wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2024 – 10:30 AM EDT

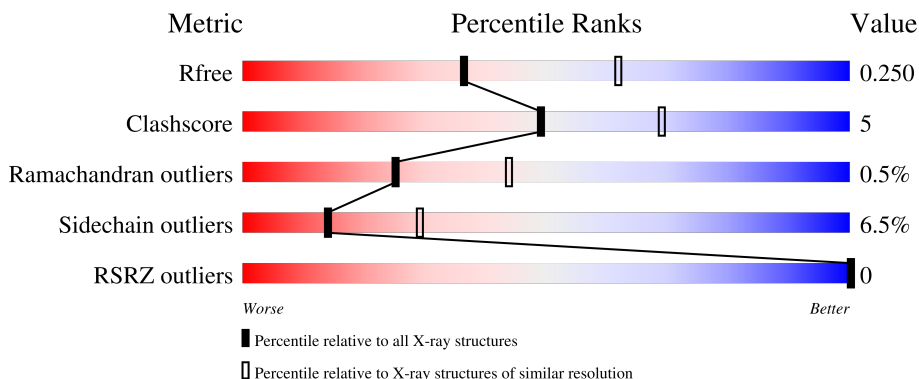|		
PDB ID	:	4JUR
Title	:	Crystal structure of the effector Tae4 from Salmonella typhimurium in complex with the immunity Tai4 from Enterobacter cloacae
Authors	:	Zhang, H.; Gao, Z.Q.; Dong, Y.H.
Deposited on	:	2013-03-25
Resolution	:	2.50 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	Percentile Ranks	Value
Rfree		0.250
Clashscore		5
Ramachandran outliers		0.5%
Sidechain outliers		6.5%
RSRZ outliers		0

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	176	80% 11% • 9%
1	B	176	79% 11% • 9%
1	C	176	74% 18% 9%
1	D	176	66% 22% • 9%
1	E	176	74% 15% • 9%

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Mol	Chain	Length	Quality of chain
1	F	176	78%　　　　　　　　　　11%　・　9%
1	G	176	75%　　　　　　　　　　13%　・　9%
1	H	176	74%　　　　　　　　　　16%　　10%
2	I	105	74%　　　　　　　　　　15%　・　8%
2	J	105	79%　　　　　　　　　　10%　・　8%
2	K	105	71%　　　　　　　　　　17%　・　8%
2	L	105	72%　　　　　　　　　　19%　・　8%
2	M	105	77%　　　　　　　　　　13%　・　8%
2	N	105	81%　　　　　　　　　　10%　・　8%
2	O	105	77%　　　　　　　　　　13%　・　9%
2	P	105	83%　　　　　　　　　　9%　・　8%

2   Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15975 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 Putative cytoplasmic protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	161	Total 1241	C 794	N 216	O 224	S 3	Se 4	0	0	0
1	B	160	Total 1231	C 786	N 217	O 222	S 3	Se 3	0	0	0
1	C	161	Total 1241	C 792	N 218	O 224	S 3	Se 4	0	0	0
1	D	160	Total 1234	C 789	N 218	O 221	S 3	Se 3	0	0	0
1	E	160	Total 1238	C 791	N 219	O 222	S 3	Se 3	0	0	0
1	F	160	Total 1228	C 785	N 215	O 222	S 3	Se 3	0	0	0
1	G	160	Total 1230	C 786	N 215	O 223	S 3	Se 3	0	0	0
1	H	159	Total 1222	C 783	N 215	O 218	S 3	Se 3	0	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP Q93IS4
A	-13	MSE	-	expression tag	UNP Q93IS4
A	-12	ALA	-	expression tag	UNP Q93IS4
A	-11	SER	-	expression tag	UNP Q93IS4
A	-10	MSE	-	expression tag	UNP Q93IS4
A	-9	THR	-	expression tag	UNP Q93IS4
A	-8	GLY	-	expression tag	UNP Q93IS4
A	-7	GLY	-	expression tag	UNP Q93IS4
A	-6	GLN	-	expression tag	UNP Q93IS4
A	-5	GLN	-	expression tag	UNP Q93IS4
A	-4	MSE	-	expression tag	UNP Q93IS4
A	-3	GLY	-	expression tag	UNP Q93IS4
A	-2	ARG	-	expression tag	UNP Q93IS4

