



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:33 am GMT

PDB ID : 1T5E
Title : The structure of MexA
Authors : Higgins, M.K.; Bokma, E.; Koronakis, E.; Hughes, C.; Koronakis, V.
Deposited on : 2004-05-04
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
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)	:	recalc28949

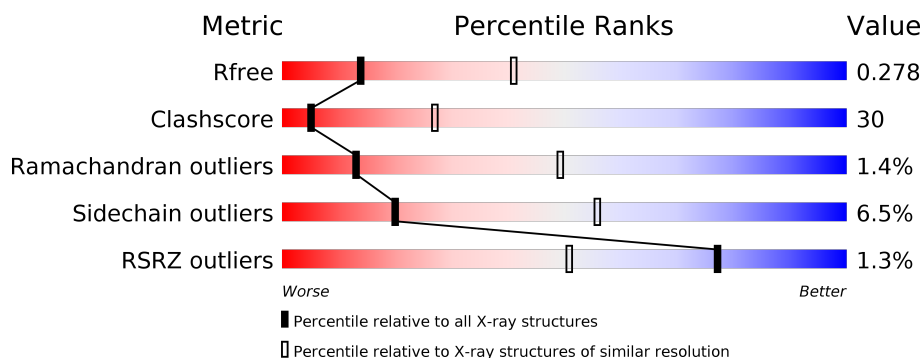
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	360	<div> <div>5%</div> <div> <div>36%</div> <div>25%</div> <div>•</div> <div>36%</div> </div> </div>
1	B	360	<div> <div>36%</div> <div>26%</div> <div>•</div> <div>36%</div> </div>
1	C	360	<div> <div>%</div> <div> <div>36%</div> <div>26%</div> <div>•</div> <div>36%</div> </div> </div>
1	D	360	<div> <div>35%</div> <div>26%</div> <div>•</div> <div>36%</div> </div>
1	E	360	<div> <div>36%</div> <div>25%</div> <div>•</div> <div>36%</div> </div>
1	F	360	<div> <div>%</div> <div> <div>33%</div> <div>28%</div> <div>•</div> <div>36%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	360	
1	H	360	
1	I	360	
1	J	360	
1	K	360	
1	L	360	
1	M	360	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	3GR	C	361	X	-	-	X
2	3GR	D	361	X	-	-	-
2	3GR	E	361	X	-	-	-
2	3GR	F	361	X	-	X	-
2	3GR	G	361	X	-	-	-
2	3GR	H	361	X	-	-	-
2	3GR	I	361	X	-	X	-
2	3GR	K	361	X	-	-	X
2	3GR	L	361	X	-	-	X
3	GOL	A	361	-	-	X	-
3	GOL	J	361	-	-	X	-

2 Entry composition

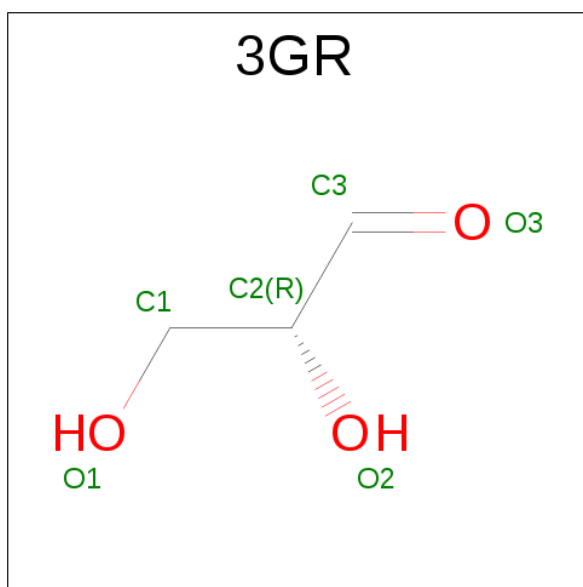
There are 3 unique types of molecules in this entry. The entry contains 23101 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Multidrug resistance protein mexA.

