wwPDB X-ray Structure Validation Summary Report (i)

Jul 31, 2017 – 12:04 PM EDT

PDB ID	:	4WL1
Title	:	Structure of WzzE Polysaccharide Co-polymerase
Authors	:	Kalynych, S.; Cherney, M.; Cygler, M.
Deposited on	:	unknown
Resolution	:	5.99 Å(reported)

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

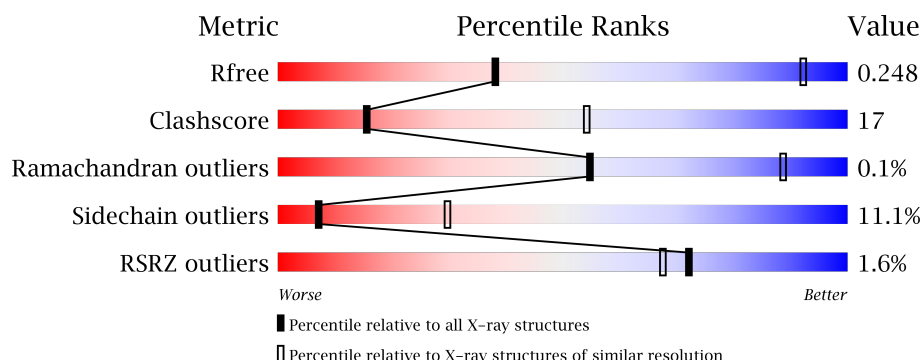|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

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 5.99 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}	100719	1084 (8.20-3.70)
Clashscore	112137	1016 (8.00-3.80)
Ramachandran outliers	110173	1001 (8.20-3.72)
Sidechain outliers	110143	1084 (8.20-3.70)
RSRZ outliers	101464	1093 (8.20-3.70)

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	356	28% 28% 6% • 38%
1	B	356	25% 33% • 38%
1	C	356	2% / 32% 26% • • 38%
1	D	356	25% 32% 5% • 38%
1	E	356	4% / 33% 24% 5% • 38%

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Mol	Chain	Length	Quality of chain
1	F	356	2% 24% 34% · · 38%
1	G	356	.% 40% 20% · 38%
1	H	356	35% 23% · · 38%
1	I	356	2% 38% 19% 5% · 38%
1	J	356	2% 38% 20% · · 38%
1	K	356	38% 20% · 38%
1	L	356	.% 33% 25% · · 38%
1	M	356	.% 38% 17% 5% · 38%
1	N	356	.% 40% 18% · · 38%
1	O	356	.% 40% 18% · · 38%
1	P	356	.% 35% 22% · · 38%
1	Q	356	37% 21% · 38%
1	R	356	3% 39% 19% · · 38%
1	S	356	38% 18% · · 38%
1	T	356	3% 38% 18% 5% · 38%
1	U	356	2% 35% 22% 5% 38%
1	V	356	41% 17% · 38%
1	W	356	.% 37% 21% · · 38%
1	X	356	.% 36% 22% · 38%
1	Y	356	2% 37% 18% 6% · 38%
1	Z	356	.% 36% 21% · · 38%
1	a	356	54% 6% · 38%
1	b	356	.% 53% 6% · 38%
1	c	356	.% 54% 6% · 38%
1	d	356	.% 55% · · 38%

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Mol	Chain	Length	Quality of chain
1	e	356	53% 6% · 38%
1	f	356	53% 5% · 38%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 57504 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 Lipopolysaccharide biosynthesis protein WzzE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	B	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	C	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	D	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	E	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	F	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	G	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	H	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	I	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	J	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	K	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	L	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	M	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	N	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	O	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			
1	P	221	Total	C	N	O	S	0	0	0
			1797	1124	321	344	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	221	Total 1797	C 1124	N 321	O 344	S 8	0	0	0
1	R	221	Total 1797	C 1124	N 321	O 344	S 8	0	0	0
1	S	221	Total 1797	C 1124	N 321	O 344	S 8	0	0	0
1	T	221	Total 1797	C 1124	N 321	O 344	S 8	0	0	0
1	U	221	Total 1797	C 1124	N 321	O 344	S 8	0	0	0
1	V	221	Total 1797	C 1124	N 321	O 344	S 8	0	0	0
1	W	221	Total 1797	C 1124	N 321	O 344	S 8	0	0	0
1	X	221	Total 1797	C 1124	N 321	O 344	S 8	0	0	0
1	Y	221	Total 1797	C 1124	N 321	O 344	S 8	0	0	0
1	Z	221	Total 1797	C 1124	N 321	O 344	S 8	0	0	0
1	a	221	Total 1797	C 1124	N 321	O 344	S 8	0	0	0
1	b	221	Total 1797	C 1124	N 321	O 344	S 8	0	0	0
1	c	221	Total 1797	C 1124	N 321	O 344	S 8	0	0	0
1	d	221	Total 1797	C 1124	N 321	O 344	S 8	0	0	0
1	e	221	Total 1797	C 1124	N 321	O 344	S 8	0	0	0
1	f	221	Total 1797	C 1124	N 321	O 344	S 8	0	0	0

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P0AG01
A	-5	GLY	-	expression tag	UNP P0AG01
A	-4	SER	-	expression tag	UNP P0AG01
A	-3	HIS	-	expression tag	UNP P0AG01
A	-2	HIS	-	expression tag	UNP P0AG01
A	-1	HIS	-	expression tag	UNP P0AG01
A	0	HIS	-	expression tag	UNP P0AG01

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	expression tag	UNP P0AG01
A	2	HIS	-	expression tag	UNP P0AG01
B	-6	MET	-	initiating methionine	UNP P0AG01
B	-5	GLY	-	expression tag	UNP P0AG01
B	-4	SER	-	expression tag	UNP P0AG01
B	-3	HIS	-	expression tag	UNP P0AG01
B	-2	HIS	-	expression tag	UNP P0AG01
B	-1	HIS	-	expression tag	UNP P0AG01
B	0	HIS	-	expression tag	UNP P0AG01
B	1	HIS	-	expression tag	UNP P0AG01
B	2	HIS	-	expression tag	UNP P0AG01
C	-6	MET	-	initiating methionine	UNP P0AG01
C	-5	GLY	-	expression tag	UNP P0AG01
C	-4	SER	-	expression tag	UNP P0AG01
C	-3	HIS	-	expression tag	UNP P0AG01
C	-2	HIS	-	expression tag	UNP P0AG01
C	-1	HIS	-	expression tag	UNP P0AG01
C	0	HIS	-	expression tag	UNP P0AG01
C	1	HIS	-	expression tag	UNP P0AG01
C	2	HIS	-	expression tag	UNP P0AG01
D	-6	MET	-	initiating methionine	UNP P0AG01
D	-5	GLY	-	expression tag	UNP P0AG01
D	-4	SER	-	expression tag	UNP P0AG01
D	-3	HIS	-	expression tag	UNP P0AG01
D	-2	HIS	-	expression tag	UNP P0AG01
D	-1	HIS	-	expression tag	UNP P0AG01
D	0	HIS	-	expression tag	UNP P0AG01
D	1	HIS	-	expression tag	UNP P0AG01
D	2	HIS	-	expression tag	UNP P0AG01
E	-6	MET	-	initiating methionine	UNP P0AG01
E	-5	GLY	-	expression tag	UNP P0AG01
E	-4	SER	-	expression tag	UNP P0AG01
E	-3	HIS	-	expression tag	UNP P0AG01
E	-2	HIS	-	expression tag	UNP P0AG01
E	-1	HIS	-	expression tag	UNP P0AG01
E	0	HIS	-	expression tag	UNP P0AG01
E	1	HIS	-	expression tag	UNP P0AG01
E	2	HIS	-	expression tag	UNP P0AG01
F	-6	MET	-	initiating methionine	UNP P0AG01
F	-5	GLY	-	expression tag	UNP P0AG01
F	-4	SER	-	expression tag	UNP P0AG01
F	-3	HIS	-	expression tag	UNP P0AG01

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	HIS	-	expression tag	UNP P0AG01
F	-1	HIS	-	expression tag	UNP P0AG01
F	0	HIS	-	expression tag	UNP P0AG01
F	1	HIS	-	expression tag	UNP P0AG01
F	2	HIS	-	expression tag	UNP P0AG01
G	-6	MET	-	initiating methionine	UNP P0AG01
G	-5	GLY	-	expression tag	UNP P0AG01
G	-4	SER	-	expression tag	UNP P0AG01
G	-3	HIS	-	expression tag	UNP P0AG01
G	-2	HIS	-	expression tag	UNP P0AG01
G	-1	HIS	-	expression tag	UNP P0AG01
G	0	HIS	-	expression tag	UNP P0AG01
G	1	HIS	-	expression tag	UNP P0AG01
G	2	HIS	-	expression tag	UNP P0AG01
H	-6	MET	-	initiating methionine	UNP P0AG01
H	-5	GLY	-	expression tag	UNP P0AG01
H	-4	SER	-	expression tag	UNP P0AG01
H	-3	HIS	-	expression tag	UNP P0AG01
H	-2	HIS	-	expression tag	UNP P0AG01
H	-1	HIS	-	expression tag	UNP P0AG01
H	0	HIS	-	expression tag	UNP P0AG01
H	1	HIS	-	expression tag	UNP P0AG01
H	2	HIS	-	expression tag	UNP P0AG01
I	-6	MET	-	initiating methionine	UNP P0AG01
I	-5	GLY	-	expression tag	UNP P0AG01
I	-4	SER	-	expression tag	UNP P0AG01
I	-3	HIS	-	expression tag	UNP P0AG01
I	-2	HIS	-	expression tag	UNP P0AG01
I	-1	HIS	-	expression tag	UNP P0AG01
I	0	HIS	-	expression tag	UNP P0AG01
I	1	HIS	-	expression tag	UNP P0AG01
I	2	HIS	-	expression tag	UNP P0AG01
J	-6	MET	-	initiating methionine	UNP P0AG01
J	-5	GLY	-	expression tag	UNP P0AG01
J	-4	SER	-	expression tag	UNP P0AG01
J	-3	HIS	-	expression tag	UNP P0AG01
J	-2	HIS	-	expression tag	UNP P0AG01
J	-1	HIS	-	expression tag	UNP P0AG01
J	0	HIS	-	expression tag	UNP P0AG01
J	1	HIS	-	expression tag	UNP P0AG01
J	2	HIS	-	expression tag	UNP P0AG01
K	-6	MET	-	initiating methionine	UNP P0AG01

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-5	GLY	-	expression tag	UNP P0AG01
K	-4	SER	-	expression tag	UNP P0AG01
K	-3	HIS	-	expression tag	UNP P0AG01
K	-2	HIS	-	expression tag	UNP P0AG01
K	-1	HIS	-	expression tag	UNP P0AG01
K	0	HIS	-	expression tag	UNP P0AG01
K	1	HIS	-	expression tag	UNP P0AG01
K	2	HIS	-	expression tag	UNP P0AG01
L	-6	MET	-	initiating methionine	UNP P0AG01
L	-5	GLY	-	expression tag	UNP P0AG01
L	-4	SER	-	expression tag	UNP P0AG01
L	-3	HIS	-	expression tag	UNP P0AG01
L	-2	HIS	-	expression tag	UNP P0AG01
L	-1	HIS	-	expression tag	UNP P0AG01
L	0	HIS	-	expression tag	UNP P0AG01
L	1	HIS	-	expression tag	UNP P0AG01
L	2	HIS	-	expression tag	UNP P0AG01
M	-6	MET	-	initiating methionine	UNP P0AG01
M	-5	GLY	-	expression tag	UNP P0AG01
M	-4	SER	-	expression tag	UNP P0AG01
M	-3	HIS	-	expression tag	UNP P0AG01
M	-2	HIS	-	expression tag	UNP P0AG01
M	-1	HIS	-	expression tag	UNP P0AG01
M	0	HIS	-	expression tag	UNP P0AG01
M	1	HIS	-	expression tag	UNP P0AG01
M	2	HIS	-	expression tag	UNP P0AG01
N	-6	MET	-	initiating methionine	UNP P0AG01
N	-5	GLY	-	expression tag	UNP P0AG01
N	-4	SER	-	expression tag	UNP P0AG01
N	-3	HIS	-	expression tag	UNP P0AG01
N	-2	HIS	-	expression tag	UNP P0AG01
N	-1	HIS	-	expression tag	UNP P0AG01
N	0	HIS	-	expression tag	UNP P0AG01
N	1	HIS	-	expression tag	UNP P0AG01
N	2	HIS	-	expression tag	UNP P0AG01
O	-6	MET	-	initiating methionine	UNP P0AG01
O	-5	GLY	-	expression tag	UNP P0AG01
O	-4	SER	-	expression tag	UNP P0AG01
O	-3	HIS	-	expression tag	UNP P0AG01
O	-2	HIS	-	expression tag	UNP P0AG01
O	-1	HIS	-	expression tag	UNP P0AG01
O	0	HIS	-	expression tag	UNP P0AG01

