:HG22	1.82	0.60
1:E:50:GLU:HB2	1:F:45:THR:HG22	1.83	0.60
1:K:53:MET:HE3	1:L:33:ILE:HG12	1.84	0.60
1:O:8:GLN:HE22	1:P:8:GLN:CD	2.05	0.60
1:G:8:GLN:HE22	1:H:8:GLN:CD	2.06	0.60
1:T:50:GLU:HB2	1:U:45:THR:HG22	1.84	0.59
1:A:33:ILE:HG23	1:Z:53:MET:CE	94.56	0.59
1:S:9:GLU:HG2	1:T:11:VAL:HG23	2.03	0.59
1:I:50:GLU:HB2	1:J:45:THR:HG22	1.84	0.59
1:Y:8:GLN:NE2	1:Z:8:GLN:CD	2.56	0.59
1:S:33:ILE:HG12	1:X:53:MET:HE3	1.84	0.59
1:U:50:GLU:HB2	1:V:45:THR:HG22	1.98	0.59
1:A:8:GLN:HE22	1:B:8:GLN:CD	2.22	0.58
1:X:112:LEU:O	1:X:113:GLU:CB	2.52	0.58
1:C:8:GLN:CD	1:D:8:GLN:HB3	2.38	0.58
1:C:67:ILE:HB	1:D:32:LYS:HE3	1.85	0.58
1:Q:33:ILE:HG12	1:V:53:MET:HE3	56.58	0.58
1:G:112:LEU:O	1:G:113:GLU:CB	2.56	0.58
1:S:8:GLN:CD	1:X:8:GLN:HE22	2.07	0.58
1:A:8:GLN:CD	1:F:8:GLN:NE2	2.57	0.58
1:Q:50:GLU:HB2	1:R:45:THR:HG22	1.98	0.58
1:Q:8:GLN:CD	1:V:8:GLN:HE22	78.22	0.58
1:J:8:GLN:HE22	1:K:8:GLN:CD	2.07	0.58
1:A:11:VAL:HG23	1:F:9:GLU:HG2	1.84	0.58
1:I:8:GLN:HE22	1:J:8:GLN:CD	2.06	0.58
1:A:9:GLU:HG2	1:B:11:VAL:HG23	2.27	0.58
1:E:8:GLN:HE22	1:F:8:GLN:CD	2.07	0.58
1:D:50:GLU:HB2	1:E:45:THR:HG22	1.86	0.57
1:L:112:LEU:O	1:L:113:GLU:CB	2.52	0.57
1:W:8:GLN:HE22	1:X:8:GLN:CD	2.08	0.57
1:D:31:LYS:CE	1:S:27:GLU:OE1	2.49	0.57
1:K:112:LEU:O	1:K:113:GLU:CB	2.52	0.57
1:N:112:LEU:O	1:N:113:GLU:CB	2.54	0.57
1:F:50:GLU:HB2	1:G:45:THR:CG2	74.88	0.57
1:D:112:LEU:O	1:D:113:GLU:CB	2.52	0.57
1:E:11:VAL:O	1:J:9:GLU:HA	58.91	0.57
1:Q:112:LEU:O	1:Q:113:GLU:CB	2.52	0.57
1:R:112:LEU:O	1:R:113:GLU:CB	2.54	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:LYS:CE	1:M:37:ASP:OD2	79.04	0.57
1:L:53:MET:HE1	1:M:78:VAL:HG21	37.94	0.57
1:T:8:GLN:NE2	1:U:8:GLN:CD	2.87	0.57
1:E:37:ASP:H	1:X:31:LYS:NZ	2.01	0.57
1:V:8:GLN:HE22	1:W:8:GLN:CD	2.08	0.56
1:D:8:GLN:HE22	1:E:8:GLN:CD	2.09	0.56
1:T:112:LEU:O	1:T:113:GLU:CB	2.52	0.56
1:U:8:GLN:HE22	1:V:8:GLN:CD	2.09	0.56
1:H:112:LEU:O	1:H:113:GLU:CB	2.52	0.56
1:N:53:MET:HE3	1:O:33:ILE:HG12	1.87	0.56
1:P:112:LEU:O	1:P:113:GLU:CB	2.53	0.56
1:Z:112:LEU:O	1:Z:113:GLU:CB	2.53	0.56
1:K:31:LYS:CE	1:M:27:GLU:OE1	2.42	0.56
1:O:112:LEU:O	1:O:113:GLU:CB	2.57	0.56
1:O:9:GLU:HA	1:P:11:VAL:O	2.05	0.56
1:F:112:LEU:O	1:F:113:GLU:CB	2.53	0.56
1:W:112:LEU:O	1:W:113:GLU:CB	2.54	0.56
1:W:57:ASP:HA	1:X:29:LEU:HD22	1.87	0.56
1:M:33:ILE:HG12	1:R:53:MET:HE3	1.88	0.56
1:U:9:GLU:HG2	1:V:11:VAL:HG23	1.90	0.56
1:S:11:VAL:O	1:X:9:GLU:HA	2.06	0.56
1:G:8:GLN:CD	1:L:8:GLN:HE22	2.09	0.56
1:C:31:LYS:HE2	1:M:37:ASP:OD2	78.21	0.56
1:A:8:GLN:HB3	1:F:8:GLN:CD	2.26	0.56
1:C:112:LEU:O	1:C:113:GLU:CB	2.54	0.55
1:K:50:GLU:HB2	1:L:45:THR:HG22	2.01	0.55
1:L:24:HIS:N	1:L:25:PRO:HD3	2.22	0.55
1:W:9:GLU:HA	1:X:11:VAL:O	2.06	0.55
1:E:37:ASP:CB	1:X:31:LYS:HZ1	2.19	0.55
1:U:112:LEU:O	1:U:113:GLU:CB	2.54	0.55
1:E:112:LEU:O	1:E:113:GLU:CB	2.55	0.55
1:M:112:LEU:O	1:M:113:GLU:CB	2.54	0.55
1:U:24:HIS:N	1:U:25:PRO:HD3	2.20	0.55
1:B:112:LEU:O	1:B:113:GLU:CB	2.55	0.55
1:J:112:LEU:O	1:J:113:GLU:CB	2.55	0.55
1:S:24:HIS:N	1:S:25:PRO:HD3	2.23	0.55
1:G:29:LEU:HD22	1:L:57:ASP:HA	1.88	0.55
1:G:24:HIS:N	1:G:25:PRO:HD3	2.21	0.55
1:D:24:HIS:N	1:D:25:PRO:HD3	2.24	0.55
1:E:24:HIS:N	1:E:25:PRO:HD3	2.22	0.54
1:H:9:GLU:HG2	1:I:11:VAL:HG23	2.13	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:ASP:N	1:X:31:LYS:HZ1	2.04	0.54
1:M:50:GLU:HB2	1:N:45:THR:CG2	2.37	0.54
1:Q:24:HIS:N	1:Q:25:PRO:HD3	2.22	0.54
1:N:24:HIS:N	1:N:25:PRO:HD3	2.22	0.54
1:V:112:LEU:O	1:V:113:GLU:CB	2.56	0.54
1:B:24:HIS:N	1:B:25:PRO:HD3	2.23	0.54
1:I:112:LEU:O	1:I:113:GLU:CB	2.54	0.54
1:G:32:LYS:HE3	1:L:67:ILE:HB	1.88	0.54
1:H:24:HIS:N	1:H:25:PRO:HD3	2.26	0.54
1:N:8:GLN:HE22	1:O:8:GLN:CD	2.33	0.54
1:Z:24:HIS:N	1:Z:25:PRO:HD3	2.22	0.54
1:C:24:HIS:N	1:C:25:PRO:HD3	2.23	0.54
1:F:24:HIS:N	1:F:25:PRO:HD3	2.24	0.54
1:G:11:VAL:O	1:L:9:GLU:HA	2.07	0.54
1:P:24:HIS:N	1:P:25:PRO:HD3	2.23	0.54
1:V:24:HIS:N	1:V:25:PRO:HD3	2.23	0.54
1:H:53:MET:CE	1:I:33:ILE:HG23	2.55	0.54
1:K:45:THR:HG22	1:P:50:GLU:HB2	48.03	0.54
1:C:53:MET:CE	1:D:33:ILE:HG23	2.38	0.54
1:L:8:GLN:HE22	1:M:8:GLN:CD	69.79	0.54
1:M:24:HIS:N	1:M:25:PRO:HD3	2.23	0.54
1:C:31:LYS:HG3	1:M:27:GLU:OE2	78.26	0.54
1:O:24:HIS:N	1:O:25:PRO:HD3	2.23	0.54
1:D:31:LYS:NZ	1:S:37:ASP:OD2	2.39	0.54
1:T:8:GLN:CD	1:U:8:GLN:HB3	2.61	0.54
1:Z:87:GLU:HA	1:Z:108:MET:HE1	1.90	0.54
1:A:24:HIS:N	1:A:25:PRO:HD3	2.23	0.53
1:I:35:VAL:HG21	1:I:41:ILE:CD1	2.21	0.53
1:W:50:GLU:HB2	1:X:45:THR:HG22	1.91	0.53
1:A:112:LEU:O	1:A:113:GLU:CB	2.54	0.53
1:R:24:HIS:N	1:R:25:PRO:HD3	2.23	0.53
1:X:24:HIS:N	1:X:25:PRO:HD3	2.22	0.53
1:F:37:ASP:OD2	1:U:31:LYS:HE2	36.01	0.53
1:R:87:GLU:HA	1:R:108:MET:HE1	1.94	0.53
1:L:31:LYS:HZ1	1:R:37:ASP:H	1.49	0.53
1:C:50:GLU:HB2	1:D:45:THR:HG22	1.95	0.53
1:D:9:GLU:HA	1:E:11:VAL:O	2.08	0.53
1:I:9:GLU:HA	1:J:11:VAL:O	2.09	0.53
1:Y:24:HIS:N	1:Y:25:PRO:HD3	2.24	0.53
1:A:33:ILE:HG12	1:Z:53:MET:HE3	93.02	0.53
1:K:9:GLU:HG2	1:L:11:VAL:HG23	2.00	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:24:HIS:N	1:T:25:PRO:HD3	2.22	0.53
1:E:31:LYS:NZ	1:V:37:ASP:HB2	46.22	0.53
1:J:24:HIS:N	1:J:25:PRO:HD3	2.24	0.53
1:S:87:GLU:HA	1:S:108:MET:HE1	1.93	0.53
1:K:31:LYS:CE	1:Y:27:GLU:OE1	111.12	0.53
1:A:87:GLU:HA	1:A:108:MET:HE1	1.90	0.53
1:E:9:GLU:HA	1:F:11:VAL:O	2.16	0.53
1:F:8:GLN:HE22	1:G:8:GLN:CD	74.07	0.53
1:J:50:GLU:HB2	1:K:45:THR:HG22	1.90	0.53
1:Q:8:GLN:CD	1:R:8:GLN:HB3	2.29	0.53
1:G:78:VAL:HG21	1:L:53:MET:HE1	1.89	0.53
1:M:11:VAL:O	1:R:9:GLU:HA	2.09	0.53
1:H:87:GLU:HA	1:H:108:MET:HE1	1.91	0.53
1:M:45:THR:HG22	1:R:50:GLU:HB2	1.91	0.53
1:M:9:GLU:HG2	1:N:11:VAL:HG23	2.14	0.53
1:F:37:ASP:OD2	1:U:31:LYS:NZ	37.92	0.52
1:M:8:GLN:CD	1:N:8:GLN:HB3	2.43	0.52
1:P:87:GLU:HA	1:P:108:MET:HE1	1.93	0.52
1:Y:112:LEU:O	1:Y:113:GLU:CB	2.53	0.52
1:P:50:GLU:HB2	1:Q:45:THR:HG22	1.91	0.52
1:P:35:VAL:HG21	1:P:41:ILE:CD1	2.19	0.52
1:S:112:LEU:O	1:S:113:GLU:CB	2.56	0.52
1:W:24:HIS:N	1:W:25:PRO:HD3	2.23	0.52
1:B:87:GLU:HA	1:B:108:MET:HE1	1.91	0.52
1:G:87:GLU:HA	1:G:108:MET:HE1	1.94	0.52