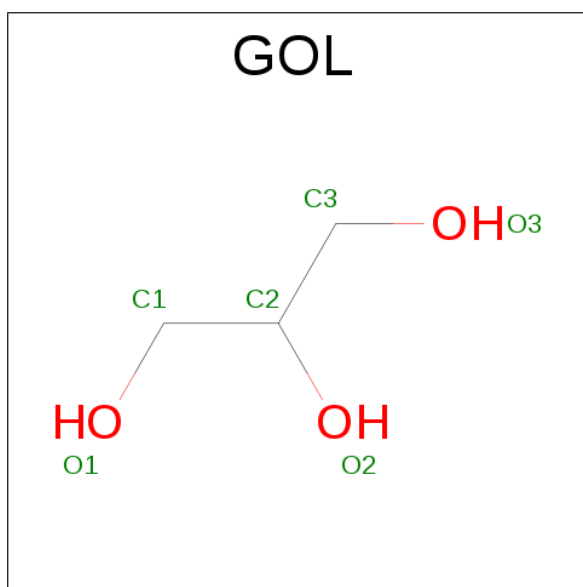
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	B	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	C	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	D	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	E	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	F	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	G	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	H	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	I	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	J	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	K	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	L	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	M	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			

- Molecule 2 is GLYCERALDEHYDE (three-letter code: 3GR) (formula: C₃H₆O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	M	1	Total	C	O	0	0
			6	3	3		

TRP
LEU
VAL
THR
GLY
GLY
LEU
ASN
ALA
ALA
GLY
ASP
LYS
LYS
ILE
ILE
THR
GLY
GLY
LEU
LEU
PHE
GLN
VAL
GLN
PRO
GLY
VAL
GLY
VAL
LYS
VAL
THR
VAL
PRO
ALA
LYS
ASN
VAL
ALA
SER
ALA
GLN
LYS
ALA
ASP
VAL
ALA
ALA
PRO
ALA
LYS
THR
ASP
SER
LYS
GLY

• Molecule 1: Multidrug resistance protein mexA

Chain C: 

CYS
GLY
LYS
SER
GLY
ALA
PRO
PRO
ALA
GLN
THR
PRO
GLY
VAL
GLY
ILE
VAL
THR
LEU
PHE
GLN
VAL
GLN
PRO
GLY
THR
THR
ASN
T29
E30
L31
R34
T35
F38
V43
R44
P45
Q46
V47
N48
L52
K53
R54
L55
S60
D61
V62
Q66
Q67
L68
Y69
Q70
I71
D72

P73
A74
Y76
Y80
N86
S89
T90
Q91
Q95
Q104
A105
V106
S107
K108
Q109
Q110
A116
A117
Y118
Q120
E126
Q127
A128
R129
L210
N130
N131
L132
R133
Y134
T135
K136
V137
L138
S139
P140
I141
S142
I145
G146
R147
Y156
T157
N158
G159
M164
A165
T166
V167

L170
D171
P172
I173
Y174
V175
D176
V177
Q178
T179
A183
R186
L187
E190
S193
G194
Q195
Q196
L196
E197
D201
N202
K205
V206
S207
L208
R209
E211
D212
E219
G220
R221
L222
E223
E226
V227
V236
T237
A240
F241
P245
N246
N247
L250
P251
G252

N253
F254
H255
H256
A257
Q258
L259
GLN
GLY
VAL
LYS
GLN
LYS
ALA
ILE
LEU
ALA
PRO
GLN
GLY
PHE
VAL
GLN
PRO
GLY
VAL
GLY
GLY
THR
THR
VAL
THR
ASN
LYS
GLY
ALA
VAL
VAL
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ALA
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LYS
VAL
THR
SER
GLN
VAL
ASP
GLY