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W O R L D W I D E
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PROTEIN DATA BANK

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q93IS4
A	0	SER	-	expression tag	UNP Q93IS4
B	-14	HIS	-	expression tag	UNP Q93IS4
B	-13	MSE	-	expression tag	UNP Q93IS4
B	-12	ALA	-	expression tag	UNP Q93IS4
B	-11	SER	-	expression tag	UNP Q93IS4
B	-10	MSE	-	expression tag	UNP Q93IS4
B	-9	THR	-	expression tag	UNP Q93IS4
B	-8	GLY	-	expression tag	UNP Q93IS4
B	-7	GLY	-	expression tag	UNP Q93IS4
B	-6	GLN	-	expression tag	UNP Q93IS4
B	-5	GLN	-	expression tag	UNP Q93IS4
B	-4	MSE	-	expression tag	UNP Q93IS4
B	-3	GLY	-	expression tag	UNP Q93IS4
B	-2	ARG	-	expression tag	UNP Q93IS4
B	-1	GLY	-	expression tag	UNP Q93IS4
B	0	SER	-	expression tag	UNP Q93IS4
C	-14	HIS	-	expression tag	UNP Q93IS4
C	-13	MSE	-	expression tag	UNP Q93IS4
C	-12	ALA	-	expression tag	UNP Q93IS4
C	-11	SER	-	expression tag	UNP Q93IS4
C	-10	MSE	-	expression tag	UNP Q93IS4
C	-9	THR	-	expression tag	UNP Q93IS4
C	-8	GLY	-	expression tag	UNP Q93IS4
C	-7	GLY	-	expression tag	UNP Q93IS4
C	-6	GLN	-	expression tag	UNP Q93IS4
C	-5	GLN	-	expression tag	UNP Q93IS4
C	-4	MSE	-	expression tag	UNP Q93IS4
C	-3	GLY	-	expression tag	UNP Q93IS4
C	-2	ARG	-	expression tag	UNP Q93IS4
C	-1	GLY	-	expression tag	UNP Q93IS4
C	0	SER	-	expression tag	UNP Q93IS4
D	-14	HIS	-	expression tag	UNP Q93IS4
D	-13	MSE	-	expression tag	UNP Q93IS4
D	-12	ALA	-	expression tag	UNP Q93IS4
D	-11	SER	-	expression tag	UNP Q93IS4
D	-10	MSE	-	expression tag	UNP Q93IS4
D	-9	THR	-	expression tag	UNP Q93IS4
D	-8	GLY	-	expression tag	UNP Q93IS4
D	-7	GLY	-	expression tag	UNP Q93IS4
D	-6	GLN	-	expression tag	UNP Q93IS4
D	-5	GLN	-	expression tag	UNP Q93IS4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	MSE	-	expression tag	UNP Q93IS4
D	-3	GLY	-	expression tag	UNP Q93IS4
D	-2	ARG	-	expression tag	UNP Q93IS4
D	-1	GLY	-	expression tag	UNP Q93IS4
D	0	SER	-	expression tag	UNP Q93IS4
E	-14	HIS	-	expression tag	UNP Q93IS4
E	-13	MSE	-	expression tag	UNP Q93IS4
E	-12	ALA	-	expression tag	UNP Q93IS4
E	-11	SER	-	expression tag	UNP Q93IS4
E	-10	MSE	-	expression tag	UNP Q93IS4
E	-9	THR	-	expression tag	UNP Q93IS4
E	-8	GLY	-	expression tag	UNP Q93IS4
E	-7	GLY	-	expression tag	UNP Q93IS4
E	-6	GLN	-	expression tag	UNP Q93IS4
E	-5	GLN	-	expression tag	UNP Q93IS4
E	-4	MSE	-	expression tag	UNP Q93IS4
E	-3	GLY	-	expression tag	UNP Q93IS4
E	-2	ARG	-	expression tag	UNP Q93IS4
E	-1	GLY	-	expression tag	UNP Q93IS4
E	0	SER	-	expression tag	UNP Q93IS4
F	-14	HIS	-	expression tag	UNP Q93IS4
F	-13	MSE	-	expression tag	UNP Q93IS4
F	-12	ALA	-	expression tag	UNP Q93IS4
F	-11	SER	-	expression tag	UNP Q93IS4
F	-10	MSE	-	expression tag	UNP Q93IS4
F	-9	THR	-	expression tag	UNP Q93IS4
F	-8	GLY	-	expression tag	UNP Q93IS4
F	-7	GLY	-	expression tag	UNP Q93IS4
F	-6	GLN	-	expression tag	UNP Q93IS4
F	-5	GLN	-	expression tag	UNP Q93IS4
F	-4	MSE	-	expression tag	UNP Q93IS4
F	-3	GLY	-	expression tag	UNP Q93IS4
F	-2	ARG	-	expression tag	UNP Q93IS4
F	-1	GLY	-	expression tag	UNP Q93IS4
F	0	SER	-	expression tag	UNP Q93IS4
G	-14	HIS	-	expression tag	UNP Q93IS4
G	-13	MSE	-	expression tag	UNP Q93IS4
G	-12	ALA	-	expression tag	UNP Q93IS4
G	-11	SER	-	expression tag	UNP Q93IS4
G	-10	MSE	-	expression tag	UNP Q93IS4
G	-9	THR	-	expression tag	UNP Q93IS4
G	-8	GLY	-	expression tag	UNP Q93IS4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	GLY	-	expression tag	UNP Q93IS4
G	-6	GLN	-	expression tag	UNP Q93IS4
G	-5	GLN	-	expression tag	UNP Q93IS4
G	-4	MSE	-	expression tag	UNP Q93IS4
G	-3	GLY	-	expression tag	UNP Q93IS4
G	-2	ARG	-	expression tag	UNP Q93IS4
G	-1	GLY	-	expression tag	UNP Q93IS4
G	0	SER	-	expression tag	UNP Q93IS4
H	-14	HIS	-	expression tag	UNP Q93IS4
H	-13	MSE	-	expression tag	UNP Q93IS4
H	-12	ALA	-	expression tag	UNP Q93IS4
H	-11	SER	-	expression tag	UNP Q93IS4
H	-10	MSE	-	expression tag	UNP Q93IS4
H	-9	THR	-	expression tag	UNP Q93IS4
H	-8	GLY	-	expression tag	UNP Q93IS4
H	-7	GLY	-	expression tag	UNP Q93IS4
H	-6	GLN	-	expression tag	UNP Q93IS4
H	-5	GLN	-	expression tag	UNP Q93IS4
H	-4	MSE	-	expression tag	UNP Q93IS4
H	-3	GLY	-	expression tag	UNP Q93IS4
H	-2	ARG	-	expression tag	UNP Q93IS4
H	-1	GLY	-	expression tag	UNP Q93IS4
H	0	SER	-	expression tag	UNP Q93IS4