1:N:9:GLU:HA	1:O:11:VAL:O	2.10	0.52
1:H:8:GLN:HE22	1:I:8:GLN:CD	2.17	0.52
1:K:24:HIS:N	1:K:25:PRO:HD3	2.23	0.52
1:N:87:GLU:HA	1:N:108:MET:HE1	1.91	0.52
1:T:87:GLU:HA	1:T:108:MET:HE1	1.92	0.52
1:G:50:GLU:HB2	1:H:45:THR:CG2	2.40	0.52
1:G:9:GLU:HA	1:H:11:VAL:O	2.10	0.52
1:I:24:HIS:N	1:I:25:PRO:HD3	2.24	0.52
1:L:87:GLU:HA	1:L:108:MET:HE1	1.92	0.52
1:M:8:GLN:NE2	1:N:8:GLN:CD	2.63	0.52
1:S:50:GLU:HB2	1:T:45:THR:CG2	2.40	0.52
1:O:87:GLU:HA	1:O:108:MET:HE1	1.96	0.51
1:Q:87:GLU:HA	1:Q:108:MET:HE1	1.91	0.51
1:Q:8:GLN:NE2	1:R:8:GLN:CD	2.71	0.51
1:C:87:GLU:HA	1:C:108:MET:HE1	1.95	0.51
1:M:8:GLN:CD	1:R:8:GLN:NE2	2.64	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:87:GLU:HA	1:U:108:MET:HE1	1.92	0.51
1:A:53:MET:HE1	1:B:78:VAL:HG21	2.06	0.51
1:B:87:GLU:HG3	1:B:108:MET:CE	2.40	0.51
1:H:87:GLU:HG3	1:H:108:MET:CE	2.44	0.51
1:O:8:GLN:CD	1:P:8:GLN:HB3	2.31	0.51
1:P:8:GLN:HE22	1:Q:8:GLN:CD	2.14	0.51
1:F:50:GLU:CB	1:G:45:THR:HG22	74.66	0.51
1:I:87:GLU:HA	1:I:108:MET:HE1	1.93	0.51
1:O:53:MET:HE3	1:P:33:ILE:HG12	1.93	0.51
1:G:37:ASP:OD2	1:Q:31:LYS:CE	2.59	0.51
1:F:87:GLU:HA	1:F:108:MET:HE1	1.93	0.51
1:A:87:GLU:HG3	1:A:108:MET:CE	2.43	0.51
1:C:35:VAL:HG21	1:C:41:ILE:CD1	2.19	0.51
1:F:27:GLU:OE1	1:U:31:LYS:CE	38.42	0.51
1:M:87:GLU:HA	1:M:108:MET:HE1	1.93	0.51
1:V:87:GLU:HA	1:V:108:MET:HE1	1.93	0.51
1:F:27:GLU:HB2	1:U:31:LYS:HE2	36.93	0.51
1:K:53:MET:CE	1:L:33:ILE:HG23	2.40	0.51
1:X:87:GLU:HA	1:X:108:MET:HE1	1.93	0.51
1:K:87:GLU:HA	1:K:108:MET:HE1	1.93	0.50
1:W:35:VAL:HG21	1:W:41:ILE:CD1	2.21	0.50
1:A:35:VAL:HG21	1:A:41:ILE:CD1	2.23	0.50
1:O:35:VAL:HG21	1:O:41:ILE:CD1	2.22	0.50
1:O:50:GLU:HB2	1:P:45:THR:CG2	2.40	0.50
1:P:53:MET:HE3	1:Q:33:ILE:HG12	1.93	0.50
1:Q:87:GLU:HG3	1:Q:108:MET:CE	2.41	0.50
1:R:50:GLU:HB2	1:S:45:THR:CG2	80.68	0.50
1:U:35:VAL:HG21	1:U:41:ILE:CD1	2.21	0.50
1:A:33:ILE:HD11	1:Z:53:MET:HB3	91.80	0.50
1:J:87:GLU:HA	1:J:108:MET:HE1	1.93	0.50
1:D:37:ASP:HB3	1:L:31:LYS:NZ	76.09	0.50
1:K:8:GLN:CD	1:L:8:GLN:HB3	2.48	0.50
1:N:53:MET:CE	1:O:33:ILE:HG23	2.42	0.50
1:D:9:GLU:HG2	1:E:11:VAL:HG23	1.94	0.50
1:H:87:GLU:HG3	1:H:108:MET:HE2	2.05	0.50
1:D:37:ASP:CB	1:L:31:LYS:HZ2	75.38	0.50
1:D:87:GLU:HA	1:D:108:MET:HE1	1.93	0.50
1:C:57:ASP:HA	1:D:29:LEU:HD22	1.92	0.50
1:E:87:GLU:HA	1:E:108:MET:HE1	1.94	0.50
1:B:50:GLU:HB2	1:C:45:THR:CG2	2.55	0.50
1:E:45:THR:CG2	1:J:50:GLU:HB2	53.62	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:GLN:NE2	1:F:8:GLN:CD	2.69	0.50
1:T:87:GLU:HG3	1:T:108:MET:CE	2.44	0.50
1:C:8:GLN:NE2	1:D:8:GLN:CD	2.64	0.50
1:D:87:GLU:HG3	1:D:108:MET:CE	2.42	0.50
1:F:87:GLU:HG3	1:F:108:MET:CE	2.42	0.49
1:N:67:ILE:HB	1:O:32:LYS:HE3	2.11	0.49
1:O:87:GLU:HG3	1:O:108:MET:CE	2.44	0.49
1:P:67:ILE:HB	1:Q:32:LYS:HE3	1.94	0.49
1:S:87:GLU:HG3	1:S:108:MET:CE	2.42	0.49
1:J:35:VAL:HG21	1:J:41:ILE:CD1	2.21	0.49
1:K:53:MET:HB3	1:L:33:ILE:HD11	1.94	0.49
1:H:80:TYR:OH	1:O:31:LYS:HE2	2.12	0.49
1:D:50:GLU:HB2	1:Y:45:THR:CG2	91.73	0.49
1:T:9:GLU:HA	1:U:11:VAL:O	2.25	0.49
1:U:87:GLU:HG3	1:U:108:MET:CE	2.42	0.49
1:W:87:GLU:HA	1:W:108:MET:HE1	1.93	0.49
1:Z:87:GLU:HG3	1:Z:108:MET:CE	2.43	0.49
1:U:53:MET:CE	1:V:33:ILE:HG23	2.43	0.49
1:V:35:VAL:HG21	1:V:41:ILE:CD1	2.21	0.49
1:V:9:GLU:HA	1:W:11:VAL:O	2.12	0.49
1:A:45:THR:HG21	1:Z:48:PRO:HG2	84.75	0.49
1:B:8:GLN:NE2	1:C:8:GLN:CD	2.73	0.49
1:U:8:GLN:CD	1:V:8:GLN:HB3	2.37	0.49
1:G:67:ILE:HB	1:H:32:LYS:HE3	2.20	0.49
1:L:50:GLU:HB2	1:M:45:THR:CG2	46.10	0.49
1:L:87:GLU:HG3	1:L:108:MET:CE	2.43	0.49
1:R:87:GLU:HG3	1:R:108:MET:CE	2.45	0.49
1:Y:87:GLU:HA	1:Y:108:MET:HE1	1.94	0.49
1:A:45:THR:HG21	1:Z:48:PRO:CG	84.46	0.49
1:A:29:LEU:CD2	1:Z:57:ASP:HB2	91.85	0.49
1:E:50:GLU:HB2	1:F:45:THR:CG2	2.44	0.48
1:G:37:ASP:OD2	1:Q:31:LYS:HE2	2.13	0.48
1:J:9:GLU:HA	1:K:11:VAL:O	2.14	0.48
1:K:35:VAL:HG21	1:K:41:ILE:CD1	2.22	0.48
1:O:87:GLU:HG3	1:O:108:MET:HE2	1.97	0.48
1:N:53:MET:CE	1:O:33:ILE:HG12	2.43	0.48
1:A:8:GLN:CD	1:B:8:GLN:HB3	2.61	0.48
1:C:53:MET:HB3	1:D:33:ILE:HD11	1.95	0.48
1:S:8:GLN:CD	1:X:8:GLN:NE2	2.67	0.48
1:C:87:GLU:HG3	1:C:108:MET:CE	2.44	0.48
1:A:67:ILE:HB	1:B:32:LYS:HE3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:50:GLU:HB2	1:I:45:THR:HG22	2.03	0.48
1:W:57:ASP:CA	1:X:29:LEU:HD22	2.44	0.48
1:Y:9:GLU:HA	1:Z:11:VAL:O	2.12	0.48
1:A:17:THR:HB	1:A:45:THR:OG1	2.15	0.48
1:S:8:GLN:CD	1:T:8:GLN:HB3	2.52	0.48
1:V:87:GLU:HG3	1:V:108:MET:CE	2.44	0.48
1:X:35:VAL:HG21	1:X:41:ILE:CD1	2.21	0.48
1:C:35:VAL:CG2	1:C:41:ILE:HD11	2.20	0.48
1:D:87:GLU:HG3	1:D:108:MET:HE2	1.96	0.48
1:V:98:GLY:O	1:V:102:ASN:HA	2.14	0.48
1:E:87:GLU:HG3	1:E:108:MET:CE	2.44	0.48
1:H:35:VAL:HG21	1:H:41:ILE:CD1	2.23	0.48
1:N:87:GLU:HG3	1:N:108:MET:CE	2.43	0.48
1:P:87:GLU:HG3	1:P:108:MET:CE	2.43	0.48
1:U:8:GLN:NE2	1:V:8:GLN:CD	2.72	0.48
1:D:17:THR:HB	1:D:45:THR:OG1	2.18	0.47
1:J:17:THR:HB	1:J:45:THR:OG1	2.16	0.47
1:J:87:GLU:HG3	1:J:108:MET:CE	2.44	0.47
1:B:39:VAL:HG12	1:S:38:ALA:HB1	37.60	0.47
1:T:17:THR:HB	1:T:45:THR:OG1	2.15	0.47
1:Q:45:THR:CG2	1:V:50:GLU:HB2	57.45	0.47
1:Y:17:THR:HB	1:Y:45:THR:OG1	2.14	0.47
1:A:33:ILE:HG12	1:Z:53:MET:CE	92.08	0.47
1:H:17:THR:HB	1:H:45:THR:OG1	2.14	0.47
1:T:35:VAL:HG21	1:T:41:ILE:CD1	2.21	0.47
1:V:8:GLN:CD	1:W:8:GLN:HB3	2.34	0.47
1:Q:8:GLN:CD	1:V:8:GLN:NE2	78.70	0.47
1:V:53:MET:HE3	1:W:33:ILE:HG12	1.95	0.47
1:C:17:THR:HB	1:C:45:THR:OG1	2.15	0.47
1:I:53:MET:HE3	1:J:33:ILE:HG12	1.98	0.47
1:M:8:GLN:NE2	1:N:8:GLN:NE2	2.55	0.47
1:Q:98:GLY:O	1:Q:102:ASN:HA	2.15	0.47
1:R:35:VAL:HG21	1:R:41:ILE:CD1	2.24	0.47
1:Y:8:GLN:NE2	1:Z:8:GLN:NE2	2.54	0.47
1:E:78:VAL:HG21	1:J:53:MET:HE1	52.01	0.47
1:M:35:VAL:HG21	1:M:41:ILE:CD1	2.21	0.47
1:R:17:THR:HB	1:R:45:THR:OG1	2.17	0.47
1:U:50:GLU:HB2	1:V:45:THR:CG2	2.64	0.47
1:P:98:GLY:O	1:P:102:ASN:HA	2.18	0.47
1:R:98:GLY:O	1:R:102:ASN:HA	2.17	0.47
1:Y:67:ILE:HB	1:Z:32:LYS:HE3	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:GLN:OE1	1:Y:5:ARG:NH2	87.58	0.47
1:D:53:MET:HE1	1:Y:78:VAL:HG21	99.14	0.47