GLY
LEU
ASN
ALA
GLY
ASP
LYS
ILE
ILE
THR
GLY
GLY
LEU
PHE
VAL
GLN
PRO
GLY
VAL
GLY
GLY
THR
THR
VAL
PRO
ALA
LYS
VAL
ASN
GLN
VAL
ALA
ASP
ALA
GLN
LYS
PRO
ALA
VAL
LYS
THR
ASP
ARG
VAL
THR
GLY

• Molecule 1: Multidrug resistance protein mexA

Chain D: 

CYS
GLY
LYS
SER
GLY
ALA
PRO
PRO
ALA
GLN
THR
PRO
GLY
VAL
GLY
ILE
VAL
THR
LEU
PHE
VAL
GLN
PRO
GLY
VAL
GLY
THR
THR
ASN
LYS
GLY
ALA
VAL
VAL
ASN
ALA
GLN
LYS
VAL
THR
SER
GLN
VAL
ASP
GLY

Y76
E77
Y80
Q81
N86
S89
T90
Q91
Q95
R96
Y97
L99
L100
V101
A102
D103
Q104
A105
V106
Q110
Y111
D113
A116
A117
Y118
E126
Q127
A128
R129
I130
N131
L132
R133
Y134
T135
K136
V137
L138
I141
S142
T145
G146
R147
Y156
T157
N158
G159
T75

V167
Q168
D171
P172
I173
Y174
V175
L184
L185
R186
R188
E190
S193
G194
Q195
L196
E197
R198
A199
K205
V206
S207
L208
K209
L210
D211
E212
Y216
P217
L218
E219
G220
R221
L222
E223
F224
S225
E226
V227
V236
T237
A240
V241
F242
P245
N246
N247
L250

N253
F254
H255
A257
L259
GLN
GLY
VAL
LYS
GLN
LYS
ALA
ILE
LEU
ALA
PRO
GLN
GLY
PHE
VAL
GLN
PRO
GLY
VAL
GLY
VAL
GLY
THR
THR
VAL
PRO
ALA
LYS
VAL
ASN
GLN
VAL
ALA
SER
GLN
LYS
VAL
ASP
ALA
GLN
LYS
THR
ASP
ARG
VAL
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GLY

GLY
LEU
ASN
GLY
ASP
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ILE
THR
GLY
GLY
LEU
PHE
VAL
GLN
PRO
GLY
VAL
GLY
VAL
GLY
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VAL
ASN
GLN
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GLN
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ASP
ARG
VAL
THR
GLY

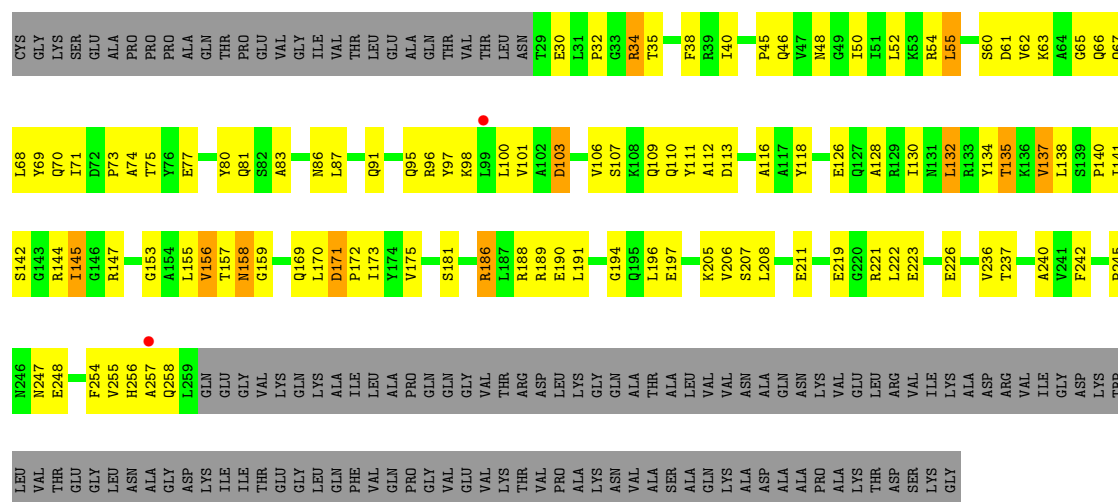
• Molecule 1: Multidrug resistance protein mexA

