Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:27 pm BST

PDB ID	:	4ZK7
Title	:	Crystal structure of rescued two-component self-assembling tetrahedral cage T33-31
Authors	:	Liu, Y.; Cascio, D.; Sawaya, M.R.; Bale, J.; Collazo, M.J.; Park, R.; King, N.; Baker, D.; Yeates, T.
Deposited on	:	2015-04-30
Resolution	:	3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

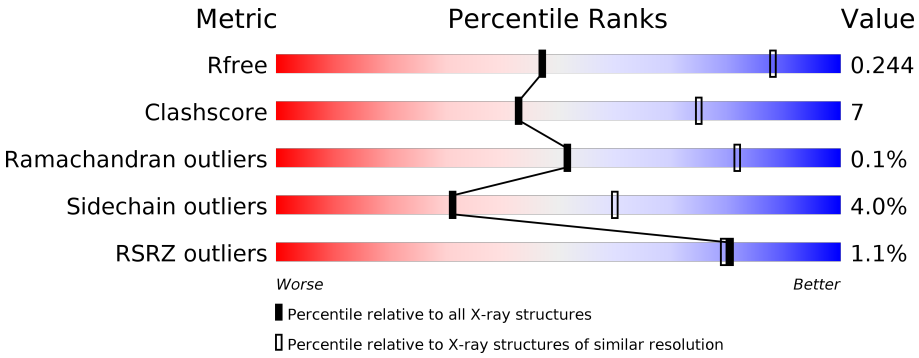
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.40 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	130	73% 16% • 10%
1	B	130	2% 71% 18% • 10%
1	C	130	72% 18% • 10%
1	D	130	75% 15% 10%
1	E	130	73% 15% • 10%
1	F	130	2% 72% 17% • 10%

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Mol	Chain	Length	Quality of chain
1	G	130	2% 75% 14% • 10%
1	H	130	% 75% 14% • 10%
1	I	130	2% 76% 13% • 10%
1	J	130	% 75% 13% • 10%
1	K	130	75% 15% • 10%
1	L	130	% 72% 16% • 10%
2	M	111	% 79% 13% • 7%
2	N	111	2% 71% 20% • 7%
2	O	111	% 74% 18% • 7%
2	P	111	74% 18% • 7%
2	Q	111	% 73% 23% • •
2	R	111	% 72% 20% • 7%
2	S	111	% 70% 21% •• 7%
2	T	111	2% 73% 19% • 7%
2	U	111	2% 74% 18% • 7%
2	V	111	% 68% 23% • 7%
2	W	111	% 80% 12% • 7%
2	X	111	75% 16% • 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20678 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 Chorismate mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	S	0	4	0
			913	584	164	162	3			
1	B	117	Total	C	N	O	S	0	4	0
			913	584	164	162	3			
1	C	117	Total	C	N	O	S	0	4	0
			913	584	164	162	3			
1	D	117	Total	C	N	O	S	0	4	0
			913	584	164	162	3			
1	E	117	Total	C	N	O	S	0	4	0
			913	584	164	162	3			
1	F	117	Total	C	N	O	S	0	4	0
			913	584	164	162	3			
1	G	117	Total	C	N	O	S	0	4	0
			913	584	164	162	3			
1	H	117	Total	C	N	O	S	0	4	0
			913	584	164	162	3			
1	I	117	Total	C	N	O	S	0	4	0
			909	582	163	161	3			
1	J	117	Total	C	N	O	S	0	4	0
			913	584	164	162	3			
1	K	117	Total	C	N	O	S	0	4	0
			913	584	164	162	3			
1	L	117	Total	C	N	O	S	0	4	0
			913	584	164	162	3			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	ALA	GLU	engineered mutation	UNP Q5SJY4
A	20	LEU	HIS	engineered mutation	UNP Q5SJY4
A	21	ALA	GLN	engineered mutation	UNP Q5SJY4
A	24	ILE	ARG	engineered mutation	UNP Q5SJY4
A	64	LEU	GLN	engineered mutation	UNP Q5SJY4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	109	ASN	ARG	engineered mutation	UNP Q5SJY4
A	123	LEU	-	expression tag	UNP Q5SJY4
A	124	GLU	-	expression tag	UNP Q5SJY4
A	125	HIS	-	expression tag	UNP Q5SJY4
A	126	HIS	-	expression tag	UNP Q5SJY4
A	127	HIS	-	expression tag	UNP Q5SJY4
A	128	HIS	-	expression tag	UNP Q5SJY4
A	129	HIS	-	expression tag	UNP Q5SJY4
A	130	HIS	-	expression tag	UNP Q5SJY4
B	17	ALA	GLU	engineered mutation	UNP Q5SJY4
B	20	LEU	HIS	engineered mutation	UNP Q5SJY4
B	21	ALA	GLN	engineered mutation	UNP Q5SJY4
B	24	ILE	ARG	engineered mutation	UNP Q5SJY4
B	64	LEU	GLN	engineered mutation	UNP Q5SJY4
B	109	ASN	ARG	engineered mutation	UNP Q5SJY4
B	123	LEU	-	expression tag	UNP Q5SJY4
B	124	GLU	-	expression tag	UNP Q5SJY4
B	125	HIS	-	expression tag	UNP Q5SJY4
B	126	HIS	-	expression tag	UNP Q5SJY4
B	127	HIS	-	expression tag	UNP Q5SJY4
B	128	HIS	-	expression tag	UNP Q5SJY4
B	129	HIS	-	expression tag	UNP Q5SJY4
B	130	HIS	-	expression tag	UNP Q5SJY4
C	17	ALA	GLU	engineered mutation	UNP Q5SJY4
C	20	LEU	HIS	engineered mutation	UNP Q5SJY4
C	21	ALA	GLN	engineered mutation	UNP Q5SJY4
C	24	ILE	ARG	engineered mutation	UNP Q5SJY4
C	64	LEU	GLN	engineered mutation	UNP Q5SJY4
C	109	ASN	ARG	engineered mutation	UNP Q5SJY4
C	123	LEU	-	expression tag	UNP Q5SJY4
C	124	GLU	-	expression tag	UNP Q5SJY4
C	125	HIS	-	expression tag	UNP Q5SJY4
C	126	HIS	-	expression tag	UNP Q5SJY4
C	127	HIS	-	expression tag	UNP Q5SJY4
C	128	HIS	-	expression tag	UNP Q5SJY4
C	129	HIS	-	expression tag	UNP Q5SJY4
C	130	HIS	-	expression tag	UNP Q5SJY4
D	17	ALA	GLU	engineered mutation	UNP Q5SJY4
D	20	LEU	HIS	engineered mutation	UNP Q5SJY4
D	21	ALA	GLN	engineered mutation	UNP Q5SJY4
D	24	ILE	ARG	engineered mutation	UNP Q5SJY4
D	64	LEU	GLN	engineered mutation	UNP Q5SJY4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	109	ASN	ARG	engineered mutation	UNP Q5SJY4
D	123	LEU	-	expression tag	UNP Q5SJY4
D	124	GLU	-	expression tag	UNP Q5SJY4
D	125	HIS	-	expression tag	UNP Q5SJY4
D	126	HIS	-	expression tag	UNP Q5SJY4
D	127	HIS	-	expression tag	UNP Q5SJY4
D	128	HIS	-	expression tag	UNP Q5SJY4
D	129	HIS	-	expression tag	UNP Q5SJY4
D	130	HIS	-	expression tag	UNP Q5SJY4
E	17	ALA	GLU	engineered mutation	UNP Q5SJY4
E	20	LEU	HIS	engineered mutation	UNP Q5SJY4
E	21	ALA	GLN	engineered mutation	UNP Q5SJY4
E	24	ILE	ARG	engineered mutation	UNP Q5SJY4
E	64	LEU	GLN	engineered mutation	UNP Q5SJY4
E	109	ASN	ARG	engineered mutation	UNP Q5SJY4
E	123	LEU	-	expression tag	UNP Q5SJY4
E	124	GLU	-	expression tag	UNP Q5SJY4
E	125	HIS	-	expression tag	UNP Q5SJY4
E	126	HIS	-	expression tag	UNP Q5SJY4
E	127	HIS	-	expression tag	UNP Q5SJY4
E	128	HIS	-	expression tag	UNP Q5SJY4
E	129	HIS	-	expression tag	UNP Q5SJY4
E	130	HIS	-	expression tag	UNP Q5SJY4
F	17	ALA	GLU	engineered mutation	UNP Q5SJY4
F	20	LEU	HIS	engineered mutation	UNP Q5SJY4
F	21	ALA	GLN	engineered mutation	UNP Q5SJY4
F	24	ILE	ARG	engineered mutation	UNP Q5SJY4
F	64	LEU	GLN	engineered mutation	UNP Q5SJY4
F	109	ASN	ARG	engineered mutation	UNP Q5SJY4
F	123	LEU	-	expression tag	UNP Q5SJY4
F	124	GLU	-	expression tag	UNP Q5SJY4
F	125	HIS	-	expression tag	UNP Q5SJY4
F	126	HIS	-	expression tag	UNP Q5SJY4
F	127	HIS	-	expression tag	UNP Q5SJY4
F	128	HIS	-	expression tag	UNP Q5SJY4
F	129	HIS	-	expression tag	UNP Q5SJY4
F	130	HIS	-	expression tag	UNP Q5SJY4
G	17	ALA	GLU	engineered mutation	UNP Q5SJY4
G	20	LEU	HIS	engineered mutation	UNP Q5SJY4
G	21	ALA	GLN	engineered mutation	UNP Q5SJY4
G	24	ILE	ARG	engineered mutation	UNP Q5SJY4
G	64	LEU	GLN	engineered mutation	UNP Q5SJY4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	109	ASN	ARG	engineered mutation	UNP Q5SJY4
G	123	LEU	-	expression tag	UNP Q5SJY4
G	124	GLU	-	expression tag	UNP Q5SJY4
G	125	HIS	-	expression tag	UNP Q5SJY4
G	126	HIS	-	expression tag	UNP Q5SJY4
G	127	HIS	-	expression tag	UNP Q5SJY4
G	128	HIS	-	expression tag	UNP Q5SJY4
G	129	HIS	-	expression tag	UNP Q5SJY4
G	130	HIS	-	expression tag	UNP Q5SJY4
H	17	ALA	GLU	engineered mutation	UNP Q5SJY4
H	20	LEU	HIS	engineered mutation	UNP Q5SJY4
H	21	ALA	GLN	engineered mutation	UNP Q5SJY4
H	24	ILE	ARG	engineered mutation	UNP Q5SJY4
H	64	LEU	GLN	engineered mutation	UNP Q5SJY4
H	109	ASN	ARG	engineered mutation	UNP Q5SJY4
H	123	LEU	-	expression tag	UNP Q5SJY4
H	124	GLU	-	expression tag	UNP Q5SJY4
H	125	HIS	-	expression tag	UNP Q5SJY4
H	126	HIS	-	expression tag	UNP Q5SJY4
H	127	HIS	-	expression tag	UNP Q5SJY4
H	128	HIS	-	expression tag	UNP Q5SJY4
H	129	HIS	-	expression tag	UNP Q5SJY4
H	130	HIS	-	expression tag	UNP Q5SJY4
I	17	ALA	GLU	engineered mutation	UNP Q5SJY4
I	20	LEU	HIS	engineered mutation	UNP Q5SJY4
I	21	ALA	GLN	engineered mutation	UNP Q5SJY4
I	24	ILE	ARG	engineered mutation	UNP Q5SJY4
I	64	LEU	GLN	engineered mutation	UNP Q5SJY4
I	109	ASN	ARG	engineered mutation	UNP Q5SJY4
I	123	LEU	-	expression tag	UNP Q5SJY4
I	124	GLU	-	expression tag	UNP Q5SJY4
I	125	HIS	-	expression tag	UNP Q5SJY4
I	126	HIS	-	expression tag	UNP Q5SJY4
I	127	HIS	-	expression tag	UNP Q5SJY4
I	128	HIS	-	expression tag	UNP Q5SJY4
I	129	HIS	-	expression tag	UNP Q5SJY4
I	130	HIS	-	expression tag	UNP Q5SJY4
J	17	ALA	GLU	engineered mutation	UNP Q5SJY4
J	20	LEU	HIS	engineered mutation	UNP Q5SJY4
J	21	ALA	GLN	engineered mutation	UNP Q5SJY4
J	24	ILE	ARG	engineered mutation	UNP Q5SJY4
J	64	LEU	GLN	engineered mutation	UNP Q5SJY4