1:W:53:MET:CE	1:X:33:ILE:HG23	2.44	0.47
1:F:17:THR:HB	1:F:45:THR:OG1	2.16	0.47
1:G:17:THR:HB	1:G:45:THR:OG1	2.13	0.47
1:G:8:GLN:NE2	1:H:8:GLN:CD	2.68	0.47
1:X:87:GLU:HG3	1:X:108:MET:CE	2.45	0.47
1:Y:87:GLU:HG3	1:Y:108:MET:CE	2.45	0.47
1:Y:8:GLN:CD	1:Z:8:GLN:HB3	2.35	0.47
1:B:35:VAL:HG21	1:B:41:ILE:CD1	2.23	0.47
1:G:29:LEU:HB2	1:L:60:LEU:HD12	1.97	0.47
1:I:87:GLU:HG3	1:I:108:MET:CE	2.44	0.47
1:M:17:THR:HB	1:M:45:THR:OG1	2.16	0.47
1:F:37:ASP:OD2	1:U:31:LYS:CE	36.63	0.47
1:W:53:MET:HB3	1:X:33:ILE:HD11	1.97	0.47
1:A:87:GLU:HG3	1:A:108:MET:HE2	1.98	0.47
1:H:53:MET:HB3	1:I:33:ILE:HD11	2.09	0.47
1:I:8:GLN:CD	1:J:8:GLN:HB3	2.36	0.47
1:L:17:THR:HB	1:L:45:THR:OG1	2.14	0.47
1:M:87:GLU:HG3	1:M:108:MET:CE	2.45	0.47
1:P:35:VAL:CG2	1:P:41:ILE:HD11	2.21	0.47
1:Q:35:VAL:HG21	1:Q:41:ILE:CD1	2.20	0.47
1:X:98:GLY:O	1:X:102:ASN:HA	2.15	0.47
1:L:35:VAL:HG21	1:L:41:ILE:CD1	2.22	0.47
1:R:8:GLN:HE22	1:S:8:GLN:CD	75.10	0.47
1:V:17:THR:HB	1:V:45:THR:OG1	2.15	0.47
1:W:17:THR:HB	1:W:45:THR:OG1	2.14	0.47
1:E:33:ILE:HG12	1:J:53:MET:HE3	57.45	0.47
1:L:57:ASP:HA	1:M:29:LEU:HD22	46.07	0.47
1:S:87:GLU:HG3	1:S:108:MET:HE1	2.06	0.47
1:U:98:GLY:O	1:U:102:ASN:HA	2.20	0.46
1:S:33:ILE:HG23	1:X:53:MET:CE	2.45	0.46
1:A:8:GLN:NE2	1:Z:8:GLN:HE22	83.90	0.46
1:A:53:MET:HE3	1:B:33:ILE:HG12	1.97	0.46
1:E:17:THR:HB	1:E:45:THR:OG1	2.14	0.46
1:E:9:GLU:HG2	1:F:11:VAL:HG23	2.13	0.46
1:A:45:THR:CG2	1:F:50:GLU:HB2	2.44	0.46
1:G:45:THR:HG21	1:L:48:PRO:HG2	1.97	0.46
1:F:35:VAL:HG21	1:F:41:ILE:CD1	2.24	0.46
1:G:98:GLY:O	1:G:102:ASN:HA	2.18	0.46
1:K:98:GLY:O	1:K:102:ASN:HA	2.17	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:THR:HB	1:B:45:THR:OG1	2.15	0.46
1:G:87:GLU:HG3	1:G:108:MET:CE	2.46	0.46
1:H:48:PRO:HG2	1:I:45:THR:HG21	2.19	0.46
1:I:17:THR:HB	1:I:45:THR:OG1	2.15	0.46
1:H:98:GLY:O	1:H:102:ASN:HA	2.15	0.46
1:W:87:GLU:HG3	1:W:108:MET:CE	2.46	0.46
1:N:17:THR:HB	1:N:45:THR:OG1	2.15	0.46
1:G:27:GLU:CD	1:Q:31:LYS:HE3	2.34	0.46
1:S:8:GLN:NE2	1:T:8:GLN:CD	2.78	0.46
1:W:8:GLN:NE2	1:X:8:GLN:CD	2.68	0.46
1:Y:98:GLY:O	1:Y:102:ASN:HA	2.16	0.46
1:E:35:VAL:HG21	1:E:41:ILE:CD1	2.22	0.46
1:I:98:GLY:O	1:I:102:ASN:HA	2.16	0.46
1:E:11:VAL:HG23	1:J:9:GLU:HG2	57.40	0.46
1:P:17:THR:HB	1:P:45:THR:OG1	2.16	0.46
1:D:8:GLN:NE2	1:E:8:GLN:CD	2.69	0.46
1:M:98:GLY:O	1:M:102:ASN:HA	2.16	0.46
1:N:8:GLN:NE2	1:O:8:GLN:CD	2.93	0.46
1:N:53:MET:HB3	1:O:33:ILE:HD11	1.97	0.46
1:K:8:GLN:CD	1:P:8:GLN:HE22	68.69	0.46
1:C:87:GLU:HG3	1:C:108:MET:HE1	2.17	0.46
1:E:8:GLN:HB3	1:J:8:GLN:CD	70.57	0.46
1:F:98:GLY:O	1:F:102:ASN:HA	2.16	0.46
1:Q:17:THR:HB	1:Q:45:THR:OG1	2.16	0.46
1:S:33:ILE:HD11	1:X:53:MET:HB3	1.98	0.46
1:V:67:ILE:HB	1:W:32:LYS:HE3	1.98	0.46
1:G:35:VAL:HG21	1:G:41:ILE:CD1	2.23	0.46
1:N:98:GLY:O	1:N:102:ASN:HA	2.17	0.46
1:O:17:THR:HB	1:O:45:THR:OG1	2.16	0.46
1:U:17:THR:HB	1:U:45:THR:OG1	2.16	0.46
1:A:45:THR:HG22	1:Z:50:GLU:HB2	86.84	0.46
1:A:31:LYS:HE2	1:N:80:TYR:OH	77.43	0.45
1:E:8:GLN:CD	1:J:8:GLN:NE2	73.21	0.45
1:M:33:ILE:HG23	1:R:53:MET:CE	2.46	0.45
1:X:17:THR:HB	1:X:45:THR:OG1	2.16	0.45
1:C:87:GLU:HG3	1:C:108:MET:HE2	1.98	0.45
1:K:87:GLU:HG3	1:K:108:MET:CE	2.47	0.45
1:K:8:GLN:NE2	1:L:8:GLN:CD	2.71	0.45
1:L:31:LYS:HZ3	1:R:37:ASP:H	1.60	0.45
1:O:98:GLY:O	1:O:102:ASN:HA	2.18	0.45
1:S:11:VAL:HG23	1:X:9:GLU:HG2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:50:GLU:HB2	1:U:45:THR:CG2	2.47	0.45
1:K:17:THR:HB	1:K:45:THR:OG1	2.17	0.45
1:O:9:GLU:HG2	1:P:11:VAL:HG23	1.99	0.45
1:J:8:GLN:NE2	1:K:8:GLN:CD	2.68	0.45
1:K:87:GLU:HG3	1:K:108:MET:HE2	1.98	0.45
1:B:8:GLN:CD	1:C:8:GLN:HB3	2.37	0.45
1:D:50:GLU:HB2	1:E:45:THR:CG2	2.47	0.45
1:C:57:ASP:CA	1:D:29:LEU:HD22	2.47	0.45
1:G:29:LEU:HD22	1:L:57:ASP:CA	2.47	0.45
1:F:82:SER:HB2	1:K:87:GLU:OE1	2.16	0.45
1:G:33:ILE:HG23	1:L:53:MET:CE	2.47	0.45
1:L:98:GLY:O	1:L:102:ASN:HA	2.17	0.45
1:P:53:MET:HE1	1:Q:78:VAL:HG21	1.99	0.45
1:A:48:PRO:HG2	1:B:45:THR:HG21	2.16	0.45
1:A:8:GLN:NE2	1:B:8:GLN:CD	2.77	0.45
1:C:67:ILE:HD12	1:D:32:LYS:HG3	1.99	0.45
1:I:50:GLU:HB2	1:J:45:THR:CG2	2.47	0.45
1:O:35:VAL:CG2	1:O:41:ILE:HD11	2.23	0.45
1:P:53:MET:CE	1:Q:33:ILE:HG23	2.46	0.45
1:S:17:THR:HB	1:S:45:THR:OG1	2.16	0.45
1:U:87:GLU:HG3	1:U:108:MET:HE1	2.13	0.45
1:C:57:ASP:HB2	1:D:29:LEU:CD2	2.47	0.45
1:D:8:GLN:CD	1:E:8:GLN:HB3	2.37	0.45
1:N:8:GLN:NE2	1:O:8:GLN:NE2	2.84	0.45
1:Q:53:MET:CE	1:R:33:ILE:HG23	2.59	0.45
1:W:87:GLU:HG3	1:W:108:MET:HE2	1.98	0.45
1:Y:50:GLU:HB2	1:Z:45:THR:CG2	2.45	0.45
1:G:27:GLU:CD	1:Q:31:LYS:CG	2.82	0.45
1:T:98:GLY:O	1:T:102:ASN:HA	2.16	0.45
1:E:31:LYS:HZ3	1:V:37:ASP:H	45.33	0.45
1:W:98:GLY:O	1:W:102:ASN:HA	2.17	0.45
1:Z:35:VAL:HG21	1:Z:41:ILE:CD1	2.23	0.45
1:B:50:GLU:CB	1:C:45:THR:HG22	2.62	0.44
1:D:98:GLY:O	1:D:102:ASN:HA	2.18	0.44
1:F:27:GLU:CD	1:U:31:LYS:CG	36.28	0.44
1:P:87:GLU:HG3	1:P:108:MET:HE2	1.99	0.44
1:O:8:GLN:NE2	1:P:8:GLN:CD	2.70	0.44
1:C:8:GLN:OE1	1:D:8:GLN:HB3	2.35	0.44
1:G:33:ILE:HD11	1:L:53:MET:HB3	1.99	0.44
1:E:37:ASP:HB2	1:X:31:LYS:HZ1	1.82	0.44
1:G:27:GLU:HB2	1:Q:31:LYS:CE	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:57:ASP:HA	1:R:29:LEU:HD22	2.33	0.44
1:S:35:VAL:HG21	1:S:41:ILE:CD1	2.21	0.44
1:J:98:GLY:O	1:J:102:ASN:HA	2.17	0.44
1:W:57:ASP:HB2	1:X:29:LEU:CD2	2.47	0.44
1:E:98:GLY:O	1:E:102:ASN:HA	2.17	0.44
1:N:87:GLU:HG3	1:N:108:MET:HE1	2.00	0.44
1:Q:53:MET:HE1	1:R:78:VAL:HG21	2.34	0.44
1:D:35:VAL:HG21	1:D:41:ILE:CD1	2.23	0.44
1:P:57:ASP:HA	1:Q:29:LEU:HD22	1.99	0.44
1:F:9:GLU:HA	1:G:11:VAL:O	85.36	0.44
1:R:50:GLU:CB	1:S:45:THR:HG22	80.37	0.44
1:S:53:MET:HB3	1:T:33:ILE:HD11	2.07	0.44
1:V:50:GLU:HB2	1:W:45:THR:CG2	2.46	0.44
1:W:67:ILE:HD12	1:X:32:LYS:HG3	1.99	0.44
1:D:50:GLU:CB	1:Y:45:THR:HG22	92.54	0.44
1:A:98:GLY:O	1:A:102:ASN:HA	2.16	0.44
1:B:9:GLU:HG2	1:C:11:VAL:HG23	2.00	0.44
1:I:9:GLU:HG2	1:J:11:VAL:HG23	2.00	0.44
1:M:50:GLU:CB	1:N:45:THR:HG22	2.44	0.44
1:S:98:GLY:O	1:S:102:ASN:HA	2.18	0.44
1:Y:57:ASP:HA	1:Z:29:LEU:HD22	1.99	0.44
1:Z:17:THR:HB	1:Z:45:THR:OG1	2.18	0.44