Chain E: 

CYS
GLY
LYS
SER
GLY
ALA
PRO
PRO
ALA
GLN
THR
PRO
GLY
VAL
GLY
ILE
VAL
THR
LEU
PHE
VAL
GLN
PRO
GLY
VAL
GLY
THR
THR
ASN
LYS
GLY
ALA
VAL
VAL
ASN
GLN
VAL
ALA
SER
GLN
LYS
VAL
ASP
ALA
GLN
LYS
THR
ASP
ARG
VAL
THR
GLY

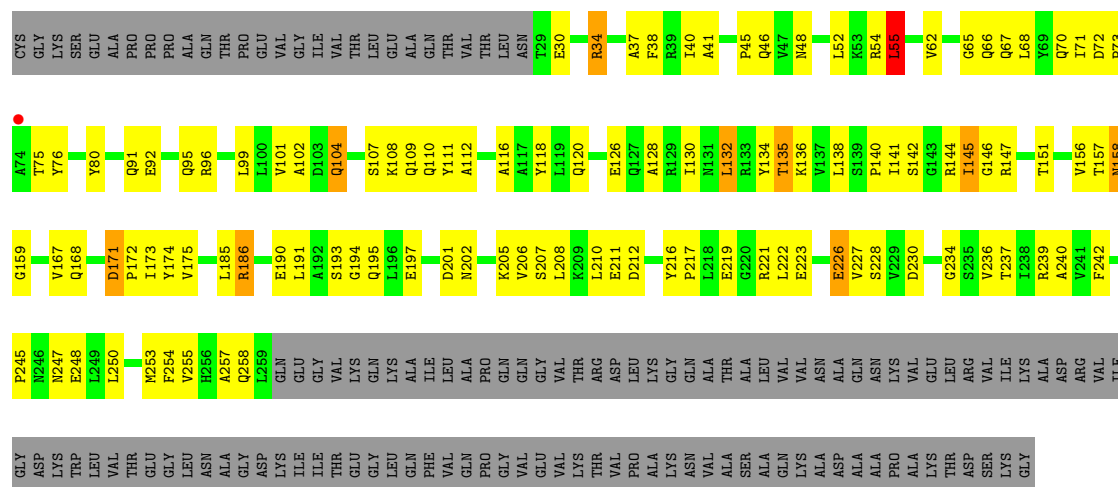
T29
E30
R34
T35
F38
V43
R44
P45
Q46
V47
N48
L52
L55
S60
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G65
Q66
Q67
L68
Y69
Q70
I71
D72
P73

A74
T75
Y76
E77
Y80
Q81
Q91
E92
Q95
R96
L99
L100
V101
A102
D103
Q104
A105
V106
Q109
Q110
Y118
E126
Q127
A128
R129
L130
N131
L132
R133
Y134
T135
K136
V137
L138
S139
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G146
R147
T151
V156
T157
N158
G159
A165
T166



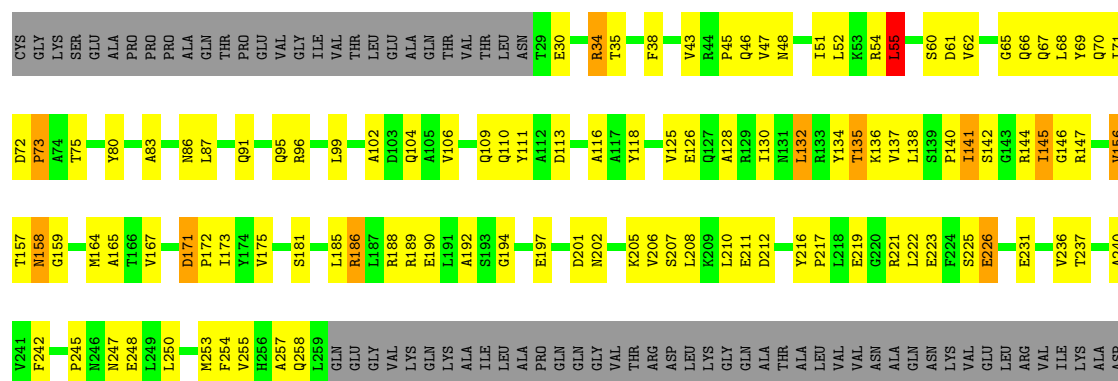
• Molecule 1: Multidrug resistance protein mexA