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Chain	Residue	Modelled	Actual	Comment	Reference
J	109	ASN	ARG	engineered mutation	UNP Q5SJY4
J	123	LEU	-	expression tag	UNP Q5SJY4
J	124	GLU	-	expression tag	UNP Q5SJY4
J	125	HIS	-	expression tag	UNP Q5SJY4
J	126	HIS	-	expression tag	UNP Q5SJY4
J	127	HIS	-	expression tag	UNP Q5SJY4
J	128	HIS	-	expression tag	UNP Q5SJY4
J	129	HIS	-	expression tag	UNP Q5SJY4
J	130	HIS	-	expression tag	UNP Q5SJY4
K	17	ALA	GLU	engineered mutation	UNP Q5SJY4
K	20	LEU	HIS	engineered mutation	UNP Q5SJY4
K	21	ALA	GLN	engineered mutation	UNP Q5SJY4
K	24	ILE	ARG	engineered mutation	UNP Q5SJY4
K	64	LEU	GLN	engineered mutation	UNP Q5SJY4
K	109	ASN	ARG	engineered mutation	UNP Q5SJY4
K	123	LEU	-	expression tag	UNP Q5SJY4
K	124	GLU	-	expression tag	UNP Q5SJY4
K	125	HIS	-	expression tag	UNP Q5SJY4
K	126	HIS	-	expression tag	UNP Q5SJY4
K	127	HIS	-	expression tag	UNP Q5SJY4
K	128	HIS	-	expression tag	UNP Q5SJY4
K	129	HIS	-	expression tag	UNP Q5SJY4
K	130	HIS	-	expression tag	UNP Q5SJY4
L	17	ALA	GLU	engineered mutation	UNP Q5SJY4
L	20	LEU	HIS	engineered mutation	UNP Q5SJY4
L	21	ALA	GLN	engineered mutation	UNP Q5SJY4
L	24	ILE	ARG	engineered mutation	UNP Q5SJY4
L	64	LEU	GLN	engineered mutation	UNP Q5SJY4
L	109	ASN	ARG	engineered mutation	UNP Q5SJY4
L	123	LEU	-	expression tag	UNP Q5SJY4
L	124	GLU	-	expression tag	UNP Q5SJY4
L	125	HIS	-	expression tag	UNP Q5SJY4
L	126	HIS	-	expression tag	UNP Q5SJY4
L	127	HIS	-	expression tag	UNP Q5SJY4
L	128	HIS	-	expression tag	UNP Q5SJY4
L	129	HIS	-	expression tag	UNP Q5SJY4
L	130	HIS	-	expression tag	UNP Q5SJY4

- Molecule 2 is a protein called Divalent-cation tolerance protein CutA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	103	Total	C	N	O	S	0	0	0
			806	518	133	153	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	103	Total	C	N	O	S	0	0	0
			806	518	133	153	2			
2	O	103	Total	C	N	O	S	0	0	0
			806	518	133	153	2			
2	P	103	Total	C	N	O	S	0	0	0
			806	518	133	153	2			
2	Q	109	Total	C	N	O	S	0	0	0
			860	550	147	161	2			
2	R	103	Total	C	N	O	S	0	0	0
			806	518	133	153	2			
2	S	103	Total	C	N	O	S	0	0	0
			806	518	133	153	2			
2	T	103	Total	C	N	O	S	0	0	0
			806	518	133	153	2			
2	U	103	Total	C	N	O	S	0	0	0
			806	518	133	153	2			
2	V	103	Total	C	N	O	S	0	0	0
			806	518	133	153	2			
2	W	103	Total	C	N	O	S	0	0	0
			806	518	133	153	2			
2	X	103	Total	C	N	O	S	0	0	0
			806	518	133	153	2			

There are 252 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	12	ALA	GLU	engineered mutation	UNP Q7SIA8
M	13	LEU	GLU	engineered mutation	UNP Q7SIA8
M	16	VAL	ARG	engineered mutation	UNP Q7SIA8
M	17	LYS	THR	engineered mutation	UNP Q7SIA8
M	20	HIS	LYS	engineered mutation	UNP Q7SIA8
M	43	GLU	TRP	engineered mutation	UNP Q7SIA8
M	44	GLU	GLN	engineered mutation	UNP Q7SIA8
M	46	SER	GLU	engineered mutation	UNP Q7SIA8
M	49	SER	GLU	engineered mutation	UNP Q7SIA8
M	51	HIS	GLN	engineered mutation	UNP Q7SIA8
M	62	ASP	HIS	engineered mutation	UNP Q7SIA8
M	73	GLU	ALA	engineered mutation	UNP Q7SIA8
M	78	GLU	THR	engineered mutation	UNP Q7SIA8
M	104	LEU	-	expression tag	UNP Q7SIA8
M	105	GLU	-	expression tag	UNP Q7SIA8
M	106	HIS	-	expression tag	UNP Q7SIA8
M	107	HIS	-	expression tag	UNP Q7SIA8

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Chain	Residue	Modelled	Actual	Comment	Reference
M	108	HIS	-	expression tag	UNP Q7SIA8
M	109	HIS	-	expression tag	UNP Q7SIA8
M	110	HIS	-	expression tag	UNP Q7SIA8
M	111	HIS	-	expression tag	UNP Q7SIA8
N	12	ALA	GLU	engineered mutation	UNP Q7SIA8
N	13	LEU	GLU	engineered mutation	UNP Q7SIA8
N	16	VAL	ARG	engineered mutation	UNP Q7SIA8
N	17	LYS	THR	engineered mutation	UNP Q7SIA8
N	20	HIS	LYS	engineered mutation	UNP Q7SIA8
N	43	GLU	TRP	engineered mutation	UNP Q7SIA8
N	44	GLU	GLN	engineered mutation	UNP Q7SIA8
N	46	SER	GLU	engineered mutation	UNP Q7SIA8
N	49	SER	GLU	engineered mutation	UNP Q7SIA8
N	51	HIS	GLN	engineered mutation	UNP Q7SIA8
N	62	ASP	HIS	engineered mutation	UNP Q7SIA8
N	73	GLU	ALA	engineered mutation	UNP Q7SIA8
N	78	GLU	THR	engineered mutation	UNP Q7SIA8
N	104	LEU	-	expression tag	UNP Q7SIA8
N	105	GLU	-	expression tag	UNP Q7SIA8
N	106	HIS	-	expression tag	UNP Q7SIA8
N	107	HIS	-	expression tag	UNP Q7SIA8
N	108	HIS	-	expression tag	UNP Q7SIA8
N	109	HIS	-	expression tag	UNP Q7SIA8
N	110	HIS	-	expression tag	UNP Q7SIA8
N	111	HIS	-	expression tag	UNP Q7SIA8
O	12	ALA	GLU	engineered mutation	UNP Q7SIA8
O	13	LEU	GLU	engineered mutation	UNP Q7SIA8
O	16	VAL	ARG	engineered mutation	UNP Q7SIA8
O	17	LYS	THR	engineered mutation	UNP Q7SIA8
O	20	HIS	LYS	engineered mutation	UNP Q7SIA8
O	43	GLU	TRP	engineered mutation	UNP Q7SIA8
O	44	GLU	GLN	engineered mutation	UNP Q7SIA8
O	46	SER	GLU	engineered mutation	UNP Q7SIA8
O	49	SER	GLU	engineered mutation	UNP Q7SIA8
O	51	HIS	GLN	engineered mutation	UNP Q7SIA8
O	62	ASP	HIS	engineered mutation	UNP Q7SIA8
O	73	GLU	ALA	engineered mutation	UNP Q7SIA8
O	78	GLU	THR	engineered mutation	UNP Q7SIA8
O	104	LEU	-	expression tag	UNP Q7SIA8
O	105	GLU	-	expression tag	UNP Q7SIA8
O	106	HIS	-	expression tag	UNP Q7SIA8
O	107	HIS	-	expression tag	UNP Q7SIA8