1:C:98:GLY:O	1:C:102:ASN:HA	2.19	0.44
1:Q:35:VAL:CG2	1:Q:41:ILE:HD11	2.21	0.44
1:A:8:GLN:NE2	1:B:8:GLN:NE2	2.59	0.43
1:G:9:GLU:HG2	1:H:11:VAL:HG23	2.00	0.43
1:I:8:GLN:NE2	1:J:8:GLN:CD	2.71	0.43
1:M:48:PRO:HG2	1:N:45:THR:HG21	2.13	0.43
1:L:50:GLU:OE2	1:M:76:ALA:HB2	37.65	0.43
1:X:105:LEU:N	1:X:105:LEU:HD12	2.33	0.43
1:W:53:MET:HE3	1:X:33:ILE:HG12	2.01	0.43
1:Y:53:MET:HB3	1:Z:33:ILE:HD11	1.99	0.43
1:B:98:GLY:O	1:B:102:ASN:HA	2.19	0.43
1:E:87:GLU:HG3	1:E:108:MET:HE2	2.05	0.43
1:S:33:ILE:HG12	1:X:53:MET:CE	2.47	0.43
1:H:53:MET:CE	1:I:33:ILE:HG12	2.48	0.43
1:L:87:GLU:HG3	1:L:108:MET:HE2	2.06	0.43
1:B:87:GLU:HG3	1:B:108:MET:HE2	2.02	0.43
1:E:45:THR:HG22	1:J:50:GLU:CB	53.78	0.43
1:E:8:GLN:NE2	1:F:8:GLN:NE2	2.61	0.43
1:W:60:LEU:HD12	1:X:29:LEU:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLU:HB2	1:B:45:THR:CG2	2.51	0.43
1:L:9:GLU:HA	1:M:11:VAL:O	59.07	0.43
1:Q:87:GLU:HG3	1:Q:108:MET:HE2	2.05	0.43
1:T:87:GLU:HG3	1:T:108:MET:HE2	2.07	0.43
1:D:8:GLN:NE2	1:Y:8:GLN:NE2	80.34	0.43
1:D:8:GLN:HE22	1:Y:8:GLN:CD	80.83	0.43
1:F:27:GLU:HB2	1:U:31:LYS:CE	37.60	0.43
1:N:57:ASP:HB2	1:O:29:LEU:CD2	2.49	0.43
1:V:8:GLN:NE2	1:W:8:GLN:CD	2.72	0.43
1:I:35:VAL:CG2	1:I:41:ILE:HD11	2.21	0.43
1:L:53:MET:CE	1:M:33:ILE:HG23	36.28	0.43
1:B:105:LEU:HD12	1:B:105:LEU:N	2.36	0.43
1:G:8:GLN:HB3	1:L:8:GLN:CD	2.40	0.43
1:J:18:LEU:O	1:J:44:MET:HA	2.22	0.43
1:L:31:LYS:NZ	1:R:37:ASP:HB3	2.30	0.43
1:L:48:PRO:HG2	1:M:45:THR:HG21	48.61	0.43
1:I:31:LYS:NZ	1:N:80:TYR:OH	2.46	0.43
1:U:87:GLU:HG3	1:U:108:MET:HE2	1.99	0.43
1:G:8:GLN:CD	1:H:8:GLN:HB3	2.40	0.42
1:L:53:MET:HB3	1:M:33:ILE:HD11	40.46	0.42
1:S:45:THR:HG22	1:X:50:GLU:HB2	2.00	0.42
1:U:53:MET:HB3	1:V:33:ILE:HD11	2.01	0.42
1:D:31:LYS:HG3	1:S:27:GLU:OE2	2.20	0.42
1:E:50:GLU:CB	1:F:45:THR:HG22	2.49	0.42
1:L:60:LEU:HD12	1:M:29:LEU:HB2	42.39	0.42
1:T:50:GLU:OE2	1:U:76:ALA:HB2	2.18	0.42
1:E:36:PRO:HA	1:V:31:LYS:NZ	39.36	0.42
1:L:67:ILE:HB	1:M:32:LYS:HE3	28.75	0.42
1:M:35:VAL:CG2	1:M:41:ILE:HD11	2.21	0.42
1:K:33:ILE:HD11	1:P:53:MET:HB3	48.29	0.42
1:A:57:ASP:HA	1:B:29:LEU:HD22	2.00	0.42
1:O:105:LEU:N	1:O:105:LEU:HD12	2.38	0.42
1:P:9:GLU:HA	1:Q:11:VAL:O	2.20	0.42
1:E:31:LYS:NZ	1:V:37:ASP:HB3	47.08	0.42
1:K:67:ILE:HB	1:L:32:LYS:HE3	2.02	0.42
1:L:8:GLN:NE2	1:M:8:GLN:CD	69.75	0.42
1:S:3:LYS:HB3	1:S:4:GLU:H	1.74	0.42
1:U:53:MET:CE	1:V:33:ILE:HG12	2.45	0.42
1:E:3:LYS:HB3	1:E:4:GLU:H	1.74	0.42
1:G:8:GLN:CD	1:L:8:GLN:NE2	2.73	0.42
1:P:8:GLN:NE2	1:Q:8:GLN:CD	2.73	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:45:THR:HG22	1:V:50:GLU:CB	57.22	0.42
1:Z:98:GLY:O	1:Z:102:ASN:HA	2.19	0.42
1:E:31:LYS:HZ1	1:V:37:ASP:CA	45.88	0.42
1:G:105:LEU:HD12	1:G:105:LEU:N	2.37	0.42
1:Q:53:MET:CE	1:R:33:ILE:HG12	2.47	0.42
1:T:67:ILE:HB	1:U:32:LYS:HE3	2.02	0.42
1:J:3:LYS:HB3	1:J:4:GLU:H	1.75	0.42
1:D:37:ASP:CA	1:L:31:LYS:NZ	75.28	0.42
1:M:78:VAL:HG21	1:R:53:MET:HE1	2.01	0.42
1:M:8:GLN:NE2	1:R:8:GLN:NE2	2.57	0.42
1:P:18:LEU:O	1:P:44:MET:HA	2.24	0.42
1:Q:105:LEU:N	1:Q:105:LEU:HD12	2.39	0.42
1:W:53:MET:HE1	1:X:78:VAL:HG21	2.01	0.42
1:K:33:ILE:HG23	1:P:53:MET:CE	40.94	0.42
1:P:18:LEU:HG	1:P:45:THR:HG23	2.02	0.42
1:R:105:LEU:HD12	1:R:105:LEU:N	2.34	0.42
1:U:35:VAL:CG2	1:U:41:ILE:HD11	2.22	0.42
1:V:14:LYS:HD2	1:V:103:TYR:CE2	2.55	0.42
1:C:53:MET:HE1	1:D:78:VAL:HG21	2.01	0.42
1:G:32:LYS:HG3	1:L:67:ILE:HD12	2.02	0.42
1:S:18:LEU:O	1:S:44:MET:HA	2.24	0.42
1:Y:50:GLU:OE2	1:Z:76:ALA:HB2	2.20	0.42
1:C:48:PRO:HG2	1:D:45:THR:HG21	2.01	0.41
1:D:53:MET:HE3	1:Y:33:ILE:HG12	102.79	0.41
1:O:18:LEU:O	1:O:44:MET:HA	2.20	0.41
1:P:105:LEU:HD12	1:P:105:LEU:N	2.36	0.41
1:Q:48:PRO:HG2	1:R:45:THR:HG21	2.15	0.41
1:Q:8:GLN:NE2	1:V:8:GLN:NE2	79.28	0.41
1:W:48:PRO:HG2	1:X:45:THR:HG21	2.01	0.41
1:A:18:LEU:O	1:A:44:MET:HA	2.22	0.41
1:G:53:MET:HB3	1:H:33:ILE:HD11	2.12	0.41
1:K:50:GLU:HB2	1:L:45:THR:CG2	2.67	0.41
1:D:31:LYS:HE2	1:S:37:ASP:OD2	2.20	0.41
1:A:14:LYS:HD2	1:A:103:TYR:CE2	2.55	0.41
1:H:48:PRO:CG	1:I:45:THR:HG21	2.71	0.41
1:H:8:GLN:CD	1:I:8:GLN:HB3	2.57	0.41
1:L:18:LEU:O	1:L:44:MET:HA	2.20	0.41
1:G:76:ALA:HB2	1:L:50:GLU:OE2	2.20	0.41
1:K:11:VAL:O	1:P:9:GLU:HA	59.16	0.41
1:L:14:LYS:HD2	1:L:103:TYR:CE2	2.57	0.41
1:K:53:MET:CE	1:L:33:ILE:HG12	2.48	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:11:VAL:O	1:V:9:GLU:HA	70.58	0.41
1:C:105:LEU:HD12	1:C:105:LEU:N	2.35	0.41
1:G:14:LYS:HD2	1:G:103:TYR:CE2	2.56	0.41
1:L:31:LYS:HZ1	1:R:37:ASP:CA	2.32	0.41
1:O:50:GLU:CB	1:P:45:THR:HG22	2.46	0.41
1:S:105:LEU:HD12	1:S:105:LEU:N	2.38	0.41
1:S:53:MET:CE	1:T:33:ILE:HG23	2.59	0.41
1:Y:105:LEU:HD12	1:Y:105:LEU:N	2.36	0.41
1:A:29:LEU:HD22	1:Z:57:ASP:HA	93.36	0.41
1:G:45:THR:CG2	1:L:50:GLU:HB2	2.49	0.41
1:W:18:LEU:O	1:W:44:MET:HA	2.20	0.41
1:C:18:LEU:HG	1:C:45:THR:HG23	2.06	0.41
1:F:105:LEU:N	1:F:105:LEU:HD12	2.35	0.41
1:K:3:LYS:HB3	1:K:4:GLU:H	1.73	0.41
1:M:53:MET:CE	1:N:33:ILE:HG23	2.61	0.41
1:N:50:GLU:HB2	1:O:45:THR:HG22	2.02	0.41
1:Z:105:LEU:N	1:Z:105:LEU:HD12	2.36	0.41
1:G:18:LEU:HG	1:G:45:THR:HG23	2.07	0.41
1:I:87:GLU:HG3	1:I:108:MET:HE2	2.01	0.41
1:M:14:LYS:HD2	1:M:103:TYR:CE2	2.59	0.41
1:Y:53:MET:CE	1:Z:33:ILE:HG23	2.50	0.41
1:G:11:VAL:HG23	1:L:9:GLU:HG2	2.02	0.41
1:S:18:LEU:HG	1:S:45:THR:HG23	2.07	0.41
1:S:53:MET:HE1	1:T:78:VAL:HG21	2.03	0.41
1:A:29:LEU:HD22	1:Z:57:ASP:CA	92.71	0.41
1:K:45:THR:CG2	1:P:50:GLU:HB2	48.79	0.41
1:V:18:LEU:O	1:V:44:MET:HA	2.21	0.41
1:E:105:LEU:N	1:E:105:LEU:HD12	2.38	0.41
1:E:14:LYS:HD2	1:E:103:TYR:CE2	2.56	0.41
1:F:48:PRO:HG2	1:G:45:THR:HG21	73.63	0.41
1:G:27:GLU:OE1	1:Q:31:LYS:CE	2.52	0.41
1:G:50:GLU:CB	1:H:45:THR:HG22	2.45	0.41
1:Q:67:ILE:HB	1:R:32:LYS:HE3	2.47	0.41
1:V:105:LEU:HD12	1:V:105:LEU:N	2.35	0.41
1:B:18:LEU:O	1:B:44:MET:HA	2.21	0.40
1:T:50:GLU:CB	1:U:45:THR:HG22	2.53	0.40
1:V:94:VAL:CG1	1:V:105:LEU:HD23	2.48	0.40
1:A:53:MET:CE	1:B:33:ILE:HG23	2.52	0.40
1:H:18:LEU:HG	1:H:45:THR:HG23	2.03	0.40
1:M:53:MET:HB3	1:N:33:ILE:HD11	2.09	0.40