Chain I: 34% 28% 36%



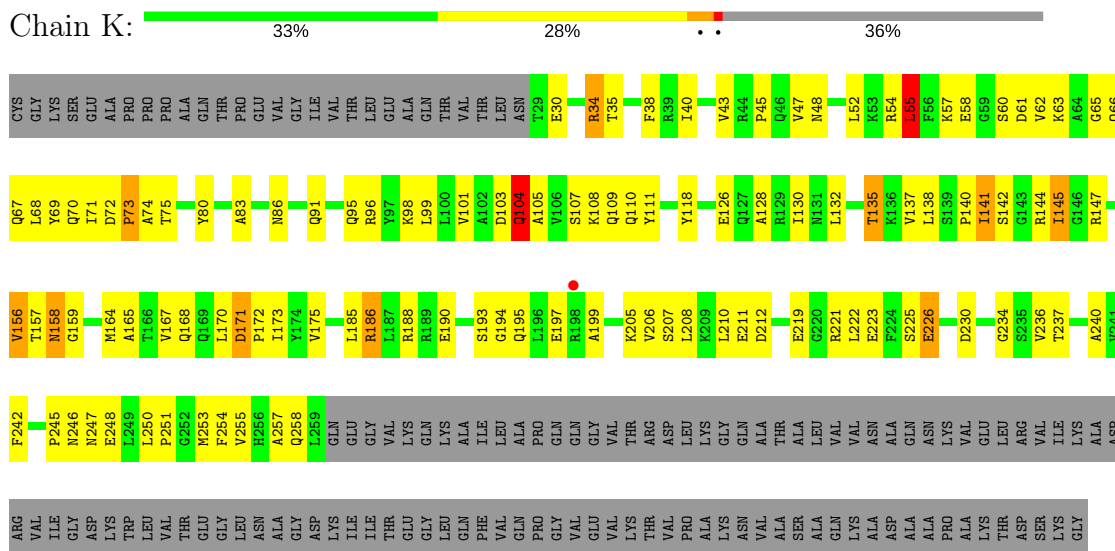
• Molecule 1: Multidrug resistance protein mexA

Chain J: 33% 28% 36%



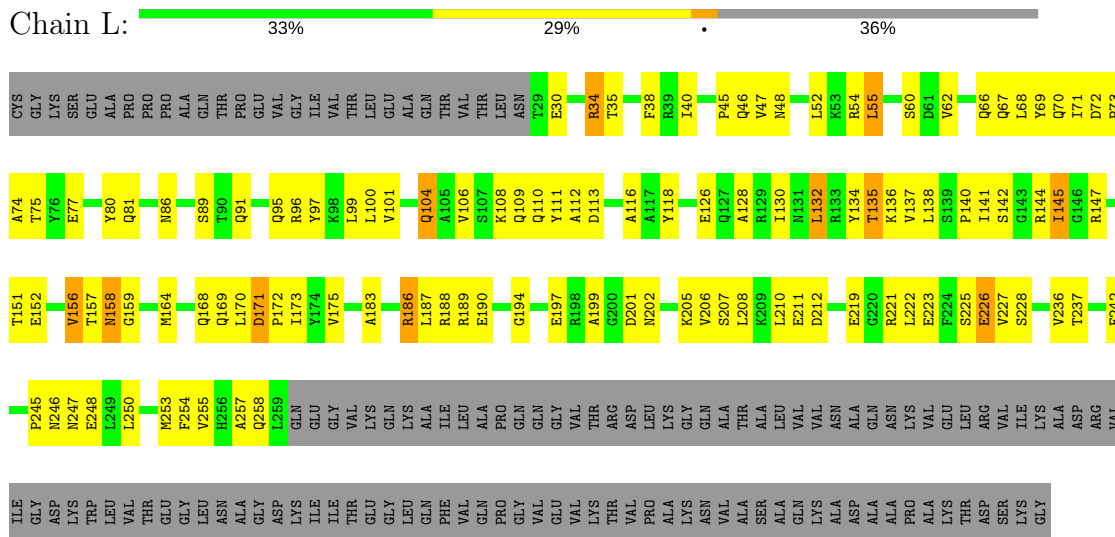
- Molecule 1: Multidrug resistance protein mexA