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Chain	Residue	Modelled	Actual	Comment	Reference
O	108	HIS	-	expression tag	UNP Q7SIA8
O	109	HIS	-	expression tag	UNP Q7SIA8
O	110	HIS	-	expression tag	UNP Q7SIA8
O	111	HIS	-	expression tag	UNP Q7SIA8
P	12	ALA	GLU	engineered mutation	UNP Q7SIA8
P	13	LEU	GLU	engineered mutation	UNP Q7SIA8
P	16	VAL	ARG	engineered mutation	UNP Q7SIA8
P	17	LYS	THR	engineered mutation	UNP Q7SIA8
P	20	HIS	LYS	engineered mutation	UNP Q7SIA8
P	43	GLU	TRP	engineered mutation	UNP Q7SIA8
P	44	GLU	GLN	engineered mutation	UNP Q7SIA8
P	46	SER	GLU	engineered mutation	UNP Q7SIA8
P	49	SER	GLU	engineered mutation	UNP Q7SIA8
P	51	HIS	GLN	engineered mutation	UNP Q7SIA8
P	62	ASP	HIS	engineered mutation	UNP Q7SIA8
P	73	GLU	ALA	engineered mutation	UNP Q7SIA8
P	78	GLU	THR	engineered mutation	UNP Q7SIA8
P	104	LEU	-	expression tag	UNP Q7SIA8
P	105	GLU	-	expression tag	UNP Q7SIA8
P	106	HIS	-	expression tag	UNP Q7SIA8
P	107	HIS	-	expression tag	UNP Q7SIA8
P	108	HIS	-	expression tag	UNP Q7SIA8
P	109	HIS	-	expression tag	UNP Q7SIA8
P	110	HIS	-	expression tag	UNP Q7SIA8
P	111	HIS	-	expression tag	UNP Q7SIA8
Q	12	ALA	GLU	engineered mutation	UNP Q7SIA8
Q	13	LEU	GLU	engineered mutation	UNP Q7SIA8
Q	16	VAL	ARG	engineered mutation	UNP Q7SIA8
Q	17	LYS	THR	engineered mutation	UNP Q7SIA8
Q	20	HIS	LYS	engineered mutation	UNP Q7SIA8
Q	43	GLU	TRP	engineered mutation	UNP Q7SIA8
Q	44	GLU	GLN	engineered mutation	UNP Q7SIA8
Q	46	SER	GLU	engineered mutation	UNP Q7SIA8
Q	49	SER	GLU	engineered mutation	UNP Q7SIA8
Q	51	HIS	GLN	engineered mutation	UNP Q7SIA8
Q	62	ASP	HIS	engineered mutation	UNP Q7SIA8
Q	73	GLU	ALA	engineered mutation	UNP Q7SIA8
Q	78	GLU	THR	engineered mutation	UNP Q7SIA8
Q	104	LEU	-	expression tag	UNP Q7SIA8
Q	105	GLU	-	expression tag	UNP Q7SIA8
Q	106	HIS	-	expression tag	UNP Q7SIA8
Q	107	HIS	-	expression tag	UNP Q7SIA8

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	108	HIS	-	expression tag	UNP Q7SIA8
Q	109	HIS	-	expression tag	UNP Q7SIA8
Q	110	HIS	-	expression tag	UNP Q7SIA8
Q	111	HIS	-	expression tag	UNP Q7SIA8
R	12	ALA	GLU	engineered mutation	UNP Q7SIA8
R	13	LEU	GLU	engineered mutation	UNP Q7SIA8
R	16	VAL	ARG	engineered mutation	UNP Q7SIA8
R	17	LYS	THR	engineered mutation	UNP Q7SIA8
R	20	HIS	LYS	engineered mutation	UNP Q7SIA8
R	43	GLU	TRP	engineered mutation	UNP Q7SIA8
R	44	GLU	GLN	engineered mutation	UNP Q7SIA8
R	46	SER	GLU	engineered mutation	UNP Q7SIA8
R	49	SER	GLU	engineered mutation	UNP Q7SIA8
R	51	HIS	GLN	engineered mutation	UNP Q7SIA8
R	62	ASP	HIS	engineered mutation	UNP Q7SIA8
R	73	GLU	ALA	engineered mutation	UNP Q7SIA8
R	78	GLU	THR	engineered mutation	UNP Q7SIA8
R	104	LEU	-	expression tag	UNP Q7SIA8
R	105	GLU	-	expression tag	UNP Q7SIA8
R	106	HIS	-	expression tag	UNP Q7SIA8
R	107	HIS	-	expression tag	UNP Q7SIA8
R	108	HIS	-	expression tag	UNP Q7SIA8
R	109	HIS	-	expression tag	UNP Q7SIA8
R	110	HIS	-	expression tag	UNP Q7SIA8
R	111	HIS	-	expression tag	UNP Q7SIA8
S	12	ALA	GLU	engineered mutation	UNP Q7SIA8
S	13	LEU	GLU	engineered mutation	UNP Q7SIA8
S	16	VAL	ARG	engineered mutation	UNP Q7SIA8
S	17	LYS	THR	engineered mutation	UNP Q7SIA8
S	20	HIS	LYS	engineered mutation	UNP Q7SIA8
S	43	GLU	TRP	engineered mutation	UNP Q7SIA8
S	44	GLU	GLN	engineered mutation	UNP Q7SIA8
S	46	SER	GLU	engineered mutation	UNP Q7SIA8
S	49	SER	GLU	engineered mutation	UNP Q7SIA8
S	51	HIS	GLN	engineered mutation	UNP Q7SIA8
S	62	ASP	HIS	engineered mutation	UNP Q7SIA8
S	73	GLU	ALA	engineered mutation	UNP Q7SIA8
S	78	GLU	THR	engineered mutation	UNP Q7SIA8
S	104	LEU	-	expression tag	UNP Q7SIA8
S	105	GLU	-	expression tag	UNP Q7SIA8
S	106	HIS	-	expression tag	UNP Q7SIA8
S	107	HIS	-	expression tag	UNP Q7SIA8

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Chain	Residue	Modelled	Actual	Comment	Reference
S	108	HIS	-	expression tag	UNP Q7SIA8
S	109	HIS	-	expression tag	UNP Q7SIA8
S	110	HIS	-	expression tag	UNP Q7SIA8
S	111	HIS	-	expression tag	UNP Q7SIA8
T	12	ALA	GLU	engineered mutation	UNP Q7SIA8
T	13	LEU	GLU	engineered mutation	UNP Q7SIA8
T	16	VAL	ARG	engineered mutation	UNP Q7SIA8
T	17	LYS	THR	engineered mutation	UNP Q7SIA8
T	20	HIS	LYS	engineered mutation	UNP Q7SIA8
T	43	GLU	TRP	engineered mutation	UNP Q7SIA8
T	44	GLU	GLN	engineered mutation	UNP Q7SIA8
T	46	SER	GLU	engineered mutation	UNP Q7SIA8
T	49	SER	GLU	engineered mutation	UNP Q7SIA8
T	51	HIS	GLN	engineered mutation	UNP Q7SIA8
T	62	ASP	HIS	engineered mutation	UNP Q7SIA8
T	73	GLU	ALA	engineered mutation	UNP Q7SIA8
T	78	GLU	THR	engineered mutation	UNP Q7SIA8
T	104	LEU	-	expression tag	UNP Q7SIA8
T	105	GLU	-	expression tag	UNP Q7SIA8
T	106	HIS	-	expression tag	UNP Q7SIA8
T	107	HIS	-	expression tag	UNP Q7SIA8
T	108	HIS	-	expression tag	UNP Q7SIA8
T	109	HIS	-	expression tag	UNP Q7SIA8
T	110	HIS	-	expression tag	UNP Q7SIA8
T	111	HIS	-	expression tag	UNP Q7SIA8
U	12	ALA	GLU	engineered mutation	UNP Q7SIA8
U	13	LEU	GLU	engineered mutation	UNP Q7SIA8
U	16	VAL	ARG	engineered mutation	UNP Q7SIA8
U	17	LYS	THR	engineered mutation	UNP Q7SIA8
U	20	HIS	LYS	engineered mutation	UNP Q7SIA8
U	43	GLU	TRP	engineered mutation	UNP Q7SIA8
U	44	GLU	GLN	engineered mutation	UNP Q7SIA8
U	46	SER	GLU	engineered mutation	UNP Q7SIA8
U	49	SER	GLU	engineered mutation	UNP Q7SIA8
U	51	HIS	GLN	engineered mutation	UNP Q7SIA8
U	62	ASP	HIS	engineered mutation	UNP Q7SIA8
U	73	GLU	ALA	engineered mutation	UNP Q7SIA8
U	78	GLU	THR	engineered mutation	UNP Q7SIA8
U	104	LEU	-	expression tag	UNP Q7SIA8
U	105	GLU	-	expression tag	UNP Q7SIA8
U	106	HIS	-	expression tag	UNP Q7SIA8
U	107	HIS	-	expression tag	UNP Q7SIA8

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Chain	Residue	Modelled	Actual	Comment	Reference
U	108	HIS	-	expression tag	UNP Q7SIA8
U	109	HIS	-	expression tag	UNP Q7SIA8
U	110	HIS	-	expression tag	UNP Q7SIA8
U	111	HIS	-	expression tag	UNP Q7SIA8
V	12	ALA	GLU	engineered mutation	UNP Q7SIA8
V	13	LEU	GLU	engineered mutation	UNP Q7SIA8
V	16	VAL	ARG	engineered mutation	UNP Q7SIA8
V	17	LYS	THR	engineered mutation	UNP Q7SIA8
V	20	HIS	LYS	engineered mutation	UNP Q7SIA8
V	43	GLU	TRP	engineered mutation	UNP Q7SIA8
V	44	GLU	GLN	engineered mutation	UNP Q7SIA8
V	46	SER	GLU	engineered mutation	UNP Q7SIA8
V	49	SER	GLU	engineered mutation	UNP Q7SIA8
V	51	HIS	GLN	engineered mutation	UNP Q7SIA8
V	62	ASP	HIS	engineered mutation	UNP Q7SIA8
V	73	GLU	ALA	engineered mutation	UNP Q7SIA8
V	78	GLU	THR	engineered mutation	UNP Q7SIA8
V	104	LEU	-	expression tag	UNP Q7SIA8
V	105	GLU	-	expression tag	UNP Q7SIA8
V	106	HIS	-	expression tag	UNP Q7SIA8
V	107	HIS	-	expression tag	UNP Q7SIA8
V	108	HIS	-	expression tag	UNP Q7SIA8
V	109	HIS	-	expression tag	UNP Q7SIA8
V	110	HIS	-	expression tag	UNP Q7SIA8
V	111	HIS	-	expression tag	UNP Q7SIA8
W	12	ALA	GLU	engineered mutation	UNP Q7SIA8
W	13	LEU	GLU	engineered mutation	UNP Q7SIA8
W	16	VAL	ARG	engineered mutation	UNP Q7SIA8
W	17	LYS	THR	engineered mutation	UNP Q7SIA8
W	20	HIS	LYS	engineered mutation	UNP Q7SIA8
W	43	GLU	TRP	engineered mutation	UNP Q7SIA8
W	44	GLU	GLN	engineered mutation	UNP Q7SIA8
W	46	SER	GLU	engineered mutation	UNP Q7SIA8
W	49	SER	GLU	engineered mutation	UNP Q7SIA8
W	51	HIS	GLN	engineered mutation	UNP Q7SIA8
W	62	ASP	HIS	engineered mutation	UNP Q7SIA8
W	73	GLU	ALA	engineered mutation	UNP Q7SIA8
W	78	GLU	THR	engineered mutation	UNP Q7SIA8
W	104	LEU	-	expression tag	UNP Q7SIA8
W	105	GLU	-	expression tag	UNP Q7SIA8
W	106	HIS	-	expression tag	UNP Q7SIA8
W	107	HIS	-	expression tag	UNP Q7SIA8