1:O:48:PRO:HG2	1:P:45:THR:HG21	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:8:GLN:OE1	1:P:8:GLN:HB3	2.22	0.40
1:P:53:MET:HB3	1:Q:33:ILE:HD11	2.04	0.40
1:U:50:GLU:CB	1:V:45:THR:HG22	2.70	0.40
1:W:9:GLU:HG2	1:X:11:VAL:HG23	2.04	0.40
1:C:31:LYS:CE	1:M:27:GLU:HB2	78.04	0.40
1:L:105:LEU:HD12	1:L:105:LEU:N	2.37	0.40
1:T:14:LYS:HD2	1:T:103:TYR:CE2	2.59	0.40
1:D:37:ASP:HB2	1:L:31:LYS:HZ2	74.91	0.40
1:H:105:LEU:HD12	1:H:105:LEU:N	2.37	0.40
1:J:14:LYS:HD2	1:J:103:TYR:CE2	2.56	0.40
1:K:57:ASP:HA	1:L:29:LEU:HD22	2.02	0.40
1:Q:18:LEU:O	1:Q:44:MET:HA	2.26	0.40
1:R:18:LEU:O	1:R:44:MET:HA	2.25	0.40
1:V:57:ASP:HA	1:W:29:LEU:HD22	2.03	0.40
1:Y:18:LEU:O	1:Y:44:MET:HA	2.22	0.40
1:C:50:GLU:HB2	1:D:45:THR:CG2	2.62	0.40
1:E:18:LEU:HG	1:E:45:THR:HG23	2.05	0.40
1:F:87:GLU:HG3	1:F:108:MET:HE1	2.03	0.40
1:G:3:LYS:HB3	1:G:4:GLU:H	1.73	0.40
1:I:53:MET:HE1	1:J:78:VAL:HG21	2.03	0.40
1:K:18:LEU:O	1:K:44:MET:HA	2.22	0.40
1:J:53:MET:CE	1:K:33:ILE:HG23	2.52	0.40
1:L:53:MET:HE3	1:M:33:ILE:HG12	35.64	0.40
1:Q:18:LEU:HG	1:Q:45:THR:HG23	2.04	0.40
1:M:32:LYS:HE3	1:R:67:ILE:HB	2.02	0.40
1:T:105:LEU:HD12	1:T:105:LEU:N	2.37	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	109/119 (92%)	109 (100%)	0	0	100	100
1	B	109/119 (92%)	107 (98%)	2 (2%)	0	100	100
1	C	109/119 (92%)	109 (100%)	0	0	100	100
1	D	109/119 (92%)	109 (100%)	0	0	100	100
1	E	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	F	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	G	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	H	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	I	109/119 (92%)	109 (100%)	0	0	100	100
1	J	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	K	109/119 (92%)	109 (100%)	0	0	100	100
1	L	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	M	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	N	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	O	109/119 (92%)	107 (98%)	2 (2%)	0	100	100
1	P	109/119 (92%)	109 (100%)	0	0	100	100
1	Q	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	R	109/119 (92%)	109 (100%)	0	0	100	100
1	S	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	T	109/119 (92%)	109 (100%)	0	0	100	100
1	U	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	V	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	W	109/119 (92%)	107 (98%)	2 (2%)	0	100	100
1	X	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	Y	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	Z	109/119 (92%)	109 (100%)	0	0	100	100
1	a	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	b	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	c	109/119 (92%)	109 (100%)	0	0	100	100
1	d	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	e	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	f	109/119 (92%)	108 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	g	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	h	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	i	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	j	109/119 (92%)	109 (100%)	0	0	100	100
1	k	109/119 (92%)	109 (100%)	0	0	100	100
1	l	109/119 (92%)	109 (100%)	0	0	100	100
1	m	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	n	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	o	109/119 (92%)	109 (100%)	0	0	100	100
1	p	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	q	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	r	109/119 (92%)	109 (100%)	0	0	100	100
1	s	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	t	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	u	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
1	v	109/119 (92%)	108 (99%)	1 (1%)	0	100	100
All	All	5232/5712 (92%)	5196 (99%)	36 (1%)	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	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	B	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	C	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	D	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	E	86/94 (92%)	83 (96%)	3 (4%)	43	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	G	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	H	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	I	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	J	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	K	86/94 (92%)	84 (98%)	2 (2%)	58	83
1	L	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	M	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	N	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	O	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	P	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	Q	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	R	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	S	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	T	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	U	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	V	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	W	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	X	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	Y	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	Z	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	a	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	b	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	c	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	d	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	e	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	f	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	g	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	h	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	i	86/94 (92%)	84 (98%)	2 (2%)	58	83
1	j	86/94 (92%)	84 (98%)	2 (2%)	58	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	k	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	l	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	m	86/94 (92%)	84 (98%)	2 (2%)	58	83