- Molecule 2 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	97	Total 735	C 462	N 124	O 147	S 2	0	0	0
2	J	97	Total 735	C 463	N 125	O 145	S 2	0	0	0
2	K	97	Total 739	C 464	N 124	O 149	S 2	0	0	0
2	L	97	Total 741	C 465	N 125	O 149	S 2	0	0	0
2	M	97	Total 741	C 466	N 126	O 147	S 2	0	0	0
2	N	97	Total 736	C 463	N 124	O 147	S 2	0	0	0
2	O	96	Total 730	C 460	N 123	O 145	S 2	0	0	0
2	P	97	Total 733	C 462	N 124	O 145	S 2	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	118	HIS	-	expression tag	UNP D5C6F7
I	119	HIS	-	expression tag	UNP D5C6F7
I	120	HIS	-	expression tag	UNP D5C6F7
I	121	HIS	-	expression tag	UNP D5C6F7
I	122	HIS	-	expression tag	UNP D5C6F7
I	123	HIS	-	expression tag	UNP D5C6F7
J	118	HIS	-	expression tag	UNP D5C6F7
J	119	HIS	-	expression tag	UNP D5C6F7
J	120	HIS	-	expression tag	UNP D5C6F7
J	121	HIS	-	expression tag	UNP D5C6F7
J	122	HIS	-	expression tag	UNP D5C6F7
J	123	HIS	-	expression tag	UNP D5C6F7
K	118	HIS	-	expression tag	UNP D5C6F7
K	119	HIS	-	expression tag	UNP D5C6F7
K	120	HIS	-	expression tag	UNP D5C6F7
K	121	HIS	-	expression tag	UNP D5C6F7
K	122	HIS	-	expression tag	UNP D5C6F7
K	123	HIS	-	expression tag	UNP D5C6F7
L	118	HIS	-	expression tag	UNP D5C6F7
L	119	HIS	-	expression tag	UNP D5C6F7
L	120	HIS	-	expression tag	UNP D5C6F7
L	121	HIS	-	expression tag	UNP D5C6F7
L	122	HIS	-	expression tag	UNP D5C6F7
L	123	HIS	-	expression tag	UNP D5C6F7
M	118	HIS	-	expression tag	UNP D5C6F7
M	119	HIS	-	expression tag	UNP D5C6F7
M	120	HIS	-	expression tag	UNP D5C6F7
M	121	HIS	-	expression tag	UNP D5C6F7
M	122	HIS	-	expression tag	UNP D5C6F7
M	123	HIS	-	expression tag	UNP D5C6F7
N	118	HIS	-	expression tag	UNP D5C6F7
N	119	HIS	-	expression tag	UNP D5C6F7
N	120	HIS	-	expression tag	UNP D5C6F7
N	121	HIS	-	expression tag	UNP D5C6F7
N	122	HIS	-	expression tag	UNP D5C6F7
N	123	HIS	-	expression tag	UNP D5C6F7
O	118	HIS	-	expression tag	UNP D5C6F7
O	119	HIS	-	expression tag	UNP D5C6F7
O	120	HIS	-	expression tag	UNP D5C6F7
O	121	HIS	-	expression tag	UNP D5C6F7
O	122	HIS	-	expression tag	UNP D5C6F7
O	123	HIS	-	expression tag	UNP D5C6F7