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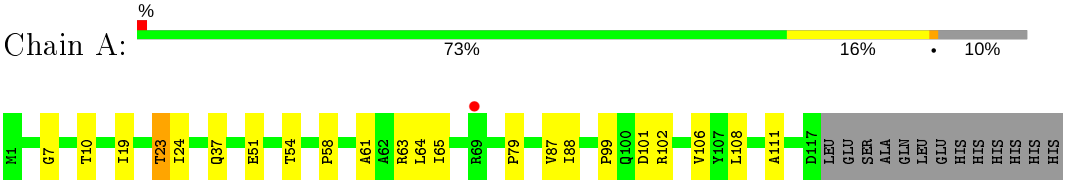
Chain	Residue	Modelled	Actual	Comment	Reference
W	108	HIS	-	expression tag	UNP Q7SIA8
W	109	HIS	-	expression tag	UNP Q7SIA8
W	110	HIS	-	expression tag	UNP Q7SIA8
W	111	HIS	-	expression tag	UNP Q7SIA8
X	12	ALA	GLU	engineered mutation	UNP Q7SIA8
X	13	LEU	GLU	engineered mutation	UNP Q7SIA8
X	16	VAL	ARG	engineered mutation	UNP Q7SIA8
X	17	LYS	THR	engineered mutation	UNP Q7SIA8
X	20	HIS	LYS	engineered mutation	UNP Q7SIA8
X	43	GLU	TRP	engineered mutation	UNP Q7SIA8
X	44	GLU	GLN	engineered mutation	UNP Q7SIA8
X	46	SER	GLU	engineered mutation	UNP Q7SIA8
X	49	SER	GLU	engineered mutation	UNP Q7SIA8
X	51	HIS	GLN	engineered mutation	UNP Q7SIA8
X	62	ASP	HIS	engineered mutation	UNP Q7SIA8
X	73	GLU	ALA	engineered mutation	UNP Q7SIA8
X	78	GLU	THR	engineered mutation	UNP Q7SIA8
X	104	LEU	-	expression tag	UNP Q7SIA8
X	105	GLU	-	expression tag	UNP Q7SIA8
X	106	HIS	-	expression tag	UNP Q7SIA8
X	107	HIS	-	expression tag	UNP Q7SIA8
X	108	HIS	-	expression tag	UNP Q7SIA8
X	109	HIS	-	expression tag	UNP Q7SIA8
X	110	HIS	-	expression tag	UNP Q7SIA8
X	111	HIS	-	expression tag	UNP Q7SIA8

3 Residue-property plots (i)

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

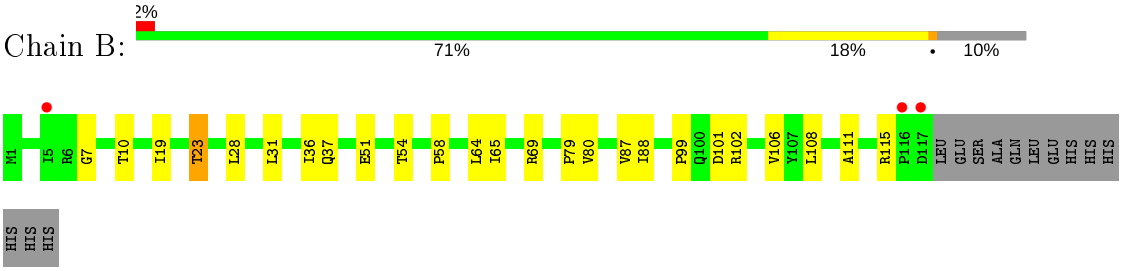
- Molecule 1: Chorismate mutase

Chain A:



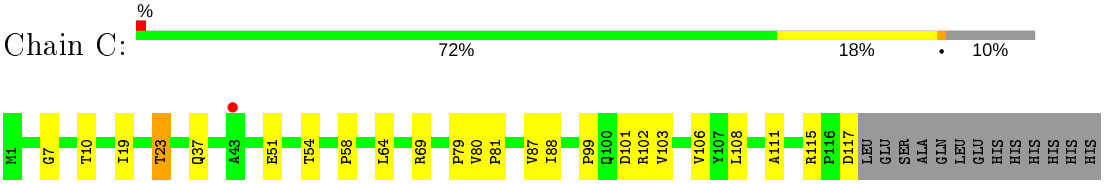
- Molecule 1: Chorismate mutase

Chain B:



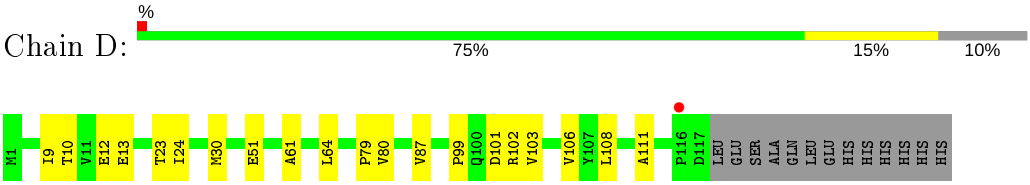
- Molecule 1: Chorismate mutase

Chain C:



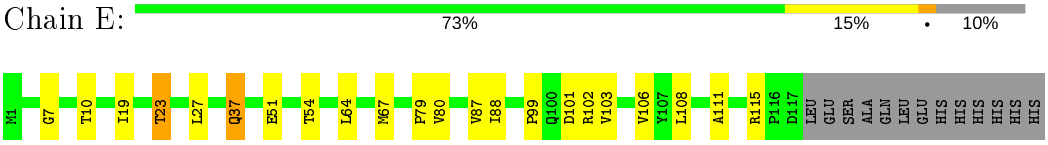
- Molecule 1: Chorismate mutase

Chain D:



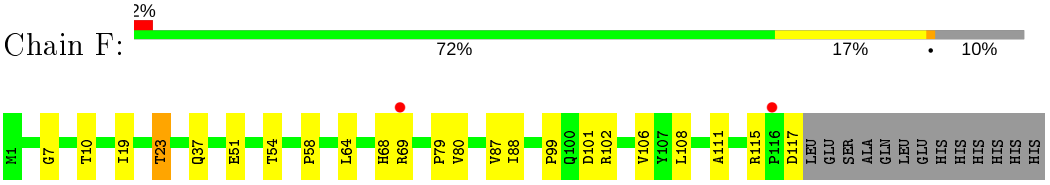
- Molecule 1: Chorismate mutase

Chain E:



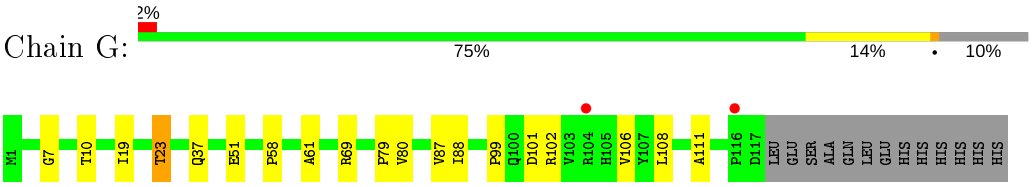
• Molecule 1: Chorismate mutase

Chain F:



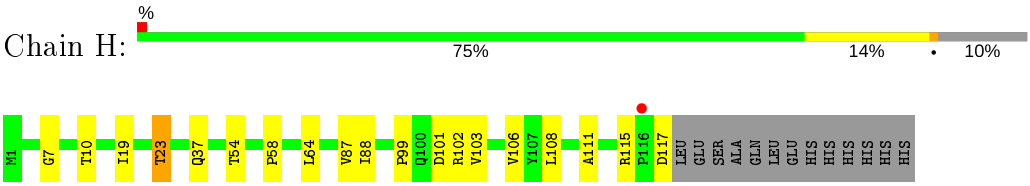
• Molecule 1: Chorismate mutase

Chain G:



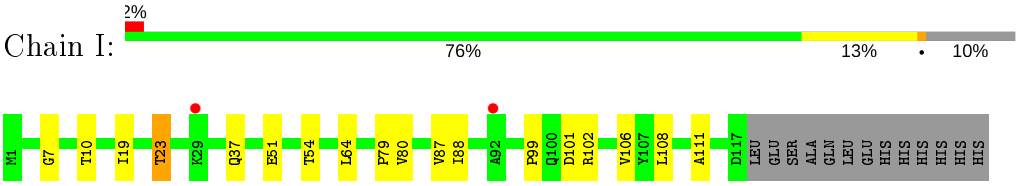
• Molecule 1: Chorismate mutase

Chain H:



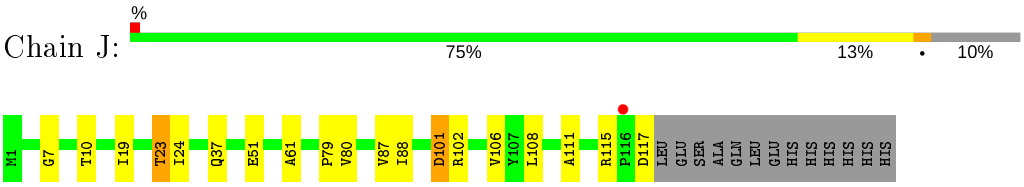
• Molecule 1: Chorismate mutase

Chain I:



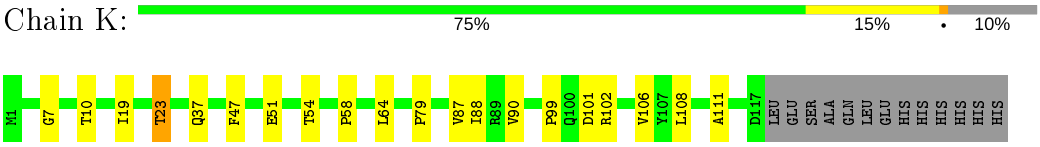
• Molecule 1: Chorismate mutase

Chain J:



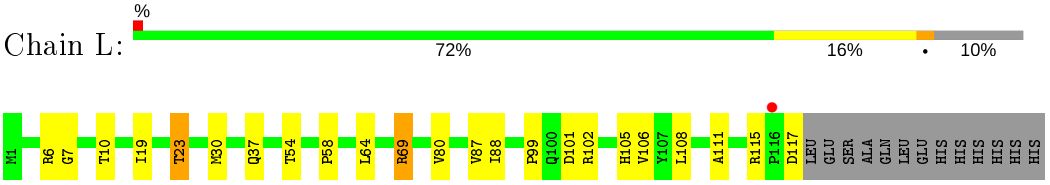
• Molecule 1: Chorismate mutase

Chain K:



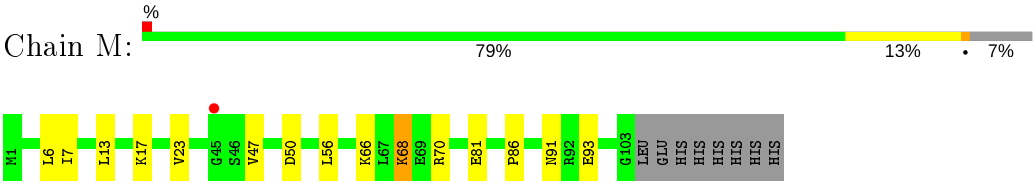
• Molecule 1: Chorismate mutase

Chain L:



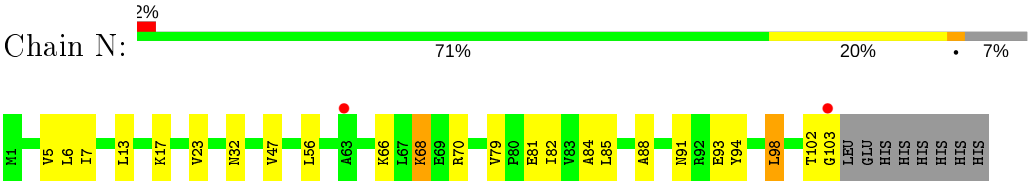
• Molecule 2: Divalent-cation tolerance protein CutA

Chain M:



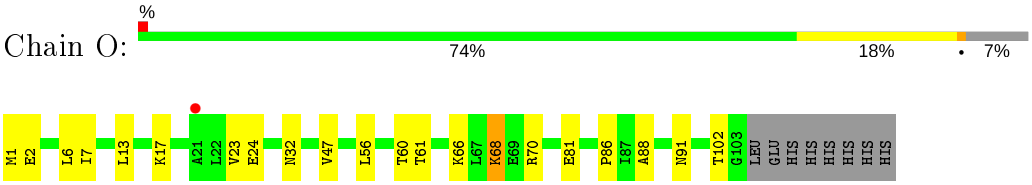
• Molecule 2: Divalent-cation tolerance protein CutA

Chain N:



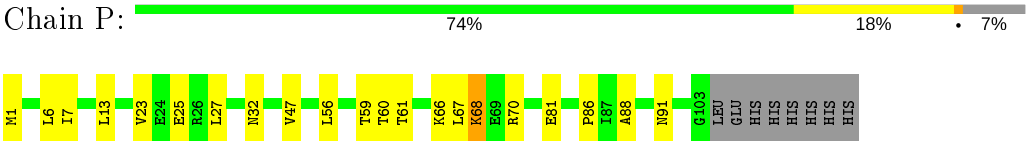
• Molecule 2: Divalent-cation tolerance protein CutA

Chain O:



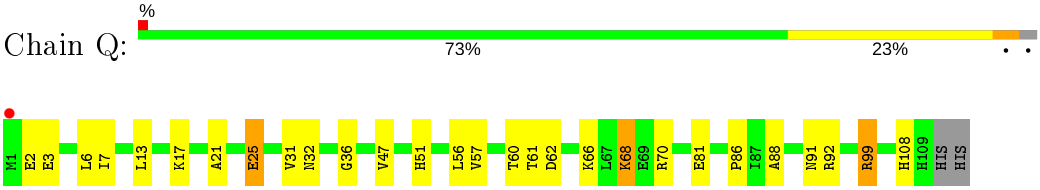
• Molecule 2: Divalent-cation tolerance protein CutA

Chain P:



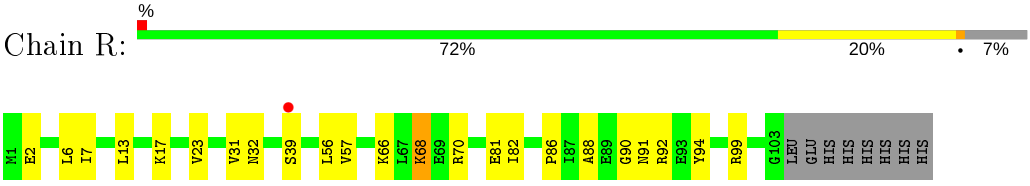
• Molecule 2: Divalent-cation tolerance protein CutA

Chain Q:



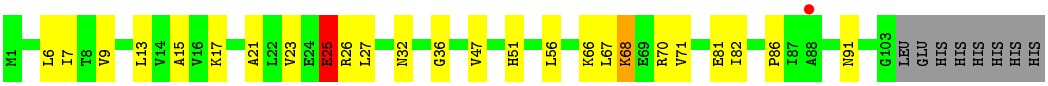
• Molecule 2: Divalent-cation tolerance protein CutA

Chain R:



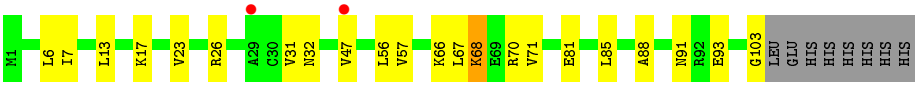
• Molecule 2: Divalent-cation tolerance protein CutA

Chain S:



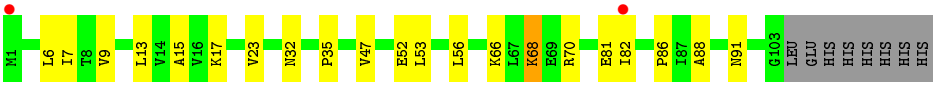
• Molecule 2: Divalent-cation tolerance protein CutA

Chain T:



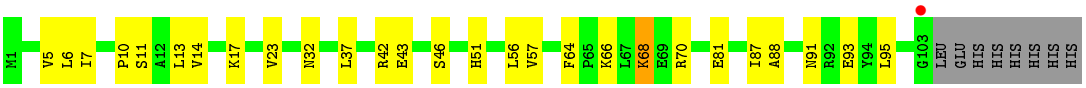
• Molecule 2: Divalent-cation tolerance protein CutA

Chain U:



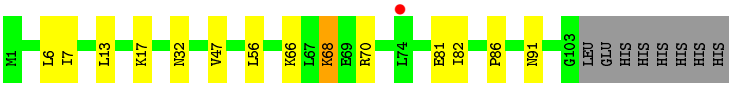
• Molecule 2: Divalent-cation tolerance protein CutA

Chain V:



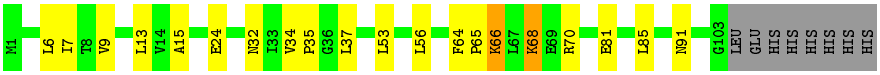
• Molecule 2: Divalent-cation tolerance protein CutA

Chain W:



• Molecule 2: Divalent-cation tolerance protein CutA

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	121.10Å 128.40Å 204.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.10 – 3.40 88.10 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (88.10-3.40) 99.1 (88.10-3.40)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 3.41Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.190 , 0.239 0.197 , 0.244	Depositor DCC
R_{free} test set	2219 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	73.9	Xtriage
Anisotropy	0.798	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 83.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	20678	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.53	0/948	0.73	0/1293
1	B	0.55	0/948	0.74	0/1293
1	C	0.48	0/948	0.71	0/1293
1	D	0.56	0/948	0.73	0/1293
1	E	0.50	0/948	0.72	0/1293
1	F	0.51	0/948	0.71	0/1293
1	G	0.53	0/948	0.71	0/1293
1	H	0.55	0/948	0.74	0/1293
1	I	0.52	0/944	0.73	0/1288
1	J	0.57	0/948	0.74	0/1293
1	K	0.53	0/948	0.73	0/1293
1	L	0.53	0/948	0.72	0/1293
2	M	0.45	0/820	0.69	0/1119
2	N	0.46	0/820	0.71	0/1119
2	O	0.48	0/820	0.72	0/1119
2	P	0.56	0/820	0.73	0/1119
2	Q	0.54	0/878	0.76	0/1198
2	R	0.53	0/820	0.74	0/1119
2	S	0.50	0/820	0.72	0/1119
2	T	0.51	0/820	0.72	0/1119
2	U	0.48	0/820	0.72	0/1119
2	V	0.53	0/820	0.73	0/1119
2	W	0.54	0/820	0.74	0/1119
2	X	0.50	0/820	0.72	0/1119
All	All	0.52	0/21270	0.73	0/29018

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	913	0	954	14	0
1	B	913	0	954	17	0
1	C	913	0	954	17	0
1	D	913	0	954	17	0
1	E	913	0	954	16	0
1	F	913	0	954	17	0
1	G	913	0	954	12	0
1	H	913	0	954	12	0
1	I	909	0	948	10	0
1	J	913	0	954	11	0
1	K	913	0	954	14	0
1	L	913	0	954	16	0
2	M	806	0	834	13	0
2	N	806	0	834	17	0
2	O	806	0	834	14	0
2	P	806	0	834	14	0
2	Q	860	0	870	16	0
2	R	806	0	834	17	0
2	S	806	0	834	15	0
2	T	806	0	834	16	0
2	U	806	0	834	15	0
2	V	806	0	834	22	0
2	W	806	0	834	11	0
2	X	806	0	834	13	0
All	All	20678	0	21486	287	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 7.