1	n	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	o	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	p	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	q	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	r	86/94 (92%)	84 (98%)	2 (2%)	58	83
1	s	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	t	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	u	86/94 (92%)	83 (96%)	3 (4%)	43	70
1	v	86/94 (92%)	84 (98%)	2 (2%)	58	83
All	All	4128/4512 (92%)	3990 (97%)	138 (3%)	45	73

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	91	SER
1	A	110	LYS
1	B	45	THR
1	B	91	SER
1	B	110	LYS
1	C	45	THR
1	C	91	SER
1	C	110	LYS
1	D	45	THR
1	D	91	SER
1	D	110	LYS
1	E	45	THR
1	E	91	SER
1	E	110	LYS
1	F	45	THR
1	F	91	SER
1	F	110	LYS
1	G	45	THR
1	G	91	SER
1	G	110	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	45	THR
1	H	91	SER
1	H	110	LYS
1	I	45	THR
1	I	91	SER
1	I	110	LYS
1	J	45	THR
1	J	91	SER
1	J	110	LYS
1	K	91	SER
1	K	110	LYS
1	L	45	THR
1	L	91	SER
1	L	110	LYS
1	M	45	THR
1	M	91	SER
1	M	110	LYS
1	N	45	THR
1	N	91	SER
1	N	110	LYS
1	O	45	THR
1	O	91	SER
1	O	110	LYS
1	P	45	THR
1	P	91	SER
1	P	110	LYS
1	Q	45	THR
1	Q	91	SER
1	Q	110	LYS
1	R	45	THR
1	R	91	SER
1	R	110	LYS
1	S	45	THR
1	S	91	SER
1	S	110	LYS
1	T	45	THR
1	T	91	SER
1	T	110	LYS
1	U	45	THR
1	U	91	SER
1	U	110	LYS
1	V	45	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	V	91	SER
1	V	110	LYS
1	W	45	THR
1	W	91	SER
1	W	110	LYS
1	X	45	THR
1	X	91	SER
1	X	110	LYS
1	Y	45	THR
1	Y	91	SER
1	Y	110	LYS
1	Z	45	THR
1	Z	91	SER
1	Z	110	LYS
1	a	45	THR
1	a	91	SER
1	a	110	LYS
1	b	45	THR
1	b	91	SER
1	b	110	LYS
1	c	45	THR
1	c	91	SER
1	c	110	LYS
1	d	45	THR
1	d	91	SER
1	d	110	LYS
1	e	45	THR
1	e	91	SER
1	e	110	LYS
1	f	45	THR
1	f	91	SER
1	f	110	LYS
1	g	45	THR
1	g	91	SER
1	g	110	LYS
1	h	45	THR
1	h	91	SER
1	h	110	LYS
1	i	91	SER
1	i	110	LYS
1	j	91	SER
1	j	110	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	k	45	THR
1	k	91	SER
1	k	110	LYS
1	l	45	THR
1	l	91	SER
1	l	110	LYS
1	m	91	SER
1	m	110	LYS
1	n	45	THR
1	n	91	SER
1	n	110	LYS
1	o	45	THR
1	o	91	SER
1	o	110	LYS
1	p	45	THR
1	p	91	SER
1	p	110	LYS
1	q	45	THR
1	q	91	SER
1	q	110	LYS
1	r	91	SER
1	r	110	LYS
1	s	45	THR
1	s	91	SER
1	s	110	LYS
1	t	45	THR
1	t	91	SER
1	t	110	LYS
1	u	45	THR
1	u	91	SER
1	u	110	LYS
1	v	91	SER
1	v	110	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	B	8	GLN
1	C	66	HIS
1	D	8	GLN
1	D	66	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	8	GLN
1	F	66	HIS
1	G	8	GLN
1	I	8	GLN
1	I	66	HIS
1	J	66	HIS
1	K	8	GLN
1	L	66	HIS
1	M	8	GLN
1	M	66	HIS
1	O	8	GLN
1	O	66	HIS
1	Q	8	GLN
1	Q	66	HIS
1	R	66	HIS
1	T	8	GLN
1	V	8	GLN
1	V	66	HIS
1	W	66	HIS
1	X	8	GLN
1	Y	8	GLN
1	Y	66	HIS
1	Z	66	HIS
1	a	8	GLN
1	a	66	HIS
1	b	66	HIS
1	c	8	GLN
1	c	66	HIS
1	d	66	HIS
1	e	66	HIS
1	f	8	GLN
1	g	66	HIS
1	h	8	GLN
1	h	66	HIS
1	j	8	GLN
1	j	66	HIS
1	k	8	GLN
1	l	66	HIS
1	m	8	GLN
1	o	8	GLN
1	o	66	HIS
1	q	8	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	r	66	HIS
1	s	8	GLN
1	t	66	HIS
1	u	8	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	111/119 (93%)	1.12	11 (9%) 9 10	53, 64, 90, 105	0
1	B	111/119 (93%)	1.24	17 (15%) 3 3	53, 63, 90, 107	0
1	C	111/119 (93%)	1.16	17 (15%) 3 3	54, 64, 90, 109	0
1	D	111/119 (93%)	1.09	16 (14%) 3 3	54, 64, 91, 106	0
1	E	111/119 (93%)	1.19	19 (17%) 2 2	50, 64, 89, 107	0
1	F	111/119 (93%)	1.12	20 (18%) 2 2	52, 62, 89, 107	0
1	G	111/119 (93%)	1.07	16 (14%) 3 3	52, 64, 89, 108	0
1	H	111/119 (93%)	1.07	18 (16%) 3 2	52, 63, 90, 104	0
1	I	111/119 (93%)	1.02	11 (9%) 9 10	52, 63, 89, 106	0
1	J	111/119 (93%)	1.20	16 (14%) 3 3	54, 63, 90, 106	0
1	K	111/119 (93%)	1.09	14 (12%) 5 5	51, 62, 91, 104	0
1	L	111/119 (93%)	1.08	8 (7%) 18 20	54, 62, 88, 106	0
1	M	111/119 (93%)	1.06	13 (11%) 6 6	51, 63, 89, 108	0
1	N	111/119 (93%)	1.14	19 (17%) 2 2	53, 64, 90, 105	0
1	O	111/119 (93%)	1.16	13 (11%) 6 6	53, 64, 88, 106	0
1	P	111/119 (93%)	1.14	13 (11%) 6 6	53, 63, 90, 107	0
1	Q	111/119 (93%)	1.13	15 (13%) 4 4	53, 64, 90, 106	0
1	R	111/119 (93%)	1.09	9 (8%) 15 16	52, 63, 89, 104	0
1	S	111/119 (93%)	1.24	21 (18%) 2 1	53, 65, 91, 108	0
1	T	111/119 (93%)	1.08	8 (7%) 18 20	51, 63, 90, 107	0
1	U	111/119 (93%)	1.11	13 (11%) 6 6	51, 63, 90, 105	0
1	V	111/119 (93%)	0.85	7 (6%) 23 26	53, 63, 90, 105	0
1	W	111/119 (93%)	0.98	9 (8%) 15 16	49, 63, 91, 105	0
1	X	111/119 (93%)	1.13	17 (15%) 3 3	54, 64, 91, 106	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	Y	111/119 (93%)	1.10	17 (15%) 3 3	51, 63, 89, 106	0
1	Z	111/119 (93%)	1.22	21 (18%) 2 1	53, 63, 90, 106	0
1	a	111/119 (93%)	1.11	18 (16%) 3 2	52, 63, 89, 107	0
1	b	111/119 (93%)	1.13	15 (13%) 4 4	54, 64, 91, 107	0
1	c	111/119 (93%)	1.10	12 (10%) 8 8	52, 64, 89, 103	0
1	d	111/119 (93%)	1.06	15 (13%) 4 4	53, 63, 90, 104	0
1	e	111/119 (93%)	1.01	13 (11%) 6 6	54, 63, 90, 106	0
1	f	111/119 (93%)	1.35	24 (21%) 1 1	54, 64, 90, 106	0
1	g	111/119 (93%)	1.12	17 (15%) 3 3	50, 64, 90, 107	0
1	h	111/119 (93%)	1.05	13 (11%) 6 6	50, 63, 90, 106	0
1	i	111/119 (93%)	1.02	12 (10%) 8 8	53, 64, 91, 105	0
1	j	111/119 (93%)	0.99	10 (9%) 12 12	50, 63, 90, 107	0
1	k	111/119 (93%)	1.04	11 (9%) 9 10	53, 63, 90, 103	0
1	l	111/119 (93%)	1.02	9 (8%) 15 16	53, 63, 88, 106	0
1	m	111/119 (93%)	1.07	16 (14%) 3 3	51, 64, 90, 108	0
1	n	111/119 (93%)	1.03	13 (11%) 6 6	53, 63, 89, 106	0
1	o	111/119 (93%)	1.03	13 (11%) 6 6	54, 63, 90, 106	0
1	p	111/119 (93%)	1.17	16 (14%) 3 3	53, 63, 91, 107	0
1	q	111/119 (93%)	1.05	15 (13%) 4 4	52, 63, 89, 107	0
1	r	111/119 (93%)	1.32	21 (18%) 2 1	53, 64, 90, 104	0
1	s	111/119 (93%)	1.43	28 (25%) 1 1	51, 64, 90, 106	0
1	t	111/119 (93%)	1.18	14 (12%) 5 5	54, 63, 89, 108	0
1	u	111/119 (93%)	1.10	11 (9%) 9 10	54, 64, 90, 108	0
1	v	111/119 (93%)	1.11	15 (13%) 4 4	52, 64, 90, 105	0
All	All	5328/5712 (93%)	1.11	709 (13%) 4 4	49, 64, 91, 109	0