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Chain	Residue	Modelled	Actual	Comment	Reference
O	1	HIS	-	expression tag	UNP P0AG01
O	2	HIS	-	expression tag	UNP P0AG01
P	-6	MET	-	initiating methionine	UNP P0AG01
P	-5	GLY	-	expression tag	UNP P0AG01
P	-4	SER	-	expression tag	UNP P0AG01
P	-3	HIS	-	expression tag	UNP P0AG01
P	-2	HIS	-	expression tag	UNP P0AG01
P	-1	HIS	-	expression tag	UNP P0AG01
P	0	HIS	-	expression tag	UNP P0AG01
P	1	HIS	-	expression tag	UNP P0AG01
P	2	HIS	-	expression tag	UNP P0AG01
Q	-6	MET	-	initiating methionine	UNP P0AG01
Q	-5	GLY	-	expression tag	UNP P0AG01
Q	-4	SER	-	expression tag	UNP P0AG01
Q	-3	HIS	-	expression tag	UNP P0AG01
Q	-2	HIS	-	expression tag	UNP P0AG01
Q	-1	HIS	-	expression tag	UNP P0AG01
Q	0	HIS	-	expression tag	UNP P0AG01
Q	1	HIS	-	expression tag	UNP P0AG01
Q	2	HIS	-	expression tag	UNP P0AG01
R	-6	MET	-	initiating methionine	UNP P0AG01
R	-5	GLY	-	expression tag	UNP P0AG01
R	-4	SER	-	expression tag	UNP P0AG01
R	-3	HIS	-	expression tag	UNP P0AG01
R	-2	HIS	-	expression tag	UNP P0AG01
R	-1	HIS	-	expression tag	UNP P0AG01
R	0	HIS	-	expression tag	UNP P0AG01
R	1	HIS	-	expression tag	UNP P0AG01
R	2	HIS	-	expression tag	UNP P0AG01
S	-6	MET	-	initiating methionine	UNP P0AG01
S	-5	GLY	-	expression tag	UNP P0AG01
S	-4	SER	-	expression tag	UNP P0AG01
S	-3	HIS	-	expression tag	UNP P0AG01
S	-2	HIS	-	expression tag	UNP P0AG01
S	-1	HIS	-	expression tag	UNP P0AG01
S	0	HIS	-	expression tag	UNP P0AG01
S	1	HIS	-	expression tag	UNP P0AG01
S	2	HIS	-	expression tag	UNP P0AG01
T	-6	MET	-	initiating methionine	UNP P0AG01
T	-5	GLY	-	expression tag	UNP P0AG01
T	-4	SER	-	expression tag	UNP P0AG01
T	-3	HIS	-	expression tag	UNP P0AG01

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-2	HIS	-	expression tag	UNP P0AG01
T	-1	HIS	-	expression tag	UNP P0AG01
T	0	HIS	-	expression tag	UNP P0AG01
T	1	HIS	-	expression tag	UNP P0AG01
T	2	HIS	-	expression tag	UNP P0AG01
U	-6	MET	-	initiating methionine	UNP P0AG01
U	-5	GLY	-	expression tag	UNP P0AG01
U	-4	SER	-	expression tag	UNP P0AG01
U	-3	HIS	-	expression tag	UNP P0AG01
U	-2	HIS	-	expression tag	UNP P0AG01
U	-1	HIS	-	expression tag	UNP P0AG01
U	0	HIS	-	expression tag	UNP P0AG01
U	1	HIS	-	expression tag	UNP P0AG01
U	2	HIS	-	expression tag	UNP P0AG01
V	-6	MET	-	initiating methionine	UNP P0AG01
V	-5	GLY	-	expression tag	UNP P0AG01
V	-4	SER	-	expression tag	UNP P0AG01
V	-3	HIS	-	expression tag	UNP P0AG01
V	-2	HIS	-	expression tag	UNP P0AG01
V	-1	HIS	-	expression tag	UNP P0AG01
V	0	HIS	-	expression tag	UNP P0AG01
V	1	HIS	-	expression tag	UNP P0AG01
V	2	HIS	-	expression tag	UNP P0AG01
W	-6	MET	-	initiating methionine	UNP P0AG01
W	-5	GLY	-	expression tag	UNP P0AG01
W	-4	SER	-	expression tag	UNP P0AG01
W	-3	HIS	-	expression tag	UNP P0AG01
W	-2	HIS	-	expression tag	UNP P0AG01
W	-1	HIS	-	expression tag	UNP P0AG01
W	0	HIS	-	expression tag	UNP P0AG01
W	1	HIS	-	expression tag	UNP P0AG01
W	2	HIS	-	expression tag	UNP P0AG01
X	-6	MET	-	initiating methionine	UNP P0AG01
X	-5	GLY	-	expression tag	UNP P0AG01
X	-4	SER	-	expression tag	UNP P0AG01
X	-3	HIS	-	expression tag	UNP P0AG01
X	-2	HIS	-	expression tag	UNP P0AG01
X	-1	HIS	-	expression tag	UNP P0AG01
X	0	HIS	-	expression tag	UNP P0AG01
X	1	HIS	-	expression tag	UNP P0AG01
X	2	HIS	-	expression tag	UNP P0AG01
Y	-6	MET	-	initiating methionine	UNP P0AG01

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	-5	GLY	-	expression tag	UNP P0AG01
Y	-4	SER	-	expression tag	UNP P0AG01
Y	-3	HIS	-	expression tag	UNP P0AG01
Y	-2	HIS	-	expression tag	UNP P0AG01
Y	-1	HIS	-	expression tag	UNP P0AG01
Y	0	HIS	-	expression tag	UNP P0AG01
Y	1	HIS	-	expression tag	UNP P0AG01
Y	2	HIS	-	expression tag	UNP P0AG01
Z	-6	MET	-	initiating methionine	UNP P0AG01
Z	-5	GLY	-	expression tag	UNP P0AG01
Z	-4	SER	-	expression tag	UNP P0AG01
Z	-3	HIS	-	expression tag	UNP P0AG01
Z	-2	HIS	-	expression tag	UNP P0AG01
Z	-1	HIS	-	expression tag	UNP P0AG01
Z	0	HIS	-	expression tag	UNP P0AG01
Z	1	HIS	-	expression tag	UNP P0AG01
Z	2	HIS	-	expression tag	UNP P0AG01
a	-6	MET	-	initiating methionine	UNP P0AG01
a	-5	GLY	-	expression tag	UNP P0AG01
a	-4	SER	-	expression tag	UNP P0AG01
a	-3	HIS	-	expression tag	UNP P0AG01
a	-2	HIS	-	expression tag	UNP P0AG01
a	-1	HIS	-	expression tag	UNP P0AG01
a	0	HIS	-	expression tag	UNP P0AG01
a	1	HIS	-	expression tag	UNP P0AG01
a	2	HIS	-	expression tag	UNP P0AG01
b	-6	MET	-	initiating methionine	UNP P0AG01
b	-5	GLY	-	expression tag	UNP P0AG01
b	-4	SER	-	expression tag	UNP P0AG01
b	-3	HIS	-	expression tag	UNP P0AG01
b	-2	HIS	-	expression tag	UNP P0AG01
b	-1	HIS	-	expression tag	UNP P0AG01
b	0	HIS	-	expression tag	UNP P0AG01
b	1	HIS	-	expression tag	UNP P0AG01
b	2	HIS	-	expression tag	UNP P0AG01
c	-6	MET	-	initiating methionine	UNP P0AG01
c	-5	GLY	-	expression tag	UNP P0AG01
c	-4	SER	-	expression tag	UNP P0AG01
c	-3	HIS	-	expression tag	UNP P0AG01
c	-2	HIS	-	expression tag	UNP P0AG01
c	-1	HIS	-	expression tag	UNP P0AG01
c	0	HIS	-	expression tag	UNP P0AG01

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Chain	Residue	Modelled	Actual	Comment	Reference
c	1	HIS	-	expression tag	UNP P0AG01
c	2	HIS	-	expression tag	UNP P0AG01
d	-6	MET	-	initiating methionine	UNP P0AG01
d	-5	GLY	-	expression tag	UNP P0AG01
d	-4	SER	-	expression tag	UNP P0AG01
d	-3	HIS	-	expression tag	UNP P0AG01
d	-2	HIS	-	expression tag	UNP P0AG01
d	-1	HIS	-	expression tag	UNP P0AG01
d	0	HIS	-	expression tag	UNP P0AG01
d	1	HIS	-	expression tag	UNP P0AG01
d	2	HIS	-	expression tag	UNP P0AG01
e	-6	MET	-	initiating methionine	UNP P0AG01
e	-5	GLY	-	expression tag	UNP P0AG01
e	-4	SER	-	expression tag	UNP P0AG01
e	-3	HIS	-	expression tag	UNP P0AG01
e	-2	HIS	-	expression tag	UNP P0AG01
e	-1	HIS	-	expression tag	UNP P0AG01
e	0	HIS	-	expression tag	UNP P0AG01
e	1	HIS	-	expression tag	UNP P0AG01
e	2	HIS	-	expression tag	UNP P0AG01
f	-6	MET	-	initiating methionine	UNP P0AG01
f	-5	GLY	-	expression tag	UNP P0AG01
f	-4	SER	-	expression tag	UNP P0AG01
f	-3	HIS	-	expression tag	UNP P0AG01
f	-2	HIS	-	expression tag	UNP P0AG01
f	-1	HIS	-	expression tag	UNP P0AG01
f	0	HIS	-	expression tag	UNP P0AG01
f	1	HIS	-	expression tag	UNP P0AG01
f	2	HIS	-	expression tag	UNP P0AG01

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: Lipopolysaccharide biosynthesis protein WzzE

Chain A:

• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain B:

MET TRP GLY ILE VAL GLY LEU ILE GLY ALA GLY ALA LEU THR ARG CYS SER LYS

● Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain C:

2%

32%   26%   · ·   38%

MET GLY SER HIS HIS HIS HIS HIS HIS THR GLN PRO MET PRO GLY LYS PRO ALA GLU ASP ALA GLU ASN GLU LEU ASP ILE ARG GLY LEU PHE ARG THR LEU TRP ALA GLY LYS LEU TRP ILE ILE GLY MET GLY LEU LEU ALA PHE ALA LEU ILE ALA LEU ALA TYR THR PHE PHE ALA ARG

GLN E55 W56 S57 A60 D63 T66 V67 N68 M69 L70 Y73 Y74 S75 Q76 Q77 Q78 F79 L80 L83 D84 V85 ARG SER ASN MET ALA SER ALA GLN P95 S96 V97 M98 A101 Y102 K103 E104 F105 V106 M107 Q108 T114 W119 L120 Q121 T122 D123 Y124 Y125 K126

Q127 R128 M129 N132 S133 K134 A135 M143 I147 I150 P151 G152 R156 D160 K163 L164 T168 A169 P170 D171 L175 A187 L191 N192 D193 E194 L195 K196 W199 R202 Q205 M206 V210 K211 R212 Q213 E214 E215 V216 Y221 M225 N226 S227