All (287) 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:D:13:GLU:HG2	2:V:51:HIS:CE1	2.12	0.84
1:D:106:VAL:HG12	1:D:108:LEU:HD21	1.63	0.78
1:B:64:LEU:HD22	2:R:17:LYS:HB2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:ILE:O	1:E:23:THR:HG23	1.83	0.77
1:G:19:ILE:O	1:G:23:THR:HG23	1.88	0.74
1:A:19:ILE:O	1:A:23:THR:HG23	1.88	0.74
1:I:19:ILE:O	1:I:23:THR:HG23	1.90	0.71
1:C:19:ILE:O	1:C:23:THR:HG23	1.90	0.71
1:H:19:ILE:O	1:H:23:THR:HG23	1.89	0.71
1:D:106:VAL:CG1	1:D:108:LEU:HD21	2.20	0.71
1:B:28:LEU:HD21	1:B:65:ILE:HD12	1.73	0.70
1:K:19:ILE:O	1:K:23:THR:HG23	1.91	0.70
1:F:19:ILE:O	1:F:23:THR:HG23	1.93	0.68
1:J:19:ILE:O	1:J:23:THR:HG23	1.93	0.67
2:N:5:VAL:HG22	2:N:84:ALA:HB2	1.77	0.67
1:L:19:ILE:O	1:L:23:THR:HG23	1.94	0.67
1:G:69:ARG:NH2	1:H:103:VAL:O	2.28	0.67
1:D:12:GLU:HB2	2:V:51:HIS:CD2	2.32	0.65
1:B:19:ILE:O	1:B:23:THR:HG23	1.97	0.65
2:P:25:GLU:HB2	2:P:27:LEU:HD12	1.78	0.64
2:P:23:VAL:HG12	2:Q:47:VAL:HG22	1.80	0.64
1:L:30:MET:HA	1:L:106:VAL:HG21	1.80	0.63
2:V:10:PRO:HG2	2:V:14:VAL:HG21	1.80	0.63
2:V:11:SER:OG	2:V:14:VAL:HG23	1.99	0.63
2:Q:31:VAL:HG22	2:Q:57:VAL:HG13	1.79	0.63
1:H:99:PRO:HD2	1:H:102:ARG:HB2	1.81	0.63
2:R:90:GLY:O	2:R:92:ARG:HD3	1.99	0.62
1:G:99:PRO:HD2	1:G:102:ARG:HB2	1.81	0.62
2:S:25:GLU:HB3	2:S:27:LEU:HD12	1.81	0.62
2:T:31:VAL:HG22	2:T:57:VAL:HG22	1.80	0.61
1:A:64:LEU:HD22	2:U:17:LYS:HB2	1.81	0.61
2:S:68:LYS:HD3	2:U:91:ASN:HA	1.82	0.61
2:V:37:LEU:HD11	2:X:34:VAL:HG22	1.83	0.61
1:E:108:LEU:O	1:E:111:ALA:HB3	2.01	0.61
2:N:6:LEU:HD11	2:N:85:LEU:HD11	1.81	0.61
2:N:94:TYR:CE2	2:N:98:LEU:HD12	2.36	0.61
2:P:88:ALA:HB2	2:Q:86:PRO:HD3	1.83	0.60
2:W:91:ASN:HA	2:X:68:LYS:HD3	1.82	0.60
1:L:99:PRO:HD2	1:L:102:ARG:HB2	1.84	0.60
2:S:23:VAL:HG12	2:T:47:VAL:HG22	1.84	0.60
2:N:88:ALA:HB2	2:O:86:PRO:HD3	1.83	0.60
2:V:10:PRO:HD2	2:V:14:VAL:HG11	1.82	0.60
2:M:86:PRO:HD3	2:O:88:ALA:HB2	1.84	0.59
1:K:7:GLY:HA2	1:K:106:VAL:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:ILE:HD12	1:D:108:LEU:HD12	1.85	0.59
1:I:99:PRO:HD2	1:I:102:ARG:HB2	1.85	0.59
2:S:91:ASN:HA	2:T:68:LYS:HD3	1.84	0.58
1:A:108:LEU:O	1:A:111:ALA:HB3	2.04	0.58
1:A:99:PRO:HD2	1:A:102:ARG:HB2	1.85	0.58
1:I:10:THR:HG22	1:I:87:VAL:HG22	1.86	0.58
1:K:64:LEU:HD22	2:W:17:LYS:HB2	1.85	0.58
1:C:7:GLY:HA2	1:C:106:VAL:O	2.05	0.57
1:F:99:PRO:HD2	1:F:102:ARG:HB2	1.86	0.57
1:C:10:THR:HG22	1:C:87:VAL:HG22	1.87	0.57
2:V:68:LYS:HD3	2:X:91:ASN:HA	1.86	0.57
2:S:86:PRO:HD3	2:U:88:ALA:HB2	1.87	0.57
1:B:99:PRO:HD2	1:B:102:ARG:HB2	1.87	0.56
2:N:102:THR:HG22	2:N:103:GLY:H	1.70	0.56
1:D:99:PRO:HD2	1:D:102:ARG:HB2	1.87	0.56
2:V:88:ALA:HB2	2:W:86:PRO:HD3	1.87	0.56
1:A:10:THR:HG22	1:A:87:VAL:HG22	1.88	0.56
1:H:10:THR:HG22	1:H:87:VAL:HG22	1.88	0.56
1:K:47:PHE:CD1	1:K:90:VAL:HG22	2.42	0.55
1:J:7:GLY:HA2	1:J:106:VAL:O	2.06	0.55
1:C:99:PRO:HD2	1:C:102:ARG:HB2	1.87	0.55
1:K:99:PRO:HD2	1:K:102:ARG:HB2	1.87	0.55
1:K:47:PHE:HD1	1:K:90:VAL:HG22	1.70	0.55
1:C:69:ARG:NH2	1:E:103:VAL:O	2.40	0.55
1:F:10:THR:HG22	1:F:87:VAL:HG22	1.89	0.55
1:E:10:THR:HG22	1:E:87:VAL:HG22	1.88	0.55
2:V:91:ASN:HA	2:W:68:LYS:HD3	1.88	0.55
1:F:108:LEU:O	1:F:111:ALA:HB3	2.07	0.55
1:B:7:GLY:HA2	1:B:106:VAL:O	2.07	0.54
1:A:54:THR:O	1:B:80:VAL:HA	2.08	0.54
2:U:35:PRO:HA	2:U:53:LEU:HG	1.90	0.54
1:E:54:THR:O	1:F:80:VAL:HA	2.08	0.54
2:P:59:THR:HG21	2:P:67:LEU:HD13	1.88	0.54
1:B:10:THR:HG22	1:B:87:VAL:HG22	1.89	0.54
2:Q:91:ASN:HA	2:R:68:LYS:HD3	1.90	0.54
1:J:10:THR:HG22	1:J:87:VAL:HG22	1.89	0.54
1:E:99:PRO:HD2	1:E:102:ARG:HB2	1.89	0.53
1:K:10:THR:HG22	1:K:87:VAL:HG22	1.88	0.53
1:G:108:LEU:O	1:G:111:ALA:HB3	2.08	0.53
2:S:66:LYS:H	2:S:66:LYS:HD2	1.73	0.53
2:T:26:ARG:HB3	2:T:103:GLY:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:66:LYS:HD2	2:T:66:LYS:H	1.73	0.53
1:B:108:LEU:O	1:B:111:ALA:HB3	2.08	0.53
1:H:108:LEU:O	1:H:111:ALA:HB3	2.09	0.52
2:T:91:ASN:HA	2:U:68:LYS:HD3	1.90	0.52
1:L:10:THR:HG22	1:L:87:VAL:HG22	1.90	0.52
1:D:9:ILE:HG13	1:D:108:LEU:HB2	1.90	0.52
1:E:23:THR:HG22	1:E:88:ILE:HD13	1.92	0.52
1:C:103:VAL:O	1:F:69:ARG:NH2	2.43	0.52
1:C:108:LEU:O	1:C:111:ALA:HB3	2.10	0.52
1:D:10:THR:HG22	1:D:87:VAL:HG22	1.91	0.52
1:L:30:MET:HA	1:L:106:VAL:CG2	2.39	0.52
1:D:99:PRO:HG2	1:D:102:ARG:HE	1.74	0.52
1:J:108:LEU:O	1:J:111:ALA:HB3	2.10	0.52
2:R:66:LYS:H	2:R:66:LYS:HD2	1.73	0.52
2:M:66:LYS:HD2	2:M:66:LYS:H	1.75	0.51
2:U:66:LYS:H	2:U:66:LYS:HD2	1.74	0.51
2:W:66:LYS:HD2	2:W:66:LYS:H	1.75	0.51
2:P:86:PRO:HD3	2:R:88:ALA:HB2	1.92	0.51
2:Q:66:LYS:HD2	2:Q:66:LYS:H	1.76	0.51
2:S:21:ALA:O	2:S:25:GLU:HB2	2.11	0.51
1:E:7:GLY:HA2	1:E:106:VAL:O	2.11	0.51
1:G:10:THR:HG22	1:G:87:VAL:HG22	1.92	0.51
1:I:108:LEU:O	1:I:111:ALA:HB3	2.11	0.51
2:P:91:ASN:HA	2:Q:68:LYS:HD3	1.91	0.51
1:C:80:VAL:HA	1:F:54:THR:O	2.11	0.51
1:L:108:LEU:O	1:L:111:ALA:HB3	2.09	0.51
2:P:47:VAL:HG22	2:R:23:VAL:HG12	1.93	0.51
2:Q:88:ALA:HB2	2:R:86:PRO:HD3	1.93	0.51
2:N:91:ASN:HA	2:O:68:LYS:HD3	1.92	0.51
2:M:47:VAL:HG22	2:O:23:VAL:HG12	1.92	0.51
1:B:51:GLU:HG3	1:B:79:PRO:HB3	1.93	0.51
1:D:30:MET:HA	1:D:106:VAL:HG21	1.91	0.51
1:K:108:LEU:O	1:K:111:ALA:HB3	2.11	0.50
2:M:68:LYS:HD3	2:O:91:ASN:HA	1.93	0.50
1:D:106:VAL:HG12	1:D:108:LEU:CD2	2.38	0.50
2:P:66:LYS:H	2:P:66:LYS:HD2	1.77	0.50
2:V:66:LYS:HD2	2:V:66:LYS:H	1.74	0.50
2:N:66:LYS:H	2:N:66:LYS:HD2	1.75	0.50
1:D:108:LEU:O	1:D:111:ALA:HB3	2.11	0.50
2:O:66:LYS:HD2	2:O:66:LYS:H	1.75	0.50
2:X:9:VAL:HG21	2:X:15:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:7:GLY:HA2	1:I:106:VAL:O	2.12	0.49
2:Q:6:LEU:HD23	2:Q:56:LEU:HD23	1.94	0.49
1:H:7:GLY:HA2	1:H:106:VAL:O	2.12	0.49
1:A:7:GLY:HA2	1:A:106:VAL:O	2.11	0.49
2:O:6:LEU:HD23	2:O:56:LEU:HD23	1.93	0.49
2:V:6:LEU:HD23	2:V:56:LEU:HD23	1.95	0.49
2:R:32:ASN:HB2	2:R:56:LEU:HB2	1.95	0.49
1:I:64:LEU:HD22	2:O:17:LYS:HB2	1.95	0.49
2:V:23:VAL:HG12	2:W:47:VAL:HG22	1.94	0.48
1:C:23:THR:HG21	1:C:58:PRO:HB3	1.96	0.48
1:K:54:THR:O	1:L:80:VAL:HA	2.13	0.48
2:W:32:ASN:HB2	2:W:56:LEU:HB2	1.95	0.48
2:M:23:VAL:HG12	2:N:47:VAL:HG22	1.94	0.48
1:B:54:THR:O	1:D:80:VAL:HA	2.13	0.48
2:N:6:LEU:HD23	2:N:56:LEU:HD23	1.95	0.48
2:O:1:MET:HG2	2:O:60:THR:HB	1.96	0.48
1:E:99:PRO:HG2	1:E:102:ARG:HE	1.79	0.48
1:F:99:PRO:HG2	1:F:102:ARG:HE	1.78	0.48
1:H:23:THR:HG22	1:H:88:ILE:HD13	1.95	0.48
1:F:23:THR:HG21	1:F:58:PRO:HB3	1.94	0.48
1:K:99:PRO:HG2	1:K:102:ARG:HE	1.79	0.48
2:O:32:ASN:HB2	2:O:56:LEU:HB2	1.96	0.48
2:Q:99:ARG:HB2	2:Q:99:ARG:HE	1.42	0.47
2:R:6:LEU:HD23	2:R:56:LEU:HD23	1.96	0.47
2:T:88:ALA:HB2	2:U:86:PRO:HD3	1.96	0.47
1:J:24:ILE:HG13	1:J:61:ALA:HB1	1.94	0.47
2:N:32:ASN:HB2	2:N:56:LEU:HB2	1.95	0.47
2:Q:91:ASN:HB2	2:R:82:ILE:HB	1.96	0.47
1:G:7:GLY:HA2	1:G:106:VAL:O	2.14	0.47
2:S:32:ASN:HB2	2:S:56:LEU:HB2	1.95	0.47
1:C:64:LEU:HD22	2:N:17:LYS:HB2	1.96	0.47
2:S:6:LEU:HD23	2:S:56:LEU:HD23	1.97	0.47
2:S:47:VAL:HG22	2:U:23:VAL:HG12	1.97	0.47
1:G:23:THR:HG22	1:G:88:ILE:HG21	1.96	0.47
2:N:23:VAL:HG12	2:O:47:VAL:HG22	1.97	0.47
2:R:31:VAL:HG22	2:R:57:VAL:HG13	1.96	0.47
2:Q:21:ALA:O	2:Q:25:GLU:HB2	2.15	0.47
2:T:32:ASN:HB2	2:T:56:LEU:HB2	1.96	0.47
1:C:51:GLU:HG3	1:C:79:PRO:HB3	1.97	0.46
1:L:6:ARG:O	1:L:105:HIS:HB3	2.14	0.46
2:X:6:LEU:HD23	2:X:56:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:ILE:HG13	1:D:61:ALA:HB1	1.97	0.46
2:P:68:LYS:HD3	2:R:91:ASN:HA	1.97	0.46
2:W:6:LEU:HD23	2:W:56:LEU:HD23	1.98	0.46
1:B:23:THR:HG21	1:B:58:PRO:HB3	1.97	0.46
2:U:9:VAL:HG21	2:U:15:ALA:HA	1.97	0.46
2:R:91:ASN:O	2:R:94:TYR:HB3	2.16	0.46
1:K:23:THR:HG22	1:K:88:ILE:HD13	1.97	0.45
1:L:64:LEU:HD22	2:M:17:LYS:HB2	1.98	0.45
1:L:7:GLY:HA2	1:L:106:VAL:O	2.16	0.45
1:E:64:LEU:HD22	2:V:17:LYS:HB2	1.98	0.45
2:M:6:LEU:HD23	2:M:56:LEU:HD23	1.98	0.45
1:B:31:LEU:HD22	1:B:36:ILE:HG21	1.97	0.45
2:N:7:ILE:HA	2:N:81:GLU:O	2.17	0.45
2:P:32:ASN:HB2	2:P:56:LEU:HB2	1.98	0.45
2:T:6:LEU:HD23	2:T:56:LEU:HD23	1.97	0.45
1:J:23:THR:HG22	1:J:88:ILE:HD13	1.99	0.45
2:X:65:PRO:HB2	2:X:66:LYS:HE3	1.98	0.45
1:A:23:THR:HG22	1:A:88:ILE:HD13	1.98	0.45
1:A:23:THR:HG21	1:A:58:PRO:HB3	1.97	0.45
2:Q:32:ASN:HB2	2:Q:56:LEU:HB2	1.98	0.45
1:B:23:THR:HG22	1:B:88:ILE:HD13	1.98	0.45
1:K:51:GLU:HG3	1:K:79:PRO:HB3	1.99	0.45
2:O:2:GLU:H	2:O:2:GLU:CD	2.20	0.45
2:P:1:MET:SD	2:P:60:THR:HB	2.57	0.45
1:L:23:THR:HG21	1:L:58:PRO:HB3	1.99	0.44
1:F:7:GLY:HA2	1:F:106:VAL:O	2.17	0.44
2:O:7:ILE:HA	2:O:81:GLU:O	2.18	0.44
2:S:82:ILE:HB	2:U:91:ASN:HB2	2.00	0.44
2:V:42:ARG:NH2	2:X:24:GLU:HA	2.33	0.44
1:F:64:LEU:HD22	2:Q:17:LYS:HB2	1.99	0.44
1:J:115:ARG:HA	1:J:115:ARG:HD2	1.91	0.44
1:E:64:LEU:HD11	2:V:13:LEU:HD23	2.00	0.44
1:H:64:LEU:HD22	2:T:17:LYS:HB2	2.00	0.44
2:T:7:ILE:HA	2:T:81:GLU:O	2.18	0.44
2:Q:2:GLU:HA	2:Q:60:THR:HG22	2.00	0.44
1:D:61:ALA:HA	1:D:64:LEU:HD12	1.99	0.44
1:H:115:ARG:HA	1:H:115:ARG:HD2	1.89	0.44
2:Q:36:GLY:HA2	2:Q:51:HIS:HE1	1.82	0.44
1:G:23:THR:HG21	1:G:58:PRO:HB3	2.00	0.43
2:U:32:ASN:HB2	2:U:56:LEU:HB2	1.99	0.43
2:V:32:ASN:HB2	2:V:56:LEU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:6:LEU:HD23	2:P:56:LEU:HD23	2.00	0.43
1:B:28:LEU:HD21	1:B:65:ILE:CD1	2.45	0.43
1:A:24:ILE:HG13	1:A:61:ALA:HB1	2.01	0.43
1:E:115:ARG:HD2	1:E:115:ARG:HA	1.88	0.43
1:C:54:THR:O	1:E:80:VAL:HA	2.19	0.43
1:F:23:THR:HG22	1:F:88:ILE:HG21	2.00	0.43
1:I:23:THR:HG22	1:I:88:ILE:HD13	1.99	0.43
2:V:93:GLU:H	2:V:93:GLU:HG3	1.64	0.43
1:G:51:GLU:HG3	1:G:79:PRO:HB3	2.00	0.43
2:X:32:ASN:HB2	2:X:56:LEU:HB2	2.00	0.43
1:B:23:THR:HG22	1:B:88:ILE:HG21	2.01	0.43
1:G:99:PRO:HG2	1:G:102:ARG:HE	1.84	0.43
1:J:101:ASP:HA	1:L:69:ARG:HD3	2.00	0.43
1:C:115:ARG:HA	1:C:115:ARG:HD2	1.93	0.43
1:J:80:VAL:HA	1:L:54:THR:O	2.19	0.43
2:S:36:GLY:HA2	2:S:51:HIS:HE1	1.84	0.43
1:B:69:ARG:NH2	1:D:103:VAL:O	2.52	0.43
1:I:51:GLU:HG3	1:I:79:PRO:HB3	2.01	0.43
2:V:91:ASN:HB2	2:W:82:ILE:HB	2.01	0.43
2:X:7:ILE:HA	2:X:81:GLU:O	2.19	0.43
2:R:92:ARG:HG2	2:R:92:ARG:H	1.25	0.42
2:U:6:LEU:HD23	2:U:56:LEU:HD23	2.01	0.42
1:C:23:THR:HG22	1:C:88:ILE:HD13	2.00	0.42
1:D:51:GLU:HG3	1:D:79:PRO:HB3	2.01	0.42
2:M:7:ILE:HA	2:M:81:GLU:O	2.19	0.42
2:S:67:LEU:O	2:S:71:VAL:HG23	2.20	0.42
2:V:7:ILE:HA	2:V:81:GLU:O	2.18	0.42
1:A:23:THR:HG22	1:A:88:ILE:HG21	2.00	0.42
1:C:115:ARG:HH22	1:F:68:HIS:HB3	1.83	0.42
2:M:93:GLU:HG3	2:M:93:GLU:H	1.64	0.42
2:Q:7:ILE:HA	2:Q:81:GLU:O	2.19	0.42
2:R:2:GLU:OE1	2:R:99:ARG:NH1	2.52	0.42
2:U:7:ILE:HA	2:U:81:GLU:O	2.18	0.42
1:C:115:ARG:HE	1:C:117:ASP:CG	2.23	0.42
1:F:115:ARG:HE	1:F:117:ASP:CG	2.22	0.42
1:H:54:THR:O	1:I:80:VAL:HA	2.20	0.42
2:W:32:ASN:HB3	2:X:37:LEU:HD23	2.01	0.42
1:A:51:GLU:HG3	1:A:79:PRO:HB3	2.01	0.42
1:E:27:LEU:HD22	1:E:67:MET:HE3	2.02	0.42
1:G:23:THR:OG1	1:G:61:ALA:HB3	2.20	0.42
1:H:115:ARG:HE	1:H:117:ASP:CG	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:23:THR:HG22	1:L:88:ILE:HD13	2.01	0.42
2:M:91:ASN:HB2	2:N:82:ILE:HB	2.01	0.42
1:E:51:GLU:HG3	1:E:79:PRO:HB3	2.01	0.42
1:C:81:PRO:HD3	1:F:54:THR:O	2.19	0.42
1:J:51:GLU:HG3	1:J:79:PRO:HB3	2.02	0.42
1:K:23:THR:HG22	1:K:88:ILE:HG21	2.00	0.42
1:L:115:ARG:HE	1:L:117:ASP:CG	2.22	0.42
2:T:67:LEU:O	2:T:71:VAL:HG23	2.19	0.42
1:K:23:THR:HG21	1:K:58:PRO:HB3	2.01	0.42
2:X:35:PRO:HA	2:X:53:LEU:HG	2.02	0.42
2:T:93:GLU:H	2:T:93:GLU:HG3	1.63	0.42
1:F:51:GLU:HG3	1:F:79:PRO:HB3	2.02	0.42
2:V:64:PHE:CE2	2:V:68:LYS:HG3	2.54	0.42
1:A:63:ARG:HD3	1:B:115:ARG:NH1	2.35	0.42
2:M:93:GLU:HB2	2:N:79:VAL:HG13	2.02	0.41
2:R:7:ILE:HA	2:R:81:GLU:O	2.20	0.41
2:S:7:ILE:HA	2:S:81:GLU:O	2.20	0.41
2:W:7:ILE:HA	2:W:81:GLU:O	2.20	0.41
1:E:37:GLN:HE21	1:E:37:GLN:H	1.68	0.41
2:P:7:ILE:HA	2:P:81:GLU:O	2.20	0.41
2:X:6:LEU:HD11	2:X:85:LEU:HD11	2.02	0.41
2:N:93:GLU:H	2:N:93:GLU:HG3	1.67	0.41
1:A:24:ILE:HG23	1:A:65:ILE:HG21	2.03	0.41
1:J:115:ARG:HE	1:J:117:ASP:CG	2.23	0.41
2:P:68:LYS:NZ	2:R:92:ARG:HE	2.18	0.41
2:T:6:LEU:HD11	2:T:85:LEU:HD11	2.03	0.41
2:V:87:ILE:HG21	2:V:95:LEU:HD21	2.03	0.41
1:H:23:THR:HG21	1:H:58:PRO:HB3	2.03	0.41
2:S:9:VAL:HG21	2:S:15:ALA:HB2	2.03	0.41
1:L:23:THR:HG22	1:L:88:ILE:HG21	2.02	0.41
1:G:80:VAL:HA	1:I:54:THR:O	2.21	0.41
2:X:64:PHE:CE2	2:X:68:LYS:HG3	2.55	0.41
1:F:23:THR:HG22	1:F:88:ILE:HD13	2.02	0.41
2:T:91:ASN:HB2	2:U:82:ILE:HB	2.02	0.41
2:M:91:ASN:HA	2:N:68:LYS:HD3	2.02	0.40
2:V:5:VAL:HB	2:V:57:VAL:HB	2.03	0.40
2:M:47:VAL:HG21	2:O:24:GLU:HA	2.04	0.40
2:T:23:VAL:HG12	2:U:47:VAL:HG22	2.03	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	119/130 (92%)	114 (96%)	5 (4%)	0	100	100
1	B	119/130 (92%)	113 (95%)	6 (5%)	0	100	100
1	C	119/130 (92%)	113 (95%)	6 (5%)	0	100	100
1	D	119/130 (92%)	113 (95%)	6 (5%)	0	100	100
1	E	119/130 (92%)	115 (97%)	4 (3%)	0	100	100
1	F	119/130 (92%)	113 (95%)	6 (5%)	0	100	100
1	G	119/130 (92%)	115 (97%)	4 (3%)	0	100	100
1	H	119/130 (92%)	113 (95%)	6 (5%)	0	100	100
1	I	119/130 (92%)	112 (94%)	6 (5%)	1 (1%)	19	51
1	J	119/130 (92%)	113 (95%)	6 (5%)	0	100	100
1	K	119/130 (92%)	113 (95%)	6 (5%)	0	100	100
1	L	119/130 (92%)	113 (95%)	6 (5%)	0	100	100
2	M	101/111 (91%)	100 (99%)	1 (1%)	0	100	100
2	N	101/111 (91%)	96 (95%)	5 (5%)	0	100	100
2	O	101/111 (91%)	101 (100%)	0	0	100	100
2	P	101/111 (91%)	101 (100%)	0	0	100	100
2	Q	107/111 (96%)	104 (97%)	3 (3%)	0	100	100
2	R	101/111 (91%)	100 (99%)	1 (1%)	0	100	100
2	S	101/111 (91%)	98 (97%)	1 (1%)	2 (2%)	7	30
2	T	101/111 (91%)	97 (96%)	4 (4%)	0	100	100
2	U	101/111 (91%)	99 (98%)	2 (2%)	0	100	100
2	V	101/111 (91%)	96 (95%)	5 (5%)	0	100	100
2	W	101/111 (91%)	99 (98%)	2 (2%)	0	100	100
2	X	101/111 (91%)	100 (99%)	1 (1%)	0	100	100
All	All	2646/2892 (92%)	2551 (96%)	92 (4%)	3 (0%)	51	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	37	GLN
2	S	26	ARG
2	S	25	GLU