All (709) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	81	GLY	6.6
1	L	81	GLY	6.5
1	P	38	ALA	6.3
1	b	81	GLY	6.2
1	W	81	GLY	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	112	LEU	5.5
1	s	38	ALA	5.5
1	C	38	ALA	5.5
1	f	19	ALA	5.5
1	l	67	ILE	5.3
1	G	67	ILE	5.3
1	k	81	GLY	5.2
1	T	3	LYS	5.2
1	t	81	GLY	5.1
1	o	112	LEU	5.0
1	o	81	GLY	4.9
1	G	3	LYS	4.9
1	r	59	ALA	4.9
1	n	112	LEU	4.8
1	T	81	GLY	4.7
1	Y	97	LEU	4.7
1	d	30	ALA	4.7
1	T	67	ILE	4.7
1	C	112	LEU	4.6
1	L	67	ILE	4.6
1	u	81	GLY	4.5
1	i	112	LEU	4.5
1	s	37	ASP	4.5
1	O	38	ALA	4.5
1	k	70	LEU	4.5
1	t	38	ALA	4.4
1	A	36	PRO	4.4
1	E	108	MET	4.4
1	M	81	GLY	4.3
1	O	67	ILE	4.3
1	m	3	LYS	4.3
1	s	81	GLY	4.3
1	c	8	GLN	4.3
1	f	79	ILE	4.3
1	o	90	LEU	4.3
1	V	59	ALA	4.2
1	H	112	LEU	4.1
1	r	70	LEU	4.1
1	u	30	ALA	4.1
1	P	67	ILE	4.1
1	Z	67	ILE	4.1
1	B	90	LEU	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	19	ALA	4.0
1	s	8	GLN	4.0
1	A	112	LEU	4.0
1	N	38	ALA	4.0
1	b	6	ILE	4.0
1	b	67	ILE	3.9
1	q	81	GLY	3.9
1	e	67	ILE	3.9
1	I	112	LEU	3.9
1	M	67	ILE	3.9
1	v	81	GLY	3.9
1	S	67	ILE	3.9
1	f	30	ALA	3.9
1	p	112	LEU	3.8
1	K	81	GLY	3.8
1	u	67	ILE	3.8
1	r	36	PRO	3.8
1	E	90	LEU	3.8
1	m	67	ILE	3.8
1	J	112	LEU	3.8
1	r	37	ASP	3.8
1	C	81	GLY	3.8
1	A	70	LEU	3.8
1	Z	90	LEU	3.8
1	S	14	LYS	3.7
1	m	7	ILE	3.7
1	Y	67	ILE	3.7
1	B	19	ALA	3.7
1	I	34	GLY	3.7
1	C	67	ILE	3.7
1	r	97	LEU	3.7
1	C	16	VAL	3.7
1	r	112	LEU	3.7
1	F	13	GLY	3.7
1	m	66	HIS	3.7
1	r	67	ILE	3.7
1	c	3	LYS	3.7
1	R	81	GLY	3.7
1	f	81	GLY	3.7
1	Z	112	LEU	3.6
1	P	17	THR	3.6
1	g	38	ALA	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	30	ALA	3.6
1	l	7	ILE	3.6
1	D	36	PRO	3.6
1	f	7	ILE	3.6
1	s	65	VAL	3.6
1	j	7	ILE	3.5
1	D	81	GLY	3.5
1	J	30	ALA	3.5
1	s	19	ALA	3.5
1	I	81	GLY	3.5
1	a	65	VAL	3.5
1	Z	111	SER	3.5
1	J	81	GLY	3.5
1	M	46	LEU	3.5
1	m	105	LEU	3.5
1	W	7	ILE	3.5
1	F	38	ALA	3.5
1	a	25	PRO	3.5
1	Z	37	ASP	3.4
1	U	35	VAL	3.4
1	O	19	ALA	3.4
1	t	36	PRO	3.4
1	d	43	ILE	3.4
1	D	17	THR	3.4
1	f	67	ILE	3.4
1	M	112	LEU	3.4
1	a	90	LEU	3.4
1	U	28	GLU	3.4
1	e	6	ILE	3.4
1	q	22	ILE	3.4
1	U	70	LEU	3.3
1	n	22	ILE	3.3
1	T	38	ALA	3.3
1	W	112	LEU	3.3
1	o	52	ALA	3.3
1	N	28	GLU	3.3
1	T	8	GLN	3.3
1	H	36	PRO	3.3
1	N	105	LEU	3.3
1	v	108	MET	3.3
1	H	25	PRO	3.3
1	J	36	PRO	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	q	46	LEU	3.3
1	t	97	LEU	3.3
1	v	22	ILE	3.3
1	B	37	ASP	3.3
1	B	25	PRO	3.3
1	F	36	PRO	3.3
1	O	97	LEU	3.3
1	b	14	LYS	3.3
1	J	84	GLY	3.3
1	R	97	LEU	3.3
1	u	43	ILE	3.3
1	f	104	THR	3.2
1	r	106	CYS	3.2
1	D	80	TYR	3.2
1	X	11	VAL	3.2
1	g	81	GLY	3.2
1	a	81	GLY	3.2
1	Z	85	ALA	3.2
1	E	111	SER	3.2
1	v	111	SER	3.2
1	d	8	GLN	3.2
1	j	16	VAL	3.2
1	Y	3	LYS	3.2
1	N	108	MET	3.2
1	B	32	LYS	3.2
1	Q	8	GLN	3.2
1	O	90	LEU	3.2
1	a	19	ALA	3.1
1	h	35	VAL	3.1
1	t	14	LYS	3.1
1	X	44	MET	3.1
1	H	21	LEU	3.1
1	h	17	THR	3.1
1	b	108	MET	3.1
1	m	78	VAL	3.1
1	B	81	GLY	3.1
1	n	67	ILE	3.1
1	Z	52	ALA	3.1
1	B	67	ILE	3.1
1	D	43	ILE	3.1
1	H	67	ILE	3.1
1	Z	108	MET	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	d	67	ILE	3.1
1	o	3	LYS	3.1
1	u	8	GLN	3.1
1	Z	77	LEU	3.1
1	c	59	ALA	3.1
1	r	19	ALA	3.1
1	P	22	ILE	3.1
1	A	59	ALA	3.1
1	T	112	LEU	3.1
1	i	65	VAL	3.1
1	f	43	ILE	3.0
1	G	96	GLY	3.0
1	d	104	THR	3.0
1	e	55	ALA	3.0
1	c	67	ILE	3.0
1	P	105	LEU	3.0
1	a	55	ALA	3.0
1	g	54	ILE	3.0
1	g	67	ILE	3.0
1	C	14	LYS	3.0
1	h	90	LEU	3.0
1	n	113	GLU	3.0
1	u	7	ILE	3.0
1	Z	3	LYS	3.0
1	H	59	ALA	3.0
1	i	95	SER	3.0
1	Q	59	ALA	3.0
1	R	104	THR	3.0
1	Y	101	LEU	3.0
1	g	92	GLN	3.0
1	J	90	LEU	3.0
1	f	18	LEU	3.0
1	X	81	GLY	3.0
1	h	81	GLY	3.0
1	H	43	ILE	2.9
1	U	90	LEU	2.9
1	C	22	ILE	2.9
1	G	22	ILE	2.9
1	J	67	ILE	2.9
1	e	7	ILE	2.9
1	i	7	ILE	2.9
1	K	106	CYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	62	ALA	2.9
1	N	52	ALA	2.9
1	g	36	PRO	2.9
1	o	38	ALA	2.9
1	R	80	TYR	2.9
1	Z	44	MET	2.9
1	Q	43	ILE	2.9
1	n	43	ILE	2.9
1	q	54	ILE	2.9
1	k	7	ILE	2.9
1	N	32	LYS	2.9
1	S	106	CYS	2.9
1	S	43	ILE	2.9
1	q	112	LEU	2.9
1	D	24	HIS	2.9
1	K	7	ILE	2.9
1	Z	38	ALA	2.9
1	B	66	HIS	2.9
1	a	32	LYS	2.9
1	k	112	LEU	2.9
1	u	16	VAL	2.8
1	q	97	LEU	2.8
1	Q	80	TYR	2.8
1	l	81	GLY	2.8
1	p	16	VAL	2.8
1	K	32	LYS	2.8
1	E	67	ILE	2.8
1	V	43	ILE	2.8
1	p	54	ILE	2.8
1	p	67	ILE	2.8
1	f	105	LEU	2.8
1	L	37	ASP	2.8
1	u	80	TYR	2.8
1	G	66	HIS	2.8
1	J	54	ILE	2.8
1	f	55	ALA	2.8
1	N	37	ASP	2.8
1	O	96	GLY	2.8
1	d	13	GLY	2.8
1	N	39	VAL	2.8
1	W	67	ILE	2.8
1	C	21	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	111	SER	2.8
1	C	3	LYS	2.8
1	O	36	PRO	2.8
1	q	16	VAL	2.8
1	e	54	ILE	2.8
1	B	28	GLU	2.8
1	E	21	LEU	2.8
1	s	111	SER	2.8
1	Y	44	MET	2.8
1	p	36	PRO	2.8
1	g	17	THR	2.8
1	i	59	ALA	2.8
1	D	99	ARG	2.8
1	D	37	ASP	2.8
1	E	25	PRO	2.8
1	E	65	VAL	2.7
1	h	16	VAL	2.7
1	E	69	PHE	2.7
1	K	70	LEU	2.7
1	P	112	LEU	2.7
1	f	97	LEU	2.7
1	r	44	MET	2.7
1	N	81	GLY	2.7
1	S	41	ILE	2.7
1	V	70	LEU	2.7
1	p	97	LEU	2.7
1	e	110	LYS	2.7
1	f	56	GLY	2.7
1	E	6	ILE	2.7
1	T	79	ILE	2.7
1	S	105	LEU	2.7
1	r	11	VAL	2.7
1	p	90	LEU	2.7
1	C	113	GLU	2.7
1	V	36	PRO	2.7
1	D	30	ALA	2.7
1	s	55	ALA	2.7
1	S	66	HIS	2.7
1	Q	81	GLY	2.7
1	G	27	GLU	2.7
1	v	30	ALA	2.7
1	f	66	HIS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	r	60	LEU	2.7
1	Q	110	LYS	2.7
1	r	81	GLY	2.7
1	s	83	VAL	2.6
1	N	90	LEU	2.6
1	j	6	ILE	2.6
1	k	25	PRO	2.6
1	X	8	GLN	2.6
1	J	16	VAL	2.6
1	Y	91	SER	2.6
1	n	21	LEU	2.6
1	D	8	GLN	2.6
1	K	113	GLU	2.6
1	i	81	GLY	2.6
1	X	101	LEU	2.6
1	L	36	PRO	2.6
1	Q	65	VAL	2.6
1	s	92	GLN	2.6
1	Q	70	LEU	2.6
1	R	46	LEU	2.6
1	s	70	LEU	2.6
1	M	48	PRO	2.6
1	f	8	GLN	2.6
1	g	39	VAL	2.6
1	r	62	ALA	2.6
1	s	16	VAL	2.6
1	I	105	LEU	2.6
1	X	112	LEU	2.6
1	A	67	ILE	2.6
1	N	55	ALA	2.6
1	Y	19	ALA	2.6
1	F	39	VAL	2.6
1	q	21	LEU	2.6
1	S	44	MET	2.6
1	f	44	MET	2.6
1	H	111	SER	2.6
1	q	13	GLY	2.6
1	D	63	ALA	2.5
1	M	52	ALA	2.5
1	b	17	THR	2.5
1	e	93	THR	2.5
1	H	90	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	Z	32	LYS	2.5
1	e	46	LEU	2.5
1	a	67	ILE	2.5
1	t	67	ILE	2.5
1	H	19	ALA	2.5
1	s	30	ALA	2.5
1	g	112	LEU	2.5
1	t	78	VAL	2.5
1	G	81	GLY	2.5
1	A	111	SER	2.5
1	P	14	LYS	2.5
1	j	47	THR	2.5