I228 E229 Q230 ALA LEU LYS ILE ALA GLU GLN HIS ASN ILE SER ARG SER ALA THR ASP VAL PRO ALA GLU GLU LEU PRO ASP SER GLU MET PHE LEU LEU GLY ARG PRO MET LEU Q266 A267 R268 L272 Q273 A274 V275 G276 P277 A278 F279 D282 Y283 D284 Q285 N286 R287 A288 M289 L290

N291 T292 L293 N294 V295 G296 P297 T298 L299 D300 P301 R302 Q304 F303 T305 Y306 L309 P312 E313 E314 P315 V316 K317 R318 D319 SER PRO ARG ALA PHE LEU MET ILE MET TRP GLY ILE VAL GLY LEU ILE GLY ALA GLY VAL ALA LEU THR ARG ARG CYS SER LYS

● Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain D:

25%   32%   5% ·   38%

MET GLY SER HIS HIS HIS HIS HIS HIS THR GLN PRO MET PRO GLY LYS PRO ALA GLU ASP ALA GLU ASN GLU LEU ASP ILE ARG GLY LEU PHE ARG THR LEU TRP ALA GLY LYS LEU TRP ILE ILE GLY MET GLY LEU LEU ALA PHE ALA LEU ILE ALA LEU ALA TYR THR PHE PHE ALA ARG

GLN E55 W56 S57 S58 T59 A60 I61 T62 D63 R64 P65 T66 V67 N68 M69 L70 G71 G72 Y73 Q76 Q77 Q78 F79 L80 R81 N82 L83 D84 V85 ARG SER ASN MET ALA SER ALA ASP GLN P95 S96 V97 M98 D99 Y102 K103 E104 F105 V106 M107 Q108 L109 A110 D113 T114 R115

W119 L120 Q121 T122 D123 Y124 Y125 K126 M129 V130 G131 N132 S133 K134 A135 D136 L140 D141 E142 M143 I144 N145 N146 I147 Q148 F149 I150 P151 G152 D153 V158 S161 V162 K163 L164 I165 A166 E167 T168 A169 P170 D171 L176 R177 V180 A181 F182 A183 S184 Q185 R186 A187 H90

L191 N192 D193 E194 L195 K196 W199 R202 T203 I204 Q205 M206 V210 K211 R212 Q213 V216 R223 R224 M225 N226 S227 I228 E229 Q230 ALA LEU LYS ILE ALA GLU GLN HIS ASN ILE SER ARG SER ALA THR ASP VAL PRO ALA GLU GLU LEU PRO ASP SER GLU MET PHE LEU LEU

GLY ARG PRO MET LEU Q266 A267 R268 L269 E270 N271 L272 Q273 A274 V275 G276 D280 Y283 D284 Q285 N286 R287 A288 M289 L290 L293 P297 T298 L299 D300 P301 R302 Q304 T305 Y306 R307 V308 L309 R310 T311 P312 E313 E314 P315 V316 R318 D319 SER PRO ARG ALA PHE LEU

MET ILE MET TRP GLY ILE VAL GLY LEU ILE GLY ALA GLY VAL ALA LEU THR ARG ARG CYS SER LYS

● Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain E:

4%

33%   24%   5% ·   38%

MET GLY SER HIS HIS HIS HIS HIS HIS THR GLN PRO MET PRO GLY LYS PRO ALA GLU ASP ALA GLU ASN GLU LEU ASP ILE ARG GLY LEU PHE ARG THR LEU TRP ALA GLY LYS LEU TRP ILE ILE GLY MET GLY LEU LEU ALA PHE ALA LEU ILE ALA LEU ALA TYR THR PHE PHE ALA ARG

• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain F:

• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain G:

ALA THR ASP PRO ALA GLU GLU LEU PRO ASP SER GLU MET PHE LEU LEU GLY ARG PRO MET LEU Q266 A267 R268 L269 E270 N271 L272 V275 G276 P277 D282 R287 T292 L293 N294 V295 G296 P297 T298 L299 D300 P301 R302 F303 Q304 T305 Y306 E313 D319 SER PRO ARG

ARG ALA PHE LEU MET ILE TRP GLY VAL GLY LEU ILE ALA VAL ALA LEU THR ARG ARG CYS SER LYS

• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain H:

35%   23%   • •   38%

MET GLY SER HIS HIS HIS HIS HIS HIS THR GLN PRO MET PRO GLY LYS PRO ALA GLU ALA GLU ASN GLU ASP LEU ASP ILE ARG GLY LEU PHE ARG THR LEU TRP ALA GLY LYS LEU ILE ILE GLY MET GLY LEU ALA PHE ALA LEU ILE ALA LEU ALA TYR THR PHE PHE ALA ARG

GLN E55 W56 S57 S58 T59 A60 I61 T62 D63 R64 Y73 Y74 S75 Q76 Q77 Q78 F79 L80 R81 D84 Y85 ARG SER ASN MET ALA SER ALA ASP GLN P95 S96 V97 M98 D99 K103 E104 F105 L109 D113 R116 E117 F118 W119 L120 Q121 T122 D123 Y124 Y125 K126 Q127 R128

M129 V130 G131 N132 S133 K134 A135 L139 L140 D141 E142 M143 I144 I147 G152 D153 F154 T155 R156 A157 V158 N159 D160 K163 L164 I165 E167 T168 A169 L176 R177 Q178 H190 L191 N192 D193 E194 L195 K196 W199 T203 I204 Q205 M206 K207 V210 K211 R212 Q213

M225 N226 S227 Q230 ALA LEU LYS ILE ALA GLU GLN HIS ASN ILE SER ARG SER ALA THR ASP VAL PRO ALA GLU GLU LEU PRO ASP SER GLU MET PHE LEU LEU GLY ARG PRO MET LEU Q266 A267 R268 L269 E270 N271 L272 Q273 A274 V275 N286 R287 A288 M289 L290 N291 T292 L293 N294

P297 T298 L299 R302 F303 Q304 T305 L309 R310 V316 D319 SER PRO ARG ALA ALA PHE LEU MET ILE TRP GLY ILE VAL GLY LEU ILE LEU GLY ALA GLY VAL ALA LEU THR ARG ARG CYS SER LYS

• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain I:

2%
38%   19%   5% •   38%

MET GLY SER HIS HIS HIS HIS HIS HIS THR GLN PRO MET PRO GLY LYS PRO ALA GLU ALA GLU ASN GLU ASP LEU ASP ILE ARG GLY LEU PHE ARG THR LEU TRP ALA GLY LYS LEU LEU TRP ILE ILE GLY MET GLY LEU ALA PHE ALA LEU ILE ALA LEU ALA TYR THR PHE PHE ALA ARG

GLN E55 W56 S57 S58 T59 A60 I61 T62 D63 R64 P65 T66 V67 N68 M69 L70 Y73 L83 D84 V85 ARG SER ASN MET ALA SER ALA ASP GLN P95 S96 V97 M98 D99 E104 F105 V106 M107 F118 W119 L120 Q121 T122 D123 Y124 Y125 K126 Q127 R128 V130 D141 E142 M143

I144 N145 N146 I147 Q148 G152 T155 V158 N159 D160 S161 V162 K163 L164 E167 T168 A169 P170 D171 N174 L175 L176 R177 Q178 Y179 E194 L195 R202 T203 I204 Q205 M206 K207 K211 V216 A217 K218 R223 R224 M225 I228 E229 Q230 ALA LEU LYS ILE ALA GLU

GLN HIS ASN ILE SER ARG SER ALA THR ASP VAL PRO ALA GLU LEU PRO ASP SER GLU MET PHE LEU LEU GLY ARG PRO MET LEU Q266 V275 D282 A288 M289 L290 N291 T292 L293 T298 L299 D300 P301 R302 T305 L309 R310 T311 P312 E313 V316 K317 R318 D319

SER PRO ARG ALA ARG ALA PHE LEU MET ILE TRP GLY VAL GLY LEU ILE LEU VAL GLY LEU ILE ALA GLY VAL ALA LEU THR ARG ARG CYS SER LYS

• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain J:

2%
38%   20%   • •   38%

MET GLY SER HIS HIS HIS HIS HIS HIS THR GLN PRO MET PRO GLY LYS PRO ALA GLU ALA GLU ASN GLU ASP LEU ASP ILE ARG GLY LEU PHE ARG THR LEU TRP ALA GLY LYS LEU ILE ILE GLY MET GLY LEU ALA PHE ALA LEU ILE ALA LEU ALA TYR THR PHE PHE ALA ARG

• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain K:

• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain L:

● Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain M:

● Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain N:

● Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain O:

ALA THR ASP VAL PRO ALA GLU GLU LEU PRO ASP SER GLU MET PHE LEU LEU GLY ARG PRO MET LEU Q266 A267 R268 L269 L272 V275 G276 P277 D282 M289 L290 L293 N294 V295 G296 P297 T298 L299 D300 D301 R302 Y308 L309 R310 T311 P312 P315 D319 SER PRO
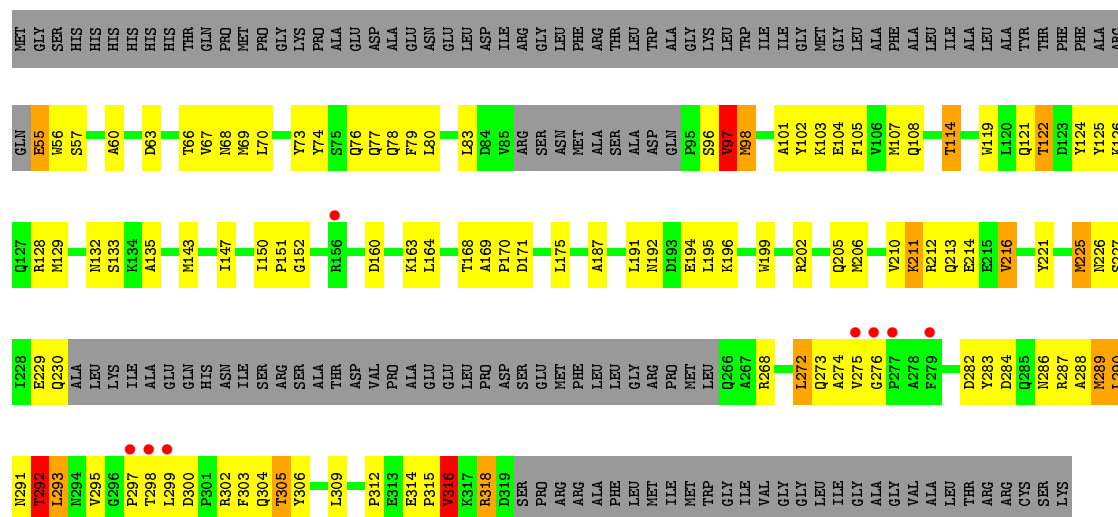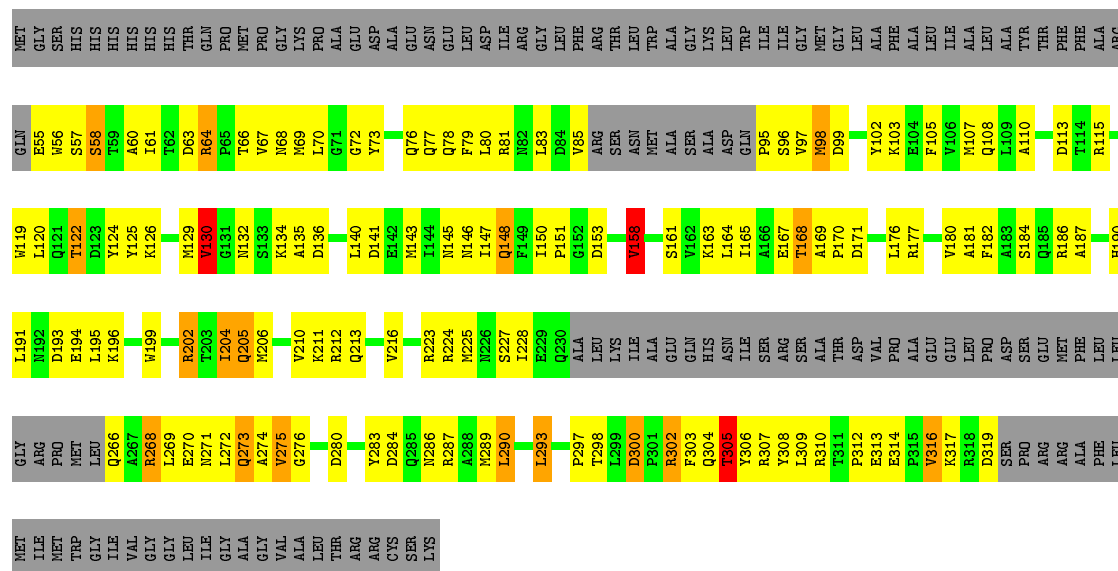
ARG ARG ALA PHE LEU MET ILE MET TRP GLY ILE VAL GLY LEU ILE GLY ILE VAL ALA LEU THR ARG ARG CYS SER LYS

• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain P:

35%   22%   ••   38%

MET GLY SER HIS HIS HIS HIS HIS HIS THR GLN PRO MET PRO GLY LYS PRO ALA GLU ASP ALA ASN GLU ASP ILE ARG GLY LEU PHE ARG THR LEU TRP ALA GLY LYS LEU TRP ILE ILE GLY MET GLY LEU ALA PHE ALA LEU ILE ALA LEU TYR THR PHE PHE ALA ARG

GLN E55 S58 T59 A60 I61 T62 D63 R64 P65 T66 V67 N68 M69 G72 Q76 F79 L83 D84 V85 ARG SER ASN MET ALA SER ALA ASP GLN P95 S96 V97 M98 A101 Y102 K103 E104 F105 V106 M107 Q108 W112 W119 L120 Q121 T122 D123 Y124 Y125 K126

M129 V130 K134 L139 L140 D141 E142 M143 I144 F149 D153 D160 S161 V162 K163 L164 I165 T168 A169 P170 D171 L176 Y179 V180 A181 F182 A183 S184 Q185 R186 A187 L191 W199 R202 T203 I204 Q205 M206 K207 K211 I220 R224 M225 S227

I228 E229 Q230 ALA LEU LYS ILE ALA GLU GLN HIS ASN ILE SER ARG SER ALA THR ASP VAL PRO ALA GLU GLU LEU PRO ASP SER GLU MET PHE LEU LEU GLY ARG PRO MET LEU Q266 A267 R268 L269 L272 Q273 A274 V275 F279 D280 Y283 D284 Q285 A288 M289 L290 N291 T292

L293 N294 V295 G296 P297 T298 L299 F303 Q304 T305 Y306 R307 Y308 L309 R310 V316 D319 SER PRO ARG ARG ALA PHE LEU MET ILE MET TRP GLY ILE VAL GLY ILE GLY ILE VAL ALA LEU THR ARG ARG CYS SER LYS
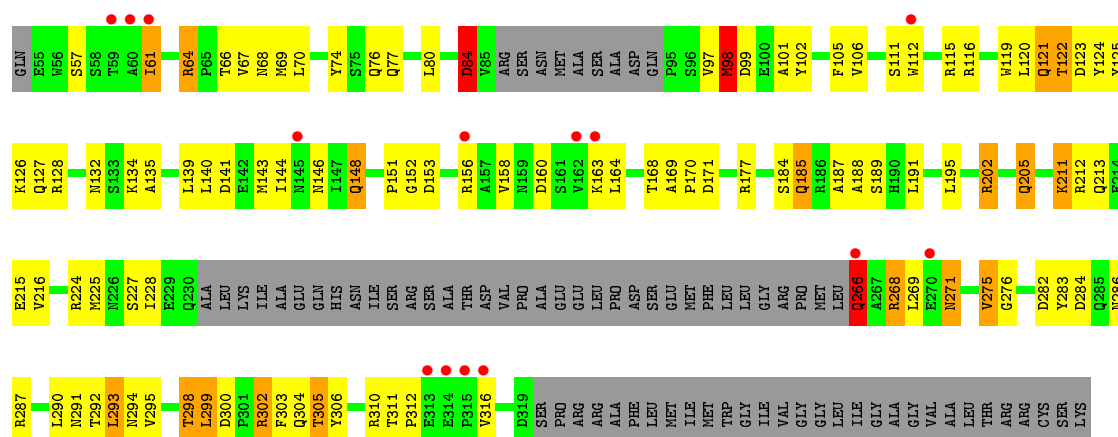
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain Q:

37%   21%   •   38%

MET GLY SER HIS HIS HIS HIS HIS HIS THR GLN PRO MET PRO GLY LYS PRO ALA GLU ASP ALA ASN GLU ASP ILE ARG GLY LEU PHE ARG THR LEU TRP ALA GLY LYS LEU TRP ILE ILE GLY MET GLY LEU ALA PHE ALA LEU ILE ALA LEU TYR THR PHE PHE ALA ARG

GLN E55 W56 S57 A60 I61 T62 D63 R64 P65 T66 V67 N68 M69 L70 F79 L80 L83 D84 V85 ARG SER ASN MET ALA SER ALA ASP GLN P95 S96 V97 M98 D99 E100 A101 Y102 F105 Q108 L109 T114 R115 R116 W119 L120 Q121 T122 D123 Y124 Y125 K126 D136

L140 D141 E142 M143 I144 N145 M146 I147 Q148 F149 G152 T155 V158 K163 L164 E167 T168 A169 P170 L175 L176 R177 Q178 Y179 R186 A187 L191 E194 L195 K196 W199 R202 T203 I204 Q205 M206 K211 R212 Q213 E214 E215 V216 I220 Q230 ALA

LEU LYS ILE ALA GLU GLN HIS ASN ILE SER ARG SER ALA THR ASP VAL PRO ALA GLU GLU LEU PRO ASP SER GLU MET PHE LEU LEU GLY ARG PRO MET LEU Q266 L272 V275 F279 D280 D281 D282 Y283 L290 N291 T292 L293 T298 L299 D300 P301 R302 F303 Q304 T305 Y306

R307 Y308 L309 P312 V316 K317 R318 D319 SER PRO ARG ARG ALA PHE LEU MET ILE MET TRP GLY ILE VAL GLY LEU ILE GLY ILE VAL ALA LEU THR ARG ARG CYS SER LYS

• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain R:

3%

39%   19%   ••   38%

MET GLY SER HIS HIS HIS HIS HIS HIS THR GLN PRO MET PRO GLY LYS PRO ALA GLU ASP ALA ASN GLU ASP ILE ARG GLY LEU PHE ARG THR LEU TRP ALA GLY LYS LEU TRP ILE ILE GLY MET GLY LEU ALA PHE ALA LEU ILE ALA LEU TYR THR PHE PHE ALA ARG

• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain S:

• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain T:

- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain U:

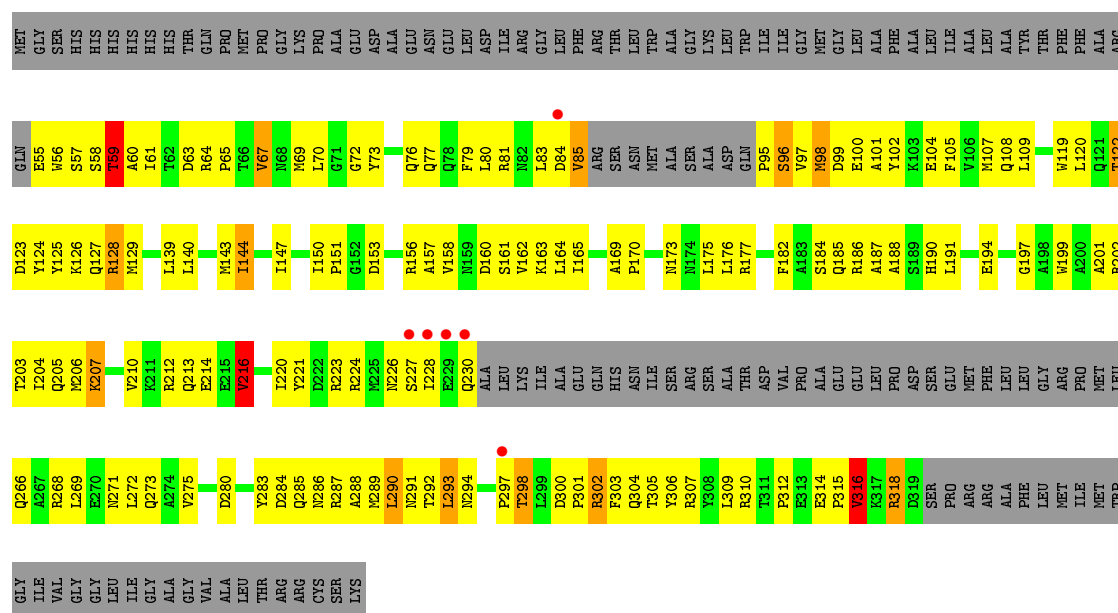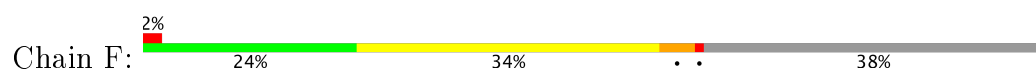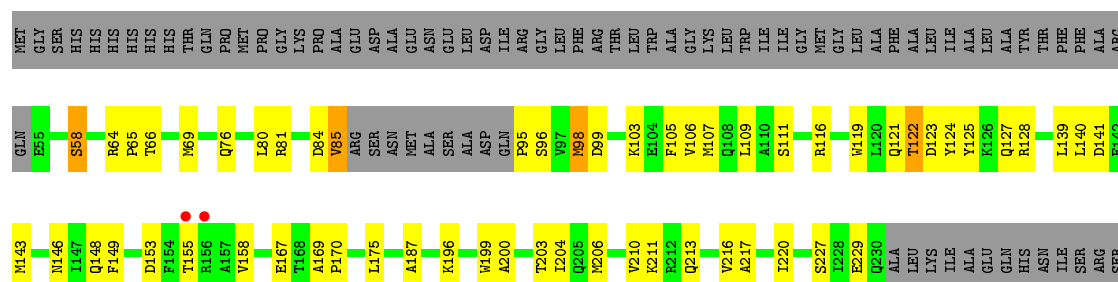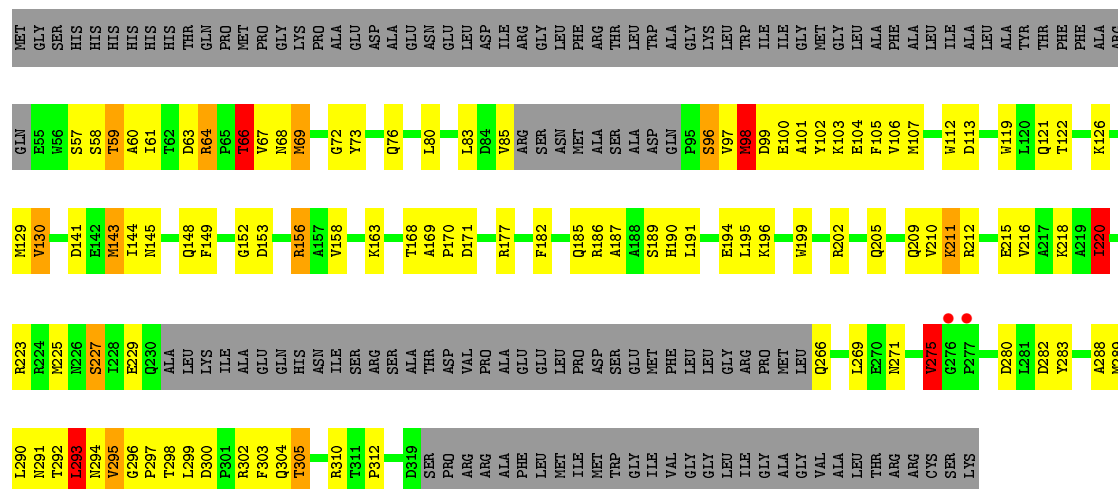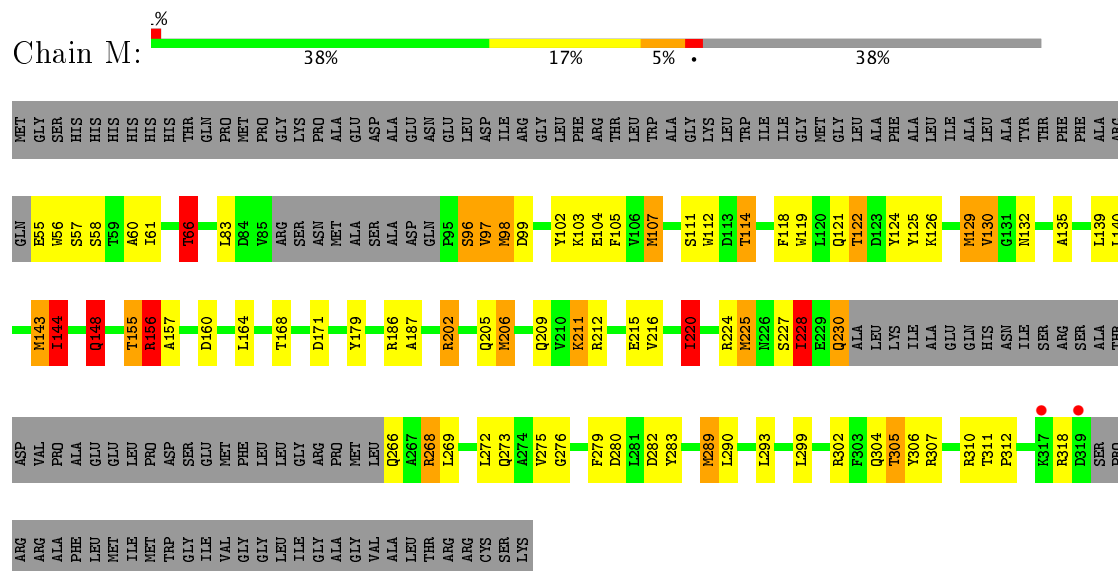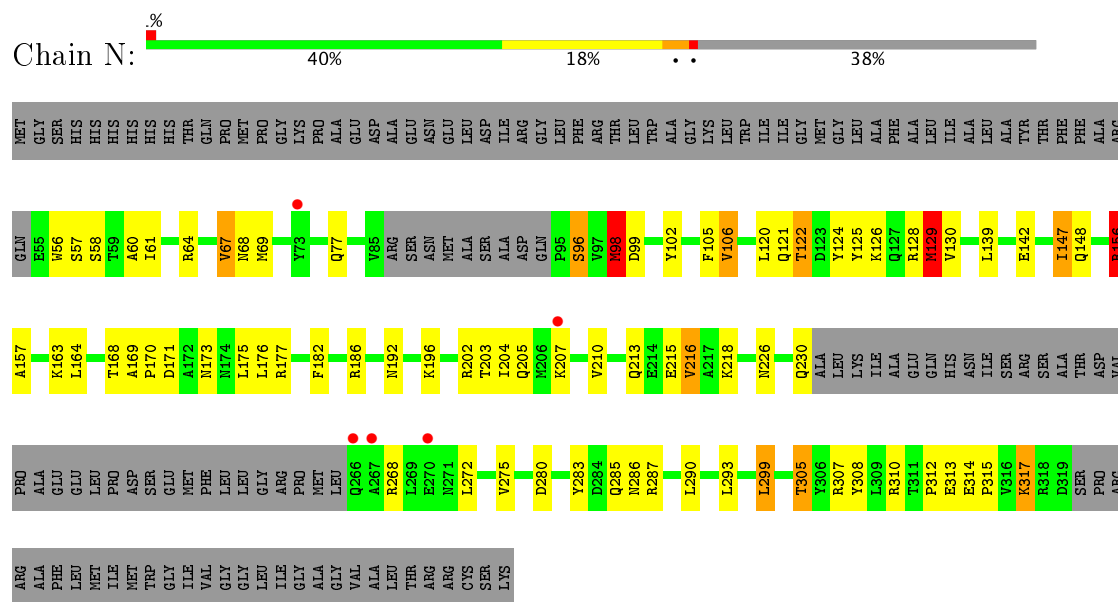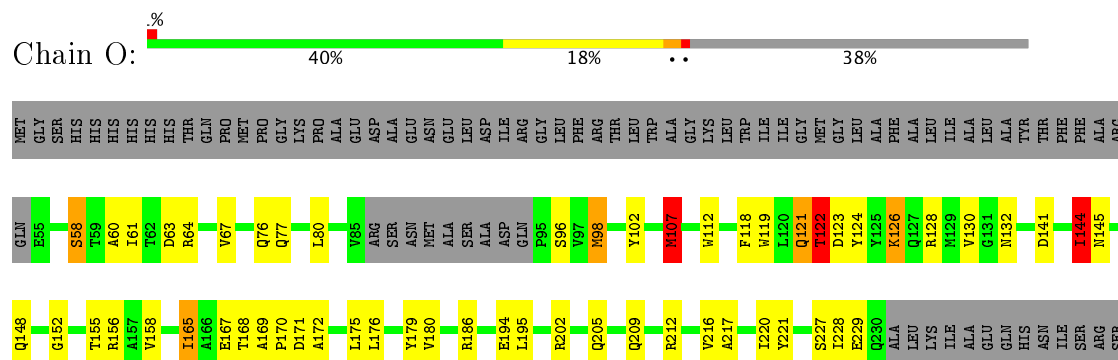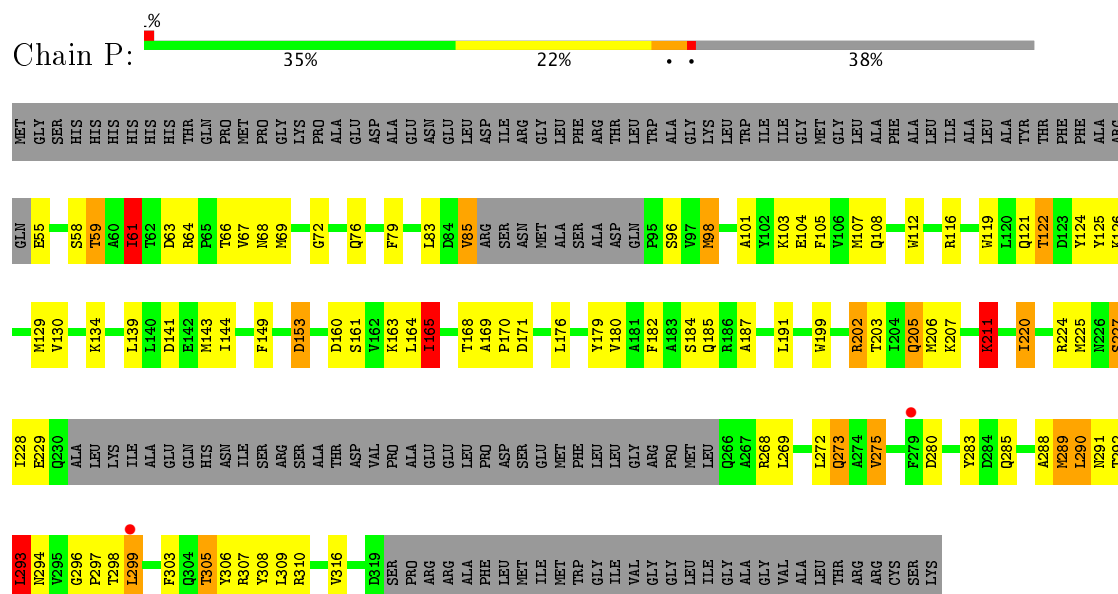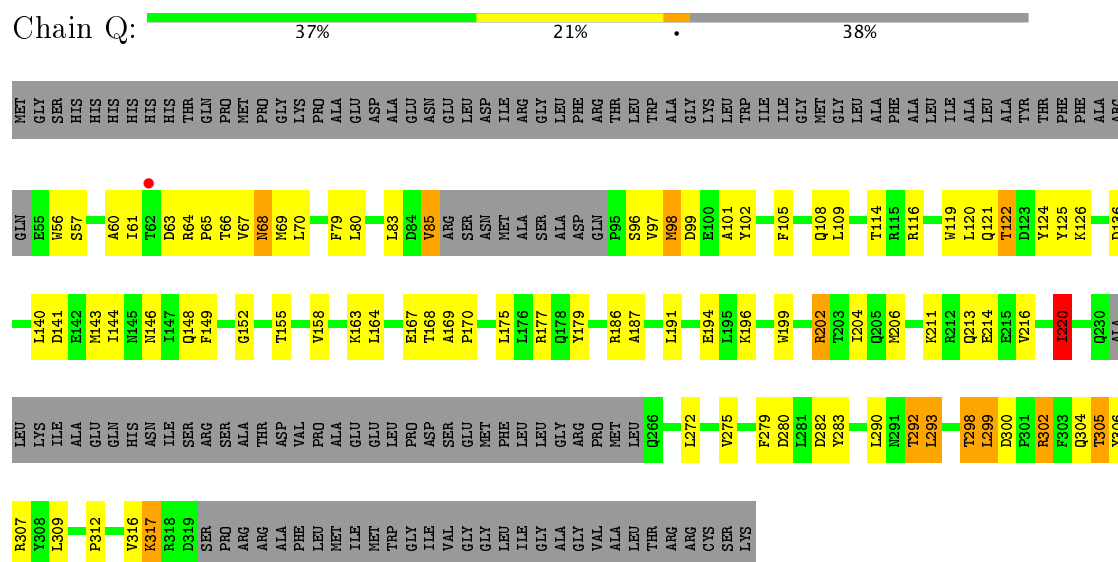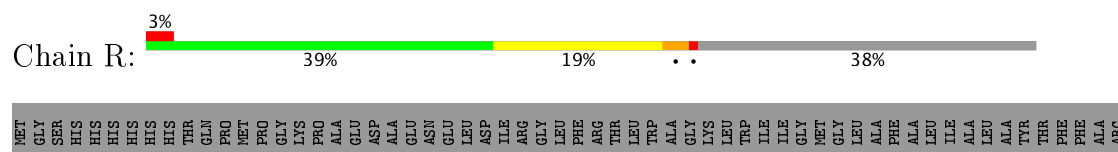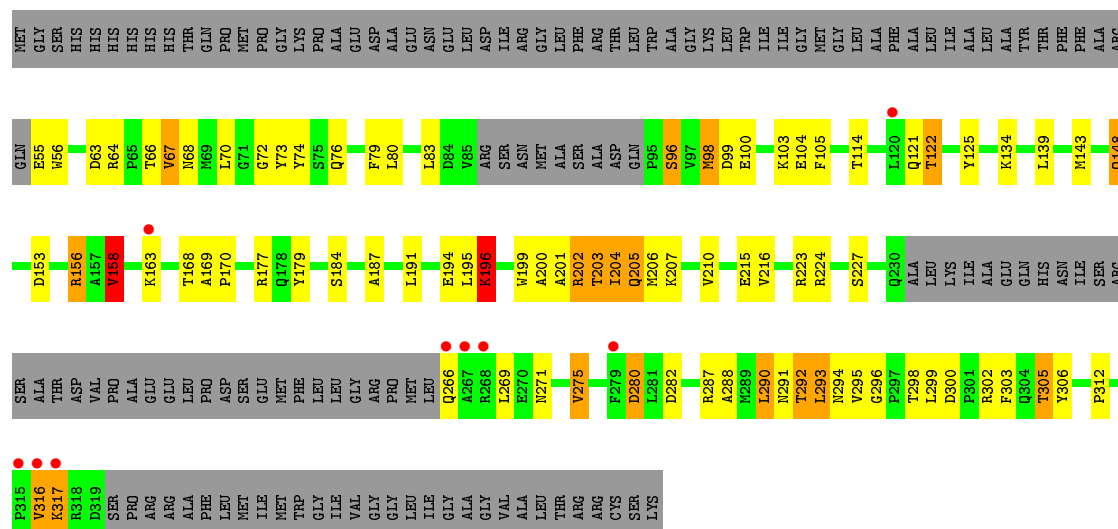- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain V:

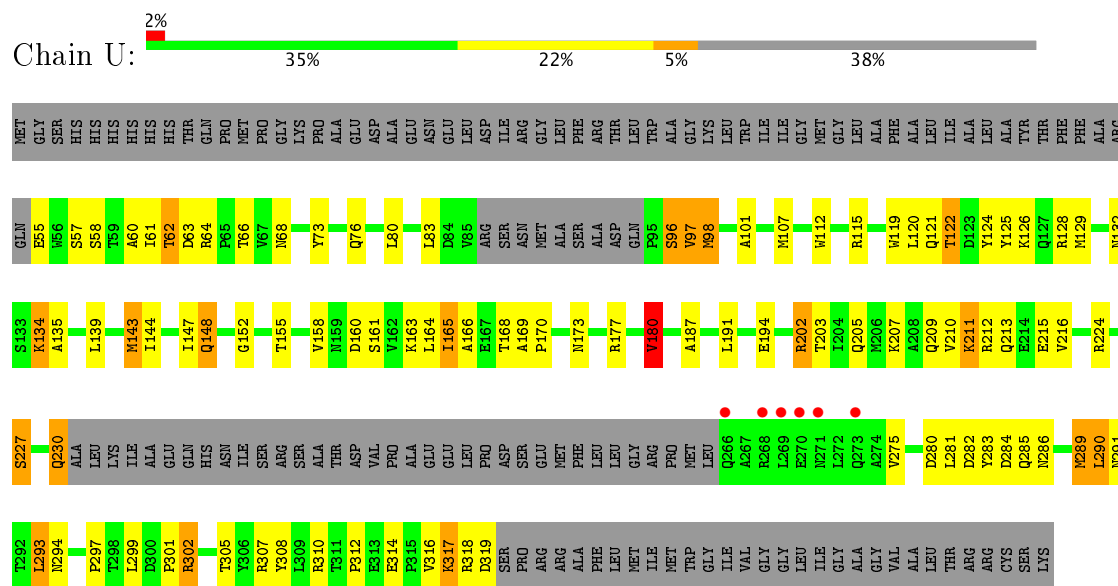- Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain W:

E229 Q230 ALA LEU LYS ILE ALA GLU GLN HIS ASN ILE SER ARG SER ALA THR ASP VAL PRO ALA GLU LEU GLU LEU PRO ASP SER MET PHE LEU LEU GLY ARG PRO MET LEU Q266 L269 V275 G276 P277 D282 M289 L290 L293 N294 V295 P297 T298 L299 D300 P301 R302

T305 R310 T311 P312 E313 E314 P315 V316 K317 R318 D319 SER PRO ARG ALA PHE LEU MET ILE MET TRP GLY ILE VAL GLY LEU ILE GLY ALA GLY VAL ALA LEU THR ARG ARG CYS SER LYS
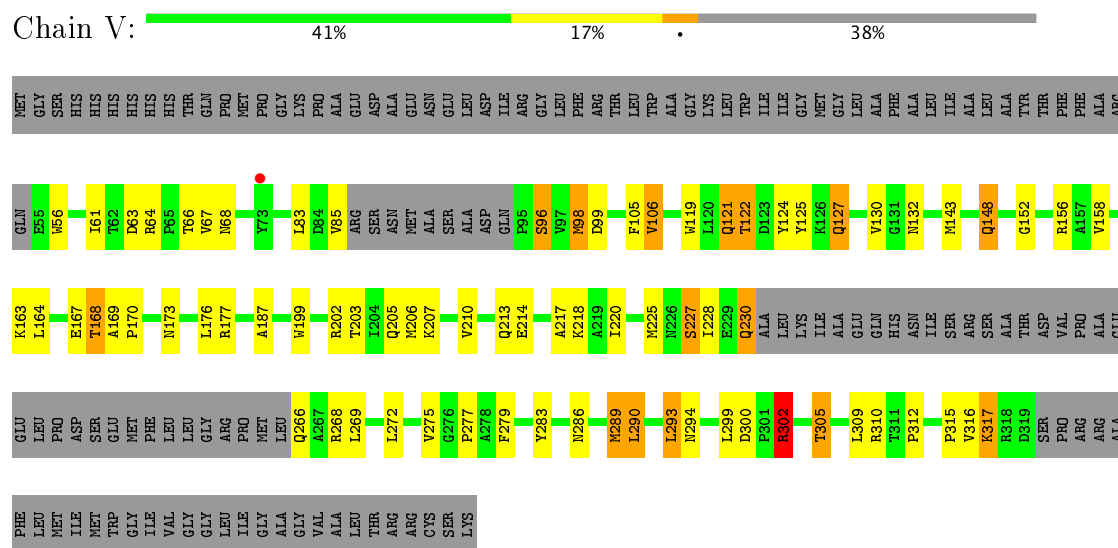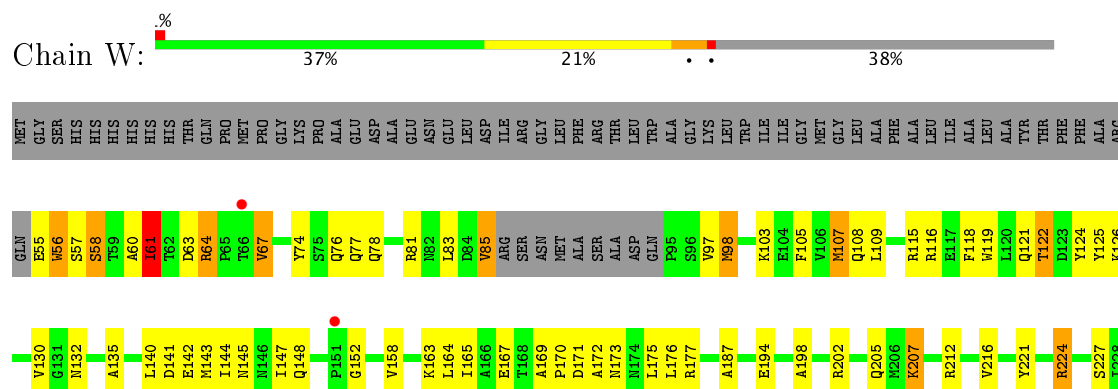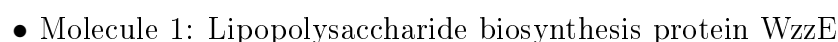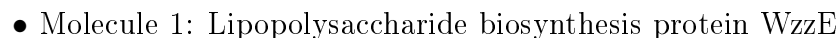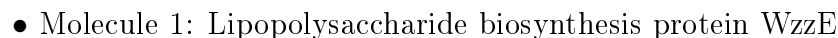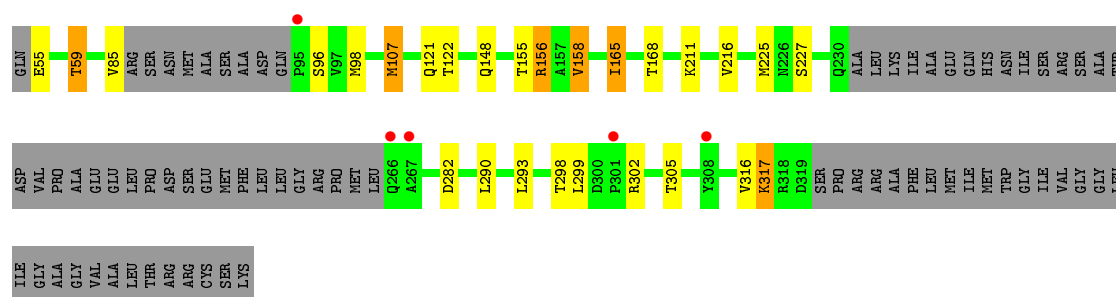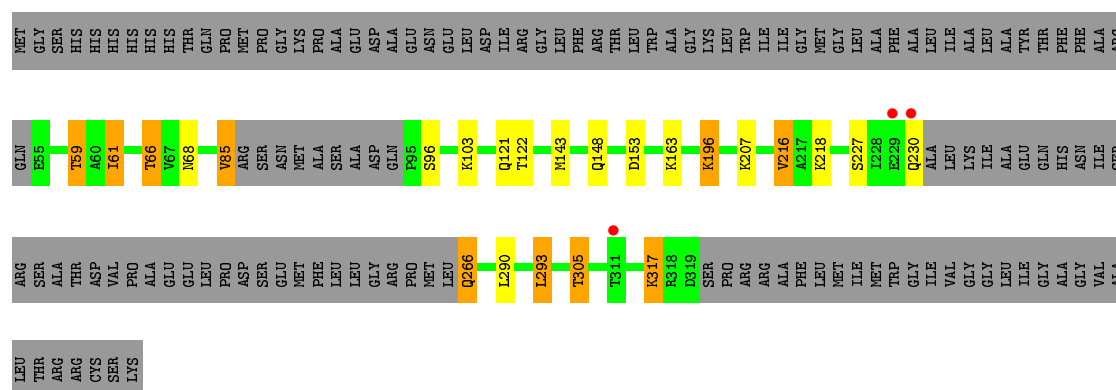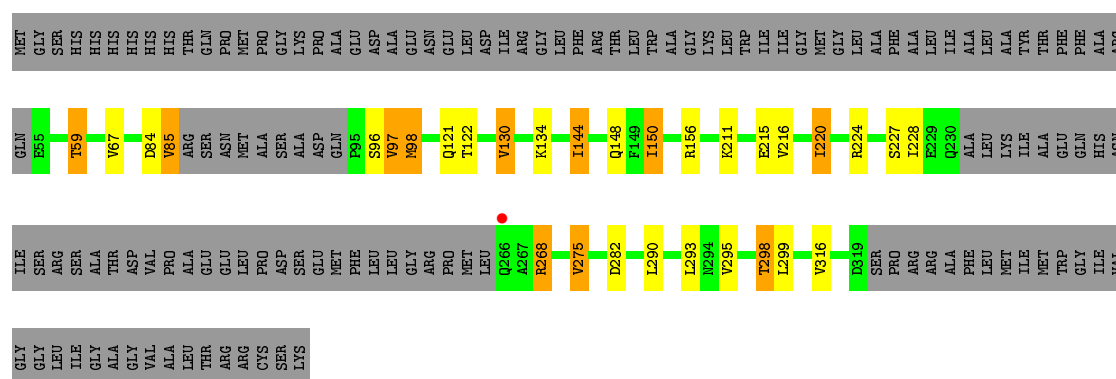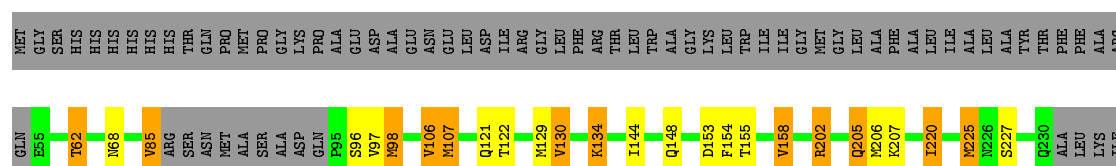
• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain X:

MET GLY SER HIS HIS HIS HIS HIS HIS THR GLN PRO MET PRO GLY LYS PRO ALA GLU ASP ALA ASN GLU ASP ILE GLY LEU PHE ARG LEU TRP ALA GLY LYS TRP ILE ILE GLY MET GLY LEU ALA PHE ALA ILE ALA LEU ALA TYR THR PHE ALA ARG

GLN E55 W56 S57 S58 T62 T66 V67 N68 M69 L70 Y74 Q77 Q78 F79 L80 R81 N82 L83 D84 V85 ARG SER ASN MET ALA SER ALA ASP P95 S96 V97 M98 D99 E100 A101 F105 V106 M107 W112 R115 W119 L120 Q121 T122 D123 Y124 Y125 K126 M129

M132 S133 K134 A135 D136 A137 L140 D141 E142 M143 I144 N145 N146 I147 G152 D153 F154 T155 V158 L164 I165 A166 E167 T168 A169 P170 D171 N174 L175 L176 R177 Q178 A188 S189 H190 L191 E194 R202 Q205 M206 K207 V210 K211 R224 S227 Q230