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	98/109 (90%)	95 (97%)	3 (3%)	40	68
1	B	98/109 (90%)	95 (97%)	3 (3%)	40	68
1	C	98/109 (90%)	95 (97%)	3 (3%)	40	68
1	D	98/109 (90%)	96 (98%)	2 (2%)	55	77
1	E	98/109 (90%)	95 (97%)	3 (3%)	40	68
1	F	98/109 (90%)	95 (97%)	3 (3%)	40	68
1	G	98/109 (90%)	95 (97%)	3 (3%)	40	68
1	H	98/109 (90%)	95 (97%)	3 (3%)	40	68
1	I	97/109 (89%)	95 (98%)	2 (2%)	53	76
1	J	98/109 (90%)	94 (96%)	4 (4%)	30	59
1	K	98/109 (90%)	95 (97%)	3 (3%)	40	68
1	L	98/109 (90%)	94 (96%)	4 (4%)	30	59
2	M	90/98 (92%)	86 (96%)	4 (4%)	28	58
2	N	90/98 (92%)	86 (96%)	4 (4%)	28	58
2	O	90/98 (92%)	85 (94%)	5 (6%)	21	51
2	P	90/98 (92%)	86 (96%)	4 (4%)	28	58
2	Q	95/98 (97%)	85 (90%)	10 (10%)	7	25
2	R	90/98 (92%)	86 (96%)	4 (4%)	28	58
2	S	90/98 (92%)	85 (94%)	5 (6%)	21	51
2	T	90/98 (92%)	87 (97%)	3 (3%)	38	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	U	90/98 (92%)	86 (96%)	4 (4%)	28 58
2	V	90/98 (92%)	86 (96%)	4 (4%)	28 58
2	W	90/98 (92%)	87 (97%)	3 (3%)	38 66
2	X	90/98 (92%)	86 (96%)	4 (4%)	28 58
All	All	2260/2484 (91%)	2170 (96%)	90 (4%)	31 60