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Chain	Residue	Modelled	Actual	Comment	Reference
P	118	HIS	-	expression tag	UNP D5C6F7
P	119	HIS	-	expression tag	UNP D5C6F7
P	120	HIS	-	expression tag	UNP D5C6F7
P	121	HIS	-	expression tag	UNP D5C6F7
P	122	HIS	-	expression tag	UNP D5C6F7
P	123	HIS	-	expression tag	UNP D5C6F7

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total 16	O 16	0	0
3	B	18	Total 18	O 18	0	0
3	C	19	Total 19	O 19	0	0
3	D	9	Total 9	O 9	0	0
3	E	12	Total 12	O 12	0	0
3	F	7	Total 7	O 7	0	0
3	G	10	Total 10	O 10	0	0
3	H	14	Total 14	O 14	0	0
3	I	21	Total 21	O 21	0	0
3	J	12	Total 12	O 12	0	0
3	K	15	Total 15	O 15	0	0
3	L	13	Total 13	O 13	0	0
3	M	15	Total 15	O 15	0	0
3	N	12	Total 12	O 12	0	0
3	O	14	Total 14	O 14	0	0
3	P	13	Total 13	O 13	0	0

3 Residue-property plots ⓘ

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

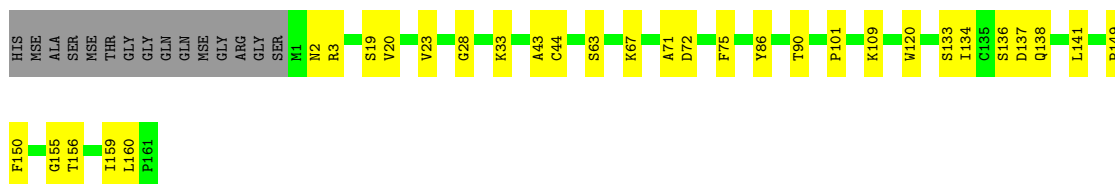• Molecule 1: Putative cytoplasmic protein

Chain A:

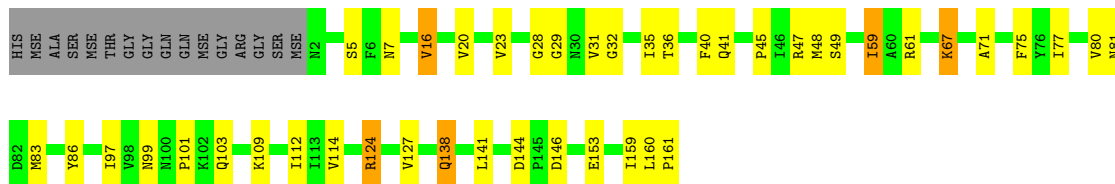• Molecule 1: Putative cytoplasmic protein

Chain B:

• Molecule 1: Putative cytoplasmic protein

Chain C:

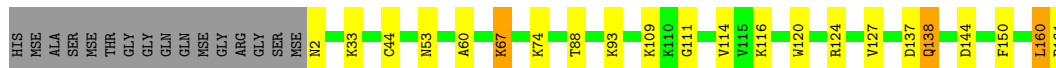• Molecule 1: Putative cytoplasmic protein

Chain D:

• Molecule 1: Putative cytoplasmic protein

Chain E:

HIS MSE ALA SER MSE THR GLY GLN GLN GLN MSE GLY ARG GLY SER MSE N2 R3 P4 S5 F13 R14 K15 S25 N30 C44 P45 M48 S49 Y50 N53 K67 V68 D72 N73 K74 F75 Y76 I77 M83 V114 R124 V127 S136 H140 L141

P149 P152 L160 P161

• Molecule 1: Putative cytoplasmic protein

Chain F: 78% 11% • 9%

HIS MSE ALA SER MSE THR GLY GLN GLN GLN MSE GLY ARG GLY SER MSE N2 K33 C44 N53 A60 K67 K74 T88 K93 K109 K110 G111 V114 V115 K116 W120 R124 V127 D137 Q138 D144 F150 L160 P161

• Molecule 1: Putative cytoplasmic protein

Chain G: 75% 13% • 9%

HIS MSE ALA SER MSE THR GLY GLN GLN GLN MSE GLY ARG GLY SER MSE N2 S5 E8 N30 V31 G32 I35 T36 Q41 C44 P45 S63 K67 V68 I77 M83 T88 H89 T90 M91 G92 K93 L96 S104 K109 D137 Q138 D144

V151 P152 W158 P161

• Molecule 1: Putative cytoplasmic protein

Chain H: 74% 16% 10%

HIS MSE ALA SER MSE THR GLY GLN GLN GLN MSE GLY ARG GLY SER MSE ASN R3 F13 S19 V23 G37 Q41 P45 M48 L52 S63 K67 I77 V80 M83 P94 D95 L96 I97 I112 I113 V114 N122 A123 R124 V127

S136 L142 V151 V154 G155 T156 L157 W158 I159 L160 P161

• Molecule 2: Uncharacterized protein

Chain I: 74% 15% • 8%

GLN T20 W36 V37 Q38 N39 R40 D47 S48 K49 S50 L51 K52 E53 S82 K85 Q86 K87 V88 T91 E92 P93 G94 K100 L103 S115 S116 LYS HIS HIS HIS HIS HIS

• Molecule 2: Uncharacterized protein

Chain J: 79% 10% • 8%

Q19 D23 T26 Q38 N39 D47 L51 W62 L63 E64 A76 I80 E92 I98 R111 K114 S115 SER LYS HIS HIS HIS HIS HIS

• Molecule 2: Uncharacterized protein

W O R L D W I D E
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Chain K:

71%   17%   •   8%

GLN T20 Q30 W36 V37 Q38 N39 R40 C41 I42 G43 K44 I45 A46 S50 L51 S58 E71 K75 A76 D77 V81 L84 E92 P93 Y96 Q97 S116 LYS HIS HIS HIS HIS HIS

• Molecule 2: Uncharacterized protein

Chain L:

72%   19%   •   8%

GLN T20 Q30 V37 Q38 N39 R40 D47 S48 K49 S50 S58 A59 A60 L68 P69 D77 I80 L84 G89 E92 H95 I98 L99 K100 K114 S115 S116 LYS HIS HIS HIS HIS HIS

• Molecule 2: Uncharacterized protein

Chain M:

77%   13%   •   8%

Q19 F33 Q38 N39 D47 L51 D54 A76 I80 I98 L103 D108 R111 P112 L113 K114 S115 SER LYS HIS HIS HIS HIS HIS

• Molecule 2: Uncharacterized protein

Chain N:

81%   10%   •   8%

GLN T20 Q38 N39 R40 D47 A55 E71 D77 L84 G89 E92 P93 G94 K100 A105 S116 LYS HIS HIS HIS HIS HIS

• Molecule 2: Uncharacterized protein

Chain O:

77%   13%   •   9%

GLN T20 E34 Q38 D47 D54 A57 L84 G89 E92 P93 G94 I98 L99 K100 R111 K114 S115 SER LYS HIS HIS HIS HIS HIS

• Molecule 2: Uncharacterized protein

Chain P:

83%   9%   •   8%

GLN T20 Q38 N39 R40 E53 A60 Q86 G89 E92 Y96 S115 S116 LYS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.95Å 89.12Å 271.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.19 – 2.50 46.19 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.19-2.50) 98.9 (46.19-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.07 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.207 , 0.261 0.198 , 0.250	Depositor DCC
R_{free} test set	3772 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	49.0	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 19.5	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.467 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15975	wwPDB-VP
Average B, all atoms (Å^2)	49.0	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.*

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[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	0.47	0/1273	0.58	0/1728
1	B	0.48	0/1263	0.60	0/1716
1	C	0.47	0/1273	0.61	0/1729
1	D	0.45	0/1266	0.63	0/1719
1	E	0.48	0/1270	0.62	0/1723
1	F	0.43	0/1260	0.58	0/1712
1	G	0.42	0/1262	0.58	0/1715
1	H	0.46	0/1254	0.58	0/1703
2	I	0.53	0/747	0.62	1/1014 (0.1%)
2	J	0.53	0/747	0.63	0/1014
2	K	0.50	0/751	0.61	0/1019
2	L	0.56	0/753	0.59	0/1021
2	M	0.53	0/753	0.60	0/1021
2	N	0.51	0/748	0.57	0/1015
2	O	0.51	0/742	0.60	0/1007
2	P	0.53	0/745	0.60	0/1011
All	All	0.48	0/16107	0.60	1/21867 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	94	GLY	N-CA-C	5.02	125.65	113.10

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	1241	0	1202	8	0
1	B	1231	0	1187	9	0
1	C	1241	0	1198	14	0
1	D	1234	0	1195	30	0
1	E	1238	0	1207	14	0
1	F	1228	0	1185	10	0
1	G	1230	0	1184	14	0
1	H	1222	0	1180	16	0
2	I	735	0	718	9	0
2	J	735	0	719	10	0
2	K	739	0	722	11	0
2	L	741	0	729	9	0
2	M	741	0	730	9	0
2	N	736	0	720	6	0
2	O	730	0	715	9	0
2	P	733	0	718	7	0
3	A	16	0	0	0	0
3	B	18	0	0	0	0
3	C	19	0	0	0	0
3	D	9	0	0	0	0
3	E	12	0	0	0	0
3	F	7	0	0	0	0
3	G	10	0	0	0	0
3	H	14	0	0	0	0
3	I	21	0	0	1	0
3	J	12	0	0	0	0
3	K	15	0	0	0	0
3	L	13	0	0	0	0
3	M	15	0	0	0	0
3	N	12	0	0	0	0
3	O	14	0	0	0	0
3	P	13	0	0	0	0
All	All	15975	0	15309	164	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 5.

The worst 5 of 164 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:49:SER:HB3	1:D:83:MSE:HE1	1.69	0.72
1:H:112:ILE:HG13	1:H:160:LEU:HD11	1.71	0.72
1:D:16:VAL:HG22	1:D:23:VAL:HG23	1.73	0.70
2:K:44:LYS:NZ	2:K:77:ASP:OD1	2.25	0.70
1:H:122:ASN:HD21	2:I:91:THR:HG22	1.58	0.69