ALA LEU LYS ILE ALA GLU GLN HIS ASN ILE SER ARG SER ALA THR ASP VAL PRO ALA GLU LEU GLU LEU PRO ASP SER GLU MET PHE LEU LEU GLY ARG PRO MET LEU Q266 L269 E270 N271 L272 Q273 A274 V275 Y283 D284 R287 A288 M289 L290 N291 T292 L293 N294 V295 L299 D300

Q304 T305 Y306 R307 T311 P312 K317 R318 D319 SER PRO ARG ALA PHE LEU MET ILE MET TRP GLY ILE VAL GLY LEU ILE GLY ALA GLY VAL ALA LEU THR ARG ARG CYS SER LYS

• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain Y:

MET GLY SER HIS HIS HIS HIS HIS HIS THR GLN PRO MET PRO GLY LYS PRO ALA GLU ASP ALA GLU ASN GLU ASP ILE GLY LEU PHE ARG LEU TRP ALA GLY LYS LEU TRP ILE ILE GLY MET GLY LEU ALA PHE ALA ILE ALA LEU ALA TYR THR PHE ALA ARG

GLN E55 W56 S57 S58 T59 A60 I61 T62 D63 R64 P65 T66 V67 N68 M69 L70 Q76 Q77 Q78 F79 L83 D84 V85 ARG SER ASN MET ALA SER ALA ASP GLN P95 S96 V97 M98 D99 E100 A101 Y102 K103 E104 F105 V106 M107 W119 L120 Q121 T122 D123 Y124 Y125 K126 Q127 R128

N132 S133 K134 A135 D141 E142 M143 I144 Q148 G152 T155 V158 N159 D160 S161 V162 K163 L164 I165 A166 E167 T168 A169 P170 L176 R177 A187 E194 R202 T203 I204 Q205 M206 V210 K211 V216 A217 K218 Y221 D222 R223 R224 M225 I228 E229 Q230 ALA

LEU LYS ILE ALA GLU GLN HIS ASN ILE SER ARG SER ALA THR ASP VAL PRO ALA GLU LEU GLU LEU PRO ASP SER GLU MET PHE LEU LEU GLY ARG PRO MET LEU Q266 N271 L272 V275 G276 P277 A278 D282 Q285 N286 M289 L290 N291 T292 L293 N294 V295 G296 P297 T298 L299

D300 P301 R302 F303 Q304 T305 Y306 R307 R310 T311 P312 V316 K317 R318 D319 SER PRO ARG ALA PHE LEU MET ILE MET TRP GLY ILE VAL GLY LEU ILE GLY ALA GLY VAL ALA LEU THR ARG ARG CYS SER LYS

• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain Z:

MET GLY SER HIS HIS HIS HIS HIS HIS THR GLN PRO MET PRO GLY LYS PRO ALA GLU ASP ALA GLU ASN GLU ASP ILE ARG GLY LEU PHE ARG LEU TRP ALA GLY LYS LEU TRP ILE ILE GLY MET GLY LEU ALA PHE ALA ILE ALA LEU ALA TYR THR PHE ALA ARG

GLN E55 W56 S57 S58 T59 A60 I61 R64 P65 T66 V67 N68 M69 L70 G71 G72 Y73 Y74 S75 Q76 Q77 Q78 F79 L80 R81 N82 L83 D84 V85 ARG SER ASN MET ALA SER ALA ASP GLN P95 S96 V97 M98 D99 Y102 K103 E104 F105 V106 M107 W119 L120 Q121 T122 D123 Y124 Y125

K126 M129 V130 D141 E142 M143 I144 Q148 F149 I150 D153 V162 K163 T168 A169 P170 D171 A172 N173 R177 Q185 H190 L191 E194 W199 R202 T203 I204 Q205 K211 E214 E215 V216 A217 K218 R223 R224 M225 N226 S227 I228 E229 Q230 ALA LEU

LYS ILE ALA GLN HIS ASN ILE SER SER ALA ASP VAL PRO ALA GLU LEU PRO ASP SER GLU PHE LEU LEU GLY ARG MET LEU Q266 N271 L272 Q273 A274 V275 F279 D280 L281 D282 Y283 D284 M289 L290 L293 D300 P301 R302 T305 Y306 R307

Y308 L309 R310 T311 P312 V316 K317 R318 D319 SER PRO ARG ALA PHE LEU MET ILE MET TRP GLY ILE VAL GLY LEU ILE GLY ALA VAL LEU THR ARG CYS SER LYS

• **Molecule 1: Lipopolysaccharide biosynthesis protein WzzE**

Chain a:

MET GLY SER HIS HIS HIS HIS HIS HIS THR GLN PRO MET PRO GLY LYS PRO ALA GLU ASP ALA GLU ASN GLU ASP LEU ASP ILE ARG GLY LEU PHE ARG THR LEU TRP ALA GLY LYS LEU LEU TRP ILE ILE GLY MET GLY LEU ALA PHE ALA LEU ILE LEU ALA LEU TYR THR PHE PHE ALA ARG

GLN E55 S58 I61 T66 V85 ARG SER ASN MET ALA SER ALA ASP GLN P95 S96 V97 M98 K103 M107 Q121 T122 M129 E142 Q148 T155 K163 R202 M206 V210 K218 S227 Q230 ALA LEU LYS ILE GLU GLN HIS

ASN ILE SER ARG SER ALA THR ASP VAL PRO ALA GLU GLU LEU PRO ASP SER GLU MET PHE LEU LEU GLY ARG PRO MET LEU Q266 L272 D282 L290 L293 T298 L299 R302 T305 V316 D319 SER PRO ARG ALA PHE LEU MET ILE MET TRP GLY ILE

VAL GLY GLY LEU ILE GLY ALA GLY VAL LEU ALA LEU THR ARG ARG CYS SER LYS

• **Molecule 1: Lipopolysaccharide biosynthesis protein WzzE**

Chain b:

MET GLY SER HIS HIS HIS HIS HIS HIS THR GLN PRO MET PRO GLY LYS PRO ALA GLU ASP ALA GLU ASN GLU ASP LEU ASP ILE ARG GLY LEU PHE ARG THR LEU TRP ALA GLY LYS LEU LEU TRP ILE ILE GLY MET GLY LEU ALA PHE ALA LEU ILE LEU ALA LEU TYR THR PHE PHE ALA ARG

GLN E55 T59 A60 I61 N68 M69 V85 ARG SER ASN MET ALA SER ALA ASP GLN P95 S96 V97 M98 K103 M107 Q108 L109 R116 W119 L120 Q121 T122 S133 I144 Q148 T155 Q205 E215 R224 S227 Q230 ALA LEU LYS ILE ALA

GLU GLN HIS ASN ILE SER ARG SER ALA THR ASP VAL PRO ALA GLU LEU GLU PRO ASP SER GLU MET PHE LEU LEU GLY ARG PRO MET LEU Q266 A267 R268 D282 L290 L293 T298 L299 D300 P301 R302 T305 T311 V316 D319 SER PRO ARG ALA PHE LEU

MET ILE MET TRP GLY ILE VAL GLY LEU ILE GLY ALA GLY VAL LEU ALA LEU THR ARG ARG CYS SER LYS

• **Molecule 1: Lipopolysaccharide biosynthesis protein WzzE**

Chain c:

MET GLY SER HIS HIS HIS HIS HIS HIS THR GLN PRO MET PRO GLY LYS PRO ALA GLU ASP ALA GLU ASN GLU ASP LEU ASP ILE ARG GLY LEU PHE ARG THR LEU TRP ALA GLY LYS LEU LEU TRP ILE ILE GLY MET GLY LEU ALA PHE ALA LEU ILE LEU ALA LEU TYR THR PHE PHE ALA ARG

• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain d:

• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain e:

• Molecule 1: Lipopolysaccharide biosynthesis protein WzzE

Chain f:

ALA GLU GLN HIS ASN ILE SER ARG SER ALA THR ASP VAL PRO ALA GLU GLU LEU PRO ASP SER GLU MET PHE LEU LEU GLY ARG PRO MET LEU Q266 L290 L293 L299 T305 V316 D319 SER PRO ARG ARG ALA PHE LEU MET ILE MET TRP GLY ILE VAL GLY GLY

LEU ILE GLY ALA VAL GLY VAL ALA LEU THR ARG ARG CYS SER LYS

GLOBAL-STATISTICS INFOmissingINFO

4 Model quality (i)

4.1 Standard geometry (i)

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	0.52	1/1830 (0.1%)	1.17	9/2475 (0.4%)
1	B	0.56	0/1830	1.05	14/2475 (0.6%)
1	C	0.51	1/1830 (0.1%)	0.98	8/2475 (0.3%)
1	D	0.53	0/1830	1.01	10/2475 (0.4%)
1	E	0.57	0/1830	1.04	15/2475 (0.6%)
1	F	0.52	0/1830	1.01	11/2475 (0.4%)
1	G	0.46	0/1830	1.05	13/2475 (0.5%)
1	H	0.46	0/1830	0.93	8/2475 (0.3%)
1	I	0.48	0/1830	1.01	21/2475 (0.8%)
1	J	0.51	0/1830	1.10	16/2475 (0.6%)
1	K	0.51	1/1830 (0.1%)	1.02	13/2475 (0.5%)
1	L	0.53	0/1830	1.10	18/2475 (0.7%)
1	M	0.55	0/1830	1.14	20/2475 (0.8%)
1	N	0.57	0/1830	1.30	17/2475 (0.7%)
1	O	0.55	0/1830	1.02	12/2475 (0.5%)
1	P	0.59	1/1830 (0.1%)	1.21	20/2475 (0.8%)
1	Q	0.50	0/1830	1.02	13/2475 (0.5%)
1	R	0.60	1/1830 (0.1%)	1.22	23/2475 (0.9%)
1	S	0.54	1/1830 (0.1%)	1.12	21/2475 (0.8%)
1	T	0.61	2/1830 (0.1%)	1.21	19/2475 (0.8%)
1	U	0.57	1/1830 (0.1%)	1.16	12/2475 (0.5%)
1	V	0.52	0/1830	1.10	13/2475 (0.5%)
1	W	0.56	1/1830 (0.1%)	1.19	19/2475 (0.8%)
1	X	0.59	1/1830 (0.1%)	1.13	15/2475 (0.6%)
1	Y	0.61	1/1830 (0.1%)	1.33	22/2475 (0.9%)
1	Z	0.53	0/1830	1.10	21/2475 (0.8%)
1	a	0.59	1/1830 (0.1%)	1.18	19/2475 (0.8%)
1	b	0.61	1/1830 (0.1%)	1.19	22/2475 (0.9%)
1	c	0.51	0/1830	1.11	21/2475 (0.8%)
1	d	0.52	1/1830 (0.1%)	1.18	22/2475 (0.9%)
1	e	0.54	0/1830	1.19	26/2475 (1.1%)
1	f	0.57	0/1830	1.19	26/2475 (1.1%)
All	All	0.55	15/58560 (0.0%)	1.12	539/79200 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	3	1
1	B	1	1
1	F	2	0
1	I	1	1
1	J	1	1
1	L	1	0
1	M	3	1
1	N	1	0
1	O	1	0
1	P	1	0
1	Q	3	0
1	R	2	0
1	S	0	1
1	T	0	1
1	U	1	0
1	V	0	1
1	W	1	1
1	X	1	1
1	Y	1	0
1	a	2	2
1	b	1	0
1	c	1	0
1	d	2	0
1	e	3	1
All	All	33	13

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	163	LYS	CD-CE	8.53	1.72	1.51
1	X	66	THR	CB-CG2	-7.76	1.26	1.52
1	b	59	THR	CB-CG2	-7.76	1.26	1.52
1	R	59	THR	CB-CG2	-6.83	1.29	1.52
1	d	305	THR	CB-CG2	-6.58	1.30	1.52

The worst 5 of 539 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	61	ILE	CG1-CB-CG2	-22.93	60.96	111.40
1	A	67	VAL	CG1-CB-CG2	-22.35	75.14	110.90
1	N	67	VAL	CG1-CB-CG2	-21.79	76.04	110.90
1	U	275	VAL	CG1-CB-CG2	-20.75	77.69	110.90
1	Y	128	ARG	NE-CZ-NH1	-20.73	109.94	120.30