1	N	77	LEU	2.5
1	b	29	LEU	2.5
1	D	79	ILE	2.5
1	S	81	GLY	2.5
1	j	81	GLY	2.5
1	p	43	ILE	2.5
1	s	106	CYS	2.5
1	M	101	LEU	2.5
1	a	39	VAL	2.5
1	r	14	LYS	2.5
1	s	97	LEU	2.5
1	d	111	SER	2.5
1	G	44	MET	2.5
1	B	18	LEU	2.5
1	S	108	MET	2.5
1	Q	85	ALA	2.5
1	B	77	LEU	2.5
1	G	11	VAL	2.5
1	J	35	VAL	2.5
1	a	28	GLU	2.5
1	v	39	VAL	2.5
1	C	7	ILE	2.5
1	E	43	ILE	2.5
1	J	44	MET	2.5
1	M	36	PRO	2.5
1	i	66	HIS	2.4
1	d	112	LEU	2.4
1	k	97	LEU	2.4
1	M	80	TYR	2.4
1	g	79	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	q	7	ILE	2.4
1	u	37	ASP	2.4
1	J	113	GLU	2.4
1	G	21	LEU	2.4
1	h	112	LEU	2.4
1	l	21	LEU	2.4
1	o	16	VAL	2.4
1	o	35	VAL	2.4
1	s	39	VAL	2.4
1	s	78	VAL	2.4
1	o	9	GLU	2.4
1	c	36	PRO	2.4
1	m	30	ALA	2.4
1	s	52	ALA	2.4
1	J	18	LEU	2.4
1	J	101	LEU	2.4
1	D	57	ASP	2.4
1	F	43	ILE	2.4
1	X	67	ILE	2.4
1	l	108	MET	2.4
1	E	81	GLY	2.4
1	N	76	ALA	2.4
1	b	30	ALA	2.4
1	F	97	LEU	2.4
1	P	29	LEU	2.4
1	Z	105	LEU	2.4
1	Q	7	ILE	2.4
1	b	80	TYR	2.4
1	S	34	GLY	2.4
1	b	26	GLY	2.4
1	O	48	PRO	2.4
1	R	36	PRO	2.4
1	b	87	GLU	2.4
1	N	97	LEU	2.4
1	Y	46	LEU	2.4
1	n	90	LEU	2.4
1	E	22	ILE	2.4
1	m	79	ILE	2.4
1	g	25	PRO	2.4
1	E	30	ALA	2.4
1	O	37	ASP	2.4
1	F	111	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	d	46	LEU	2.4
1	B	65	VAL	2.4
1	U	81	GLY	2.4
1	b	113	GLU	2.4
1	h	88	GLU	2.4
1	m	96	GLY	2.4
1	S	79	ILE	2.4
1	X	25	PRO	2.4
1	c	41	ILE	2.4
1	i	80	TYR	2.4
1	p	48	PRO	2.4
1	X	37	ASP	2.4
1	Y	52	ALA	2.4
1	q	23	ALA	2.4
1	S	97	LEU	2.4
1	F	81	GLY	2.3
1	H	79	ILE	2.3
1	P	79	ILE	2.3
1	e	37	ASP	2.3
1	i	79	ILE	2.3
1	t	79	ILE	2.3
1	R	111	SER	2.3
1	F	101	LEU	2.3
1	G	78	VAL	2.3
1	S	24	HIS	2.3
1	F	25	PRO	2.3
1	l	37	ASP	2.3
1	n	48	PRO	2.3
1	m	22	ILE	2.3
1	v	8	GLN	2.3
1	I	32	LYS	2.3
1	c	105	LEU	2.3
1	f	70	LEU	2.3
1	H	113	GLU	2.3
1	N	57	ASP	2.3
1	U	113	GLU	2.3
1	B	16	VAL	2.3
1	D	39	VAL	2.3
1	o	78	VAL	2.3
1	Z	106	CYS	2.3
1	F	7	ILE	2.3
1	Z	22	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	s	67	ILE	2.3
1	N	85	ALA	2.3
1	t	111	SER	2.3
1	m	21	LEU	2.3
1	n	46	LEU	2.3
1	o	70	LEU	2.3
1	M	86	VAL	2.3
1	S	65	VAL	2.3
1	k	11	VAL	2.3
1	C	44	MET	2.3
1	a	44	MET	2.3
1	F	22	ILE	2.3
1	J	22	ILE	2.3
1	S	104	THR	2.3
1	s	90	LEU	2.3
1	v	112	LEU	2.3
1	U	36	PRO	2.3
1	X	86	VAL	2.3
1	g	44	MET	2.3
1	o	43	ILE	2.3
1	s	43	ILE	2.3
1	C	95	SER	2.3
1	F	23	ALA	2.3
1	l	76	ALA	2.3
1	s	80	TYR	2.3
1	F	70	LEU	2.3
1	G	46	LEU	2.3
1	K	46	LEU	2.3
1	O	66	HIS	2.3
1	a	36	PRO	2.3
1	l	36	PRO	2.3
1	C	110	LYS	2.3
1	f	14	LYS	2.3
1	H	81	GLY	2.3
1	I	67	ILE	2.3
1	f	54	ILE	2.3
1	v	79	ILE	2.3
1	g	63	ALA	2.3
1	q	40	ALA	2.3
1	E	109	THR	2.3
1	s	24	HIS	2.3
1	j	46	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	v	46	LEU	2.3
1	X	110	LYS	2.2
1	g	3	LYS	2.2
1	R	86	VAL	2.2
1	U	8	GLN	2.2
1	h	19	ALA	2.2
1	u	63	ALA	2.2
1	E	70	LEU	2.2
1	K	21	LEU	2.2
1	S	77	LEU	2.2
1	m	46	LEU	2.2
1	v	90	LEU	2.2
1	b	75	GLY	2.2
1	E	16	VAL	2.2
1	I	44	MET	2.2
1	d	22	ILE	2.2
1	j	67	ILE	2.2
1	n	6	ILE	2.2
1	q	52	ALA	2.2
1	r	89	ALA	2.2
1	s	79	ILE	2.2
1	c	24	HIS	2.2
1	Z	70	LEU	2.2
1	e	105	LEU	2.2
1	B	3	LYS	2.2
1	B	39	VAL	2.2
1	I	35	VAL	2.2
1	Y	86	VAL	2.2
1	q	94	VAL	2.2
1	L	7	ILE	2.2
1	k	79	ILE	2.2
1	U	77	LEU	2.2
1	X	97	LEU	2.2
1	d	97	LEU	2.2
1	g	97	LEU	2.2
1	t	57	ASP	2.2
1	V	95	SER	2.2
1	S	39	VAL	2.2
1	m	63	ALA	2.2
1	n	76	ALA	2.2
1	r	28	GLU	2.2
1	F	37	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	P	36	PRO	2.2
1	i	48	PRO	2.2
1	p	95	SER	2.2
1	O	44	MET	2.2
1	c	85	ALA	2.2
1	j	59	ALA	2.2
1	I	43	ILE	2.2
1	s	22	ILE	2.2
1	M	49	GLY	2.2
1	X	21	LEU	2.2
1	Y	13	GLY	2.2
1	Z	36	PRO	2.2
1	m	97	LEU	2.2
1	W	80	TYR	2.2
1	W	8	GLN	2.2
1	R	67	ILE	2.2
1	E	112	LEU	2.2
1	J	21	LEU	2.2
1	h	100	LEU	2.2
1	I	3	LYS	2.1
1	Q	24	HIS	2.1
1	d	80	TYR	2.1
1	M	39	VAL	2.1
1	A	30	ALA	2.1
1	U	76	ALA	2.1
1	p	30	ALA	2.1
1	t	63	ALA	2.1
1	K	22	ILE	2.1
1	S	7	ILE	2.1
1	p	79	ILE	2.1
1	r	43	ILE	2.1
1	r	84	GLY	2.1
1	G	97	LEU	2.1
1	K	90	LEU	2.1
1	U	29	LEU	2.1
1	s	46	LEU	2.1
1	U	32	LYS	2.1
1	O	111	SER	2.1
1	k	8	GLN	2.1
1	a	64	ASP	2.1
1	L	16	VAL	2.1
1	T	4	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	a	93	THR	2.1
1	n	25	PRO	2.1
1	F	46	LEU	2.1
1	L	8	GLN	2.1
1	c	112	LEU	2.1
1	g	8	GLN	2.1
1	r	18	LEU	2.1
1	f	107	GLU	2.1
1	I	108	MET	2.1
1	A	106	CYS	2.1
1	G	39	VAL	2.1
1	v	59	ALA	2.1
1	Q	41	ILE	2.1
1	S	36	PRO	2.1
1	Y	54	ILE	2.1
1	F	21	LEU	2.1
1	L	77	LEU	2.1
1	j	112	LEU	2.1
1	D	9	GLU	2.1
1	F	24	HIS	2.1
1	u	57	ASP	2.1
1	Y	81	GLY	2.1
1	D	103	TYR	2.1
1	X	55	ALA	2.1
1	a	76	ALA	2.1
1	N	6	ILE	2.1
1	Y	79	ILE	2.1
1	p	7	ILE	2.1
1	v	6	ILE	2.1
1	Q	21	LEU	2.1
1	Q	112	LEU	2.1
1	d	77	LEU	2.1
1	h	70	LEU	2.1
1	n	10	PHE	2.1
1	v	69	PHE	2.1
1	P	66	HIS	2.1
1	m	81	GLY	2.1
1	o	49	GLY	2.1
1	E	44	MET	2.1
1	p	44	MET	2.1
1	U	39	VAL	2.1
1	W	52	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	X	59	ALA	2.1
1	c	55	ALA	2.1
1	h	94	VAL	2.1
1	l	59	ALA	2.1
1	q	85	ALA	2.1
1	P	48	PRO	2.1
1	Y	103	TYR	2.1
1	C	57	ASP	2.1
1	K	43	ILE	2.1
1	a	57	ASP	2.1
1	k	6	ILE	2.1
1	F	100	LEU	2.1
1	K	111	SER	2.1
1	O	106	CYS	2.1
1	Q	66	HIS	2.1
1	d	70	LEU	2.1
1	h	65	VAL	2.1
1	G	79	ILE	2.1
1	X	54	ILE	2.1
1	r	66	HIS	2.1
1	t	22	ILE	2.1
1	t	24	HIS	2.1
1	V	18	LEU	2.1
1	V	90	LEU	2.1
1	i	111	SER	2.1
1	S	28	GLU	2.1
1	s	113	GLU	2.1
1	N	44	MET	2.0
1	G	57	ASP	2.0
1	N	25	PRO	2.0
1	W	37	ASP	2.0
1	k	30	ALA	2.0
1	W	16	VAL	2.0
1	e	39	VAL	2.0
1	H	6	ILE	2.0
1	H	80	TYR	2.0
1	K	67	ILE	2.0
1	p	103	TYR	2.0
1	A	90	LEU	2.0
1	b	112	LEU	2.0
1	t	28	GLU	2.0
1	Y	49	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	d	81	GLY	2.0
1	H	44	MET	2.0
1	f	106	CYS	2.0
1	a	37	ASP	2.0
1	f	48	PRO	2.0
1	H	24	HIS	2.0
1	e	8	GLN	2.0
1	f	111	SER	2.0
1	Y	112	LEU	2.0
1	a	7	ILE	2.0
1	b	79	ILE	2.0
1	c	46	LEU	2.0
1	h	7	ILE	2.0
1	i	90	LEU	2.0
1	j	80	TYR	2.0
1	m	48	PRO	2.0
1	A	31	LYS	2.0
1	C	30	ALA	2.0
1	E	8	GLN	2.0
1	F	106	CYS	2.0
1	p	23	ALA	2.0
1	H	17	THR	2.0
1	Z	65	VAL	2.0
1	Z	86	VAL	2.0
1	Z	21	LEU	2.0
1	s	21	LEU	2.0
1	v	70	LEU	2.0
1	f	69	PHE	2.0
1	g	80	TYR	2.0
1	B	8	GLN	2.0
1	X	48	PRO	2.0
1	e	44	MET	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.