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	159/176 (90%)	153 (96%)	5 (3%)	1 (1%)	22	39
1	B	158/176 (90%)	153 (97%)	5 (3%)	0	100	100
1	C	159/176 (90%)	150 (94%)	7 (4%)	2 (1%)	10	19
1	D	158/176 (90%)	146 (92%)	10 (6%)	2 (1%)	10	19
1	E	158/176 (90%)	154 (98%)	4 (2%)	0	100	100
1	F	158/176 (90%)	150 (95%)	8 (5%)	0	100	100
1	G	158/176 (90%)	153 (97%)	5 (3%)	0	100	100
1	H	157/176 (89%)	148 (94%)	9 (6%)	0	100	100
2	I	95/105 (90%)	92 (97%)	1 (1%)	2 (2%)	5	10
2	J	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
2	K	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
2	L	95/105 (90%)	95 (100%)	0	0	100	100
2	M	95/105 (90%)	92 (97%)	3 (3%)	0	100	100
2	N	95/105 (90%)	94 (99%)	0	1 (1%)	12	23
2	O	94/105 (90%)	91 (97%)	1 (1%)	2 (2%)	5	10
2	P	95/105 (90%)	95 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2024/2248 (90%)	1954 (96%)	60 (3%)	10 (0%)	25 44

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2	ASN
2	I	93	PRO
2	I	94	GLY
1	C	72	ASP
1	D	29	GLY

5.3.2   Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	132/138 (96%)	126 (96%)	6 (4%)	23	46
1	B	131/138 (95%)	121 (92%)	10 (8%)	11	22
1	C	132/138 (96%)	126 (96%)	6 (4%)	23	46
1	D	131/138 (95%)	124 (95%)	7 (5%)	19	38
1	E	133/138 (96%)	122 (92%)	11 (8%)	9	19
1	F	131/138 (95%)	122 (93%)	9 (7%)	13	26
1	G	131/138 (95%)	121 (92%)	10 (8%)	11	22
1	H	128/138 (93%)	121 (94%)	7 (6%)	18	37
2	I	79/90 (88%)	73 (92%)	6 (8%)	11	22
2	J	78/90 (87%)	73 (94%)	5 (6%)	14	30
2	K	80/90 (89%)	71 (89%)	9 (11%)	4	9
2	L	81/90 (90%)	74 (91%)	7 (9%)	8	18
2	M	80/90 (89%)	75 (94%)	5 (6%)	15	30
2	N	79/90 (88%)	75 (95%)	4 (5%)	20	40
2	O	78/90 (87%)	75 (96%)	3 (4%)	28	53
2	P	78/90 (87%)	74 (95%)	4 (5%)	20	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1682/1824 (92%)	1573 (94%)	109 (6%)	14 29

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	144	ASP
2	I	115	SER
2	N	47	ASP
1	H	52	LEU
1	H	156	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	I	38	GLN
2	J	39	ASN
2	K	38	GLN
2	K	39	ASN
2	L	39	ASN

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 oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	157/176 (89%)	-1.34	0	100	100	37, 48, 63, 78	0
1	B	157/176 (89%)	-1.30	0	100	100	39, 49, 62, 73	0
1	C	157/176 (89%)	-1.33	0	100	100	38, 49, 63, 76	0
1	D	157/176 (89%)	-1.30	0	100	100	40, 50, 63, 71	0
1	E	157/176 (89%)	-1.26	0	100	100	40, 49, 62, 74	0
1	F	157/176 (89%)	-1.22	0	100	100	45, 54, 66, 71	0
1	G	157/176 (89%)	-1.24	0	100	100	45, 54, 66, 76	0
1	H	156/176 (88%)	-1.27	0	100	100	39, 50, 61, 73	0
2	I	97/105 (92%)	-1.36	0	100	100	32, 43, 63, 70	0
2	J	97/105 (92%)	-1.32	0	100	100	32, 46, 66, 72	0
2	K	97/105 (92%)	-1.33	0	100	100	31, 43, 62, 68	0
2	L	97/105 (92%)	-1.39	0	100	100	34, 45, 59, 65	0
2	M	97/105 (92%)	-1.26	0	100	100	33, 46, 68, 73	0
2	N	97/105 (92%)	-1.34	0	100	100	35, 48, 65, 73	0
2	O	96/105 (91%)	-1.33	0	100	100	36, 48, 64, 74	0
2	P	97/105 (92%)	-1.36	0	100	100	34, 44, 60, 69	0
All	All	2030/2248 (90%)	-1.30	0	100	100	31, 49, 64, 78	0

There are no RSRZ outliers to report.

6.2　Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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.