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	THR
1	A	37	GLN
1	A	101	ASP
1	B	23	THR
1	B	37	GLN
1	B	101	ASP
1	C	23	THR
1	C	37	GLN
1	C	101	ASP
1	D	23	THR
1	D	101	ASP
1	E	23	THR
1	E	37	GLN
1	E	101	ASP
1	F	23	THR
1	F	37	GLN
1	F	101	ASP
1	G	23	THR
1	G	37	GLN
1	G	101	ASP
1	H	23	THR
1	H	37	GLN
1	H	101	ASP
1	I	23	THR
1	I	101	ASP
1	J	23	THR
1	J	37	GLN
1	J	101	ASP
1	J	102	ARG
1	K	23	THR
1	K	37	GLN
1	K	101	ASP

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Mol	Chain	Res	Type
1	L	23	THR
1	L	37	GLN
1	L	69	ARG
1	L	101	ASP
2	M	13	LEU
2	M	50	ASP
2	M	68	LYS
2	M	70	ARG
2	N	13	LEU
2	N	68	LYS
2	N	70	ARG
2	N	98	LEU
2	O	13	LEU
2	O	61	THR
2	O	68	LYS
2	O	70	ARG
2	O	102	THR
2	P	13	LEU
2	P	61	THR
2	P	68	LYS
2	P	70	ARG
2	Q	3	GLU
2	Q	13	LEU
2	Q	25	GLU
2	Q	61	THR
2	Q	62	ASP
2	Q	68	LYS
2	Q	70	ARG
2	Q	92	ARG
2	Q	99	ARG
2	Q	108	HIS
2	R	13	LEU
2	R	39	SER
2	R	68	LYS
2	R	70	ARG
2	S	13	LEU
2	S	17	LYS
2	S	25	GLU
2	S	68	LYS
2	S	70	ARG
2	T	13	LEU
2	T	68	LYS

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Mol	Chain	Res	Type
2	T	70	ARG
2	U	13	LEU
2	U	52	GLU
2	U	68	LYS
2	U	70	ARG
2	V	43	GLU
2	V	46	SER
2	V	68	LYS
2	V	70	ARG
2	W	13	LEU
2	W	68	LYS
2	W	70	ARG
2	X	13	LEU
2	X	66	LYS
2	X	68	LYS
2	X	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	B	37	GLN
1	C	37	GLN
1	E	37	GLN
1	F	37	GLN
1	G	37	GLN
1	H	37	GLN
1	K	37	GLN
1	L	37	GLN
2	O	51	HIS
2	P	51	HIS
2	Q	51	HIS
2	Q	107	HIS
2	R	20	HIS
2	R	51	HIS
2	S	51	HIS
2	T	51	HIS
2	V	20	HIS
2	V	51	HIS

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	117/130 (90%)	0.01	1 (0%) 84 83	40, 63, 86, 126	9 (7%)
1	B	117/130 (90%)	0.17	3 (2%) 56 54	45, 64, 85, 147	9 (7%)
1	C	117/130 (90%)	0.21	1 (0%) 84 83	53, 73, 102, 139	9 (7%)
1	D	117/130 (90%)	0.07	1 (0%) 84 83	43, 62, 86, 125	9 (7%)
1	E	117/130 (90%)	0.20	0 100 100	51, 69, 93, 142	9 (7%)
1	F	117/130 (90%)	0.23	2 (1%) 70 68	48, 68, 98, 119	9 (7%)
1	G	117/130 (90%)	0.18	2 (1%) 70 68	48, 66, 94, 124	9 (7%)
1	H	117/130 (90%)	0.39	1 (0%) 84 83	47, 63, 90, 124	9 (7%)
1	I	117/130 (90%)	0.32	2 (1%) 70 68	46, 65, 86, 113	9 (7%)
1	J	117/130 (90%)	0.01	1 (0%) 84 83	48, 65, 87, 141	9 (7%)
1	K	117/130 (90%)	-0.13	0 100 100	47, 64, 90, 111	9 (7%)
1	L	117/130 (90%)	-0.07	1 (0%) 84 83	52, 69, 91, 137	9 (7%)
2	M	103/111 (92%)	0.31	1 (0%) 82 81	56, 80, 108, 120	0
2	N	103/111 (92%)	0.19	2 (1%) 66 65	57, 82, 110, 135	0
2	O	103/111 (92%)	0.32	1 (0%) 82 81	58, 77, 109, 138	0
2	P	103/111 (92%)	-0.03	0 100 100	48, 67, 96, 122	0
2	Q	109/111 (98%)	0.23	1 (0%) 84 83	51, 71, 98, 114	0
2	R	103/111 (92%)	0.19	1 (0%) 82 81	51, 67, 91, 114	0
2	S	103/111 (92%)	0.06	1 (0%) 82 81	45, 67, 100, 119	0
2	T	103/111 (92%)	0.58	2 (1%) 66 65	54, 70, 103, 124	0
2	U	103/111 (92%)	0.35	2 (1%) 66 65	52, 72, 98, 115	0
2	V	103/111 (92%)	0.09	1 (0%) 82 81	48, 70, 105, 117	0
2	W	103/111 (92%)	0.09	1 (0%) 82 81	52, 71, 99, 117	0
2	X	103/111 (92%)	0.17	0 100 100	43, 70, 100, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	2646/2892 (91%)	0.17	28 (1%)	80	79	40, 69, 102, 147	108 (4%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	116	PRO	4.4
1	F	116	PRO	3.7
1	G	116	PRO	3.3
2	N	103	GLY	3.2
2	N	63	ALA	3.0
1	J	116	PRO	3.0
1	H	116	PRO	3.0
2	M	45	GLY	2.9
2	U	1	MET	2.8
1	L	116	PRO	2.7
1	F	69	ARG	2.5
1	I	92	ALA	2.4
2	W	74	LEU	2.4
1	D	116	PRO	2.4
1	B	117	ASP	2.3
2	T	47	VAL	2.3
2	V	103	GLY	2.3
2	R	39	SER	2.3
2	U	82	ILE	2.2
2	S	88	ALA	2.2
1	A	69	ARG	2.2
2	Q	1	MET	2.1
1	C	43	ALA	2.0
2	T	29	ALA	2.0
2	O	21	ALA	2.0
1	I	29	LYS	2.0
1	B	5	ILE	2.0
1	G	104	ARG	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.