5 of 33 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	59	THR	CB
1	A	168	THR	CB
1	A	305	THR	CB
1	B	62	THR	CB
1	F	59	THR	CB

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	GLU	Sidechain
1	B	279	PHE	Sidechain
1	I	148	GLN	Sidechain
1	J	300	ASP	Sidechain
1	M	148	GLN	Sidechain

4.2 Too-close contacts (i)

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	1797	0	1748	121	0
1	B	1797	0	1748	140	0
1	C	1797	0	1748	95	0
1	D	1797	0	1748	125	1
1	E	1797	0	1748	103	0
1	F	1797	0	1748	154	0
1	G	1797	0	1748	68	0
1	H	1797	0	1748	77	0
1	I	1797	0	1748	50	0
1	J	1797	0	1748	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1797	0	1748	55	0
1	L	1797	0	1748	66	1
1	M	1797	0	1748	65	0
1	N	1797	0	1748	51	0
1	O	1797	0	1748	60	0
1	P	1797	0	1748	78	0
1	Q	1797	0	1748	63	0
1	R	1797	0	1748	60	0
1	S	1797	0	1748	77	0
1	T	1797	0	1747	78	0
1	U	1797	0	1748	80	0
1	V	1797	0	1748	57	0
1	W	1797	0	1748	74	0
1	X	1797	0	1748	63	0
1	Y	1797	0	1748	57	0
1	Z	1797	0	1748	64	0
1	a	1797	0	1748	0	0
1	b	1797	0	1748	0	0
1	c	1797	0	1748	0	0
1	d	1797	0	1748	0	0
1	e	1797	0	1748	0	0
1	f	1797	0	1748	0	0
All	All	57504	0	55935	1873	1

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 17.

The worst 5 of 1873 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:T:96:SER:OG	1:T:98:MET:SD	1.93	1.26
1:T:196:LYS:HG3	1:T:299:LEU:HD21	1.38	1.04
1:Q:105:PHE:HB2	1:Q:305:THR:HG23	1.35	1.03
1:X:126:LYS:HA	1:X:129:MET:HG3	1.40	1.01
1:B:225:MET:HE1	1:B:273:GLN:HG2	1.38	1.01

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:LYS:NZ	1:L:296:GLY:O[2_546]	1.93	0.27

4.3 Torsion angles (i)

4.3.1 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	215/356 (60%)	209 (97%)	6 (3%)	0	100	100
1	B	215/356 (60%)	212 (99%)	3 (1%)	0	100	100
1	C	215/356 (60%)	213 (99%)	2 (1%)	0	100	100
1	D	215/356 (60%)	211 (98%)	4 (2%)	0	100	100
1	E	215/356 (60%)	212 (99%)	2 (1%)	1 (0%)	32	74
1	F	215/356 (60%)	210 (98%)	4 (2%)	1 (0%)	32	74
1	G	215/356 (60%)	211 (98%)	3 (1%)	1 (0%)	32	74
1	H	215/356 (60%)	211 (98%)	3 (1%)	1 (0%)	32	74
1	I	215/356 (60%)	209 (97%)	6 (3%)	0	100	100
1	J	215/356 (60%)	210 (98%)	5 (2%)	0	100	100
1	K	215/356 (60%)	209 (97%)	6 (3%)	0	100	100
1	L	215/356 (60%)	210 (98%)	5 (2%)	0	100	100
1	M	215/356 (60%)	207 (96%)	8 (4%)	0	100	100
1	N	215/356 (60%)	208 (97%)	7 (3%)	0	100	100
1	O	215/356 (60%)	210 (98%)	5 (2%)	0	100	100
1	P	215/356 (60%)	209 (97%)	6 (3%)	0	100	100
1	Q	215/356 (60%)	210 (98%)	5 (2%)	0	100	100
1	R	215/356 (60%)	211 (98%)	4 (2%)	0	100	100
1	S	215/356 (60%)	209 (97%)	6 (3%)	0	100	100
1	T	215/356 (60%)	210 (98%)	5 (2%)	0	100	100
1	U	215/356 (60%)	209 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	215/356 (60%)	210 (98%)	5 (2%)	0	100	100
1	W	215/356 (60%)	209 (97%)	6 (3%)	0	100	100
1	X	215/356 (60%)	209 (97%)	6 (3%)	0	100	100
1	Y	215/356 (60%)	210 (98%)	5 (2%)	0	100	100
1	Z	215/356 (60%)	211 (98%)	4 (2%)	0	100	100
1	a	215/356 (60%)	208 (97%)	7 (3%)	0	100	100
1	b	215/356 (60%)	211 (98%)	4 (2%)	0	100	100
1	c	215/356 (60%)	209 (97%)	6 (3%)	0	100	100
1	d	215/356 (60%)	210 (98%)	5 (2%)	0	100	100
1	e	215/356 (60%)	209 (97%)	6 (3%)	0	100	100
1	f	215/356 (60%)	209 (97%)	6 (3%)	0	100	100
All	All	6880/11392 (60%)	6715 (98%)	161 (2%)	4 (0%)	55	89

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	275	VAL
1	H	303	PHE
1	F	318	ARG
1	G	269	LEU

4.3.2　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	190/296 (64%)	165 (87%)	25 (13%)	5	24
1	B	190/296 (64%)	174 (92%)	16 (8%)	13	43
1	C	190/296 (64%)	169 (89%)	21 (11%)	7	30
1	D	190/296 (64%)	173 (91%)	17 (9%)	11	39
1	E	190/296 (64%)	166 (87%)	24 (13%)	5	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	190/296 (64%)	175 (92%)	15 (8%)	14	46
1	G	190/296 (64%)	175 (92%)	15 (8%)	14	46
1	H	190/296 (64%)	167 (88%)	23 (12%)	6	27
1	I	190/296 (64%)	165 (87%)	25 (13%)	5	24
1	J	190/296 (64%)	169 (89%)	21 (11%)	7	30
1	K	190/296 (64%)	167 (88%)	23 (12%)	6	27
1	L	190/296 (64%)	164 (86%)	26 (14%)	4	23
1	M	190/296 (64%)	162 (85%)	28 (15%)	3	21
1	N	190/296 (64%)	174 (92%)	16 (8%)	13	43
1	O	190/296 (64%)	172 (90%)	18 (10%)	10	36
1	P	190/296 (64%)	166 (87%)	24 (13%)	5	26
1	Q	190/296 (64%)	172 (90%)	18 (10%)	10	36
1	R	190/296 (64%)	170 (90%)	20 (10%)	8	32
1	S	190/296 (64%)	167 (88%)	23 (12%)	6	27
1	T	190/296 (64%)	171 (90%)	19 (10%)	9	34
1	U	190/296 (64%)	165 (87%)	25 (13%)	5	24
1	V	190/296 (64%)	172 (90%)	18 (10%)	10	36
1	W	190/296 (64%)	173 (91%)	17 (9%)	11	39
1	X	190/296 (64%)	171 (90%)	19 (10%)	9	34
1	Y	190/296 (64%)	161 (85%)	29 (15%)	3	19
1	Z	190/296 (64%)	166 (87%)	24 (13%)	5	26
1	a	190/296 (64%)	168 (88%)	22 (12%)	6	28
1	b	190/296 (64%)	167 (88%)	23 (12%)	6	27
1	c	190/296 (64%)	169 (89%)	21 (11%)	7	30
1	d	190/296 (64%)	171 (90%)	19 (10%)	9	34
1	e	190/296 (64%)	168 (88%)	22 (12%)	6	28
1	f	190/296 (64%)	169 (89%)	21 (11%)	7	30
All	All	6080/9472 (64%)	5403 (89%)	677 (11%)	7	30

5 of 677 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	227	SER

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Mol	Chain	Res	Type
1	S	85	VAL
1	d	216	VAL
1	P	61	ILE
1	Q	202	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 312 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	192	ASN
1	R	78	GLN
1	d	148	GLN
1	N	294	ASN
1	P	192	ASN

4.3.3   RNA (i)

There are no RNA molecules in this entry.

4.4   Non-standard residues in protein, DNA, RNA chains (i)

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

4.5   Carbohydrates (i)

There are no carbohydrates in this entry.

4.6   Ligand geometry (i)

There are no ligands in this entry.

4.7   Other polymers (i)

There are no such residues in this entry.

4.8   Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

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	221/356 (62%)	-0.23	0	100	100	232, 286, 334, 403	0
1	B	221/356 (62%)	-0.31	0	100	100	200, 271, 345, 382	0
1	C	221/356 (62%)	-0.00	8 (3%)	43	41	248, 300, 381, 438	0
1	D	221/356 (62%)	-0.30	0	100	100	223, 281, 331, 361	0
1	E	221/356 (62%)	0.22	14 (6%)	21	23	255, 337, 447, 534	0
1	F	221/356 (62%)	-0.14	6 (2%)	55	51	208, 275, 322, 362	0
1	G	221/356 (62%)	-0.10	3 (1%)	75	70	229, 279, 337, 357	0
1	H	221/356 (62%)	-0.24	1 (0%)	90	88	228, 263, 309, 327	0
1	I	221/356 (62%)	-0.13	6 (2%)	55	51	245, 316, 404, 442	0
1	J	221/356 (62%)	-0.23	6 (2%)	55	51	244, 286, 351, 372	0
1	K	221/356 (62%)	-0.30	1 (0%)	90	88	249, 287, 346, 389	0
1	L	221/356 (62%)	-0.18	2 (0%)	84	80	223, 284, 405, 432	0
1	M	221/356 (62%)	-0.26	2 (0%)	84	80	205, 265, 333, 351	0
1	N	221/356 (62%)	-0.06	5 (2%)	61	58	206, 290, 339, 361	0
1	O	221/356 (62%)	-0.14	3 (1%)	75	70	214, 267, 337, 376	0
1	P	221/356 (62%)	-0.20	2 (0%)	84	80	245, 283, 320, 341	0
1	Q	221/356 (62%)	-0.30	1 (0%)	90	88	204, 276, 333, 350	0
1	R	221/356 (62%)	0.00	10 (4%)	34	34	229, 322, 389, 429	0
1	S	221/356 (62%)	-0.36	0	100	100	236, 300, 344, 456	0
1	T	221/356 (62%)	0.08	9 (4%)	38	37	205, 313, 404, 456	0
1	U	221/356 (62%)	-0.22	6 (2%)	55	51	199, 286, 401, 509	0
1	V	221/356 (62%)	-0.17	1 (0%)	90	88	237, 309, 351, 378	0
1	W	221/356 (62%)	-0.24	3 (1%)	75	70	211, 301, 375, 398	0
1	X	221/356 (62%)	-0.17	5 (2%)	61	58	240, 303, 398, 414	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9
1	Y	221/356 (62%)	-0.04	7 (3%)	48 45	236, 326, 449, 465	0
1	Z	221/356 (62%)	-0.28	2 (0%)	84 80	228, 310, 395, 408	0
1	a	221/356 (62%)	-0.27	0	100 100	231, 299, 363, 391	0
1	b	221/356 (62%)	-0.00	4 (1%)	69 65	256, 348, 475, 550	0
1	c	221/356 (62%)	-0.16	5 (2%)	61 58	256, 314, 369, 399	0
1	d	221/356 (62%)	-0.39	3 (1%)	75 70	235, 284, 331, 372	0
1	e	221/356 (62%)	-0.29	1 (0%)	90 88	237, 321, 358, 384	0
1	f	221/356 (62%)	-0.31	0	100 100	214, 289, 334, 393	0
All	All	7072/11392 (62%)	-0.18	116 (1%)	72 67	199, 295, 383, 550	0

The worst 5 of 116 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	c	266	GLN	6.1
1	Y	277	PRO	6.0
1	X	305	THR	5.8
1	M	319	ASP	5.3
1	G	156	ARG	5.1

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

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

5.3　Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.4　Ligands ⓘ

There are no ligands in this entry.

5.5　Other polymers ⓘ

There are no such residues in this entry.