Chain K:



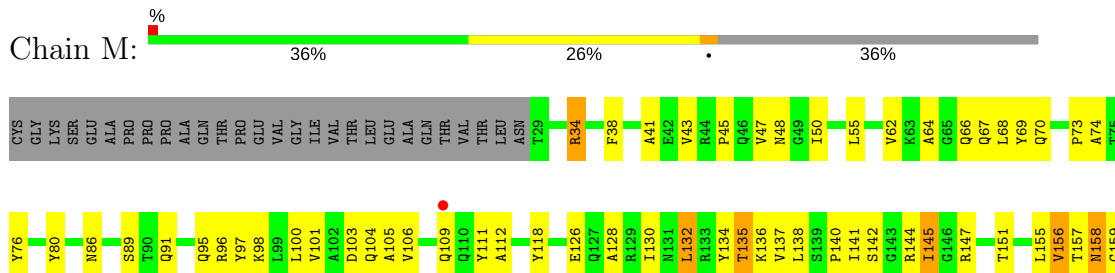
- Molecule 1: Multidrug resistance protein mexA

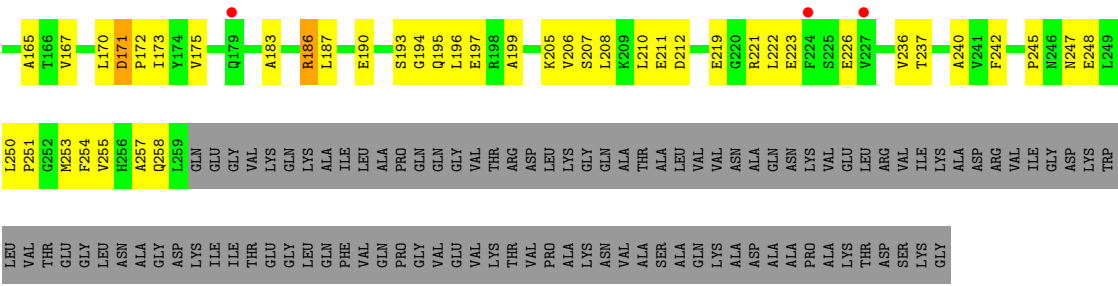
Chain L:



- Molecule 1: Multidrug resistance protein mexA

Chain M:





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	130.55Å 183.59Å 213.31Å 90.00° 107.38° 90.00°	Depositor
Resolution (Å)	95.00 – 3.00 83.48 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.8 (95.00-3.00) 98.3 (83.48-2.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.273 , 0.285 0.268 , 0.278	Depositor DCC
R_{free} test set	9310 reflections (4.91%)	DCC
Wilson B-factor (Å ²)	75.0	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.005 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	23101	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 3GR

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	0.48	1/1795 (0.1%)	0.62	0/2434
1	B	0.39	0/1795	0.65	0/2434
1	C	0.40	0/1795	0.66	0/2434
1	D	0.42	0/1795	0.69	0/2434
1	E	0.47	0/1795	0.71	0/2434
1	F	0.38	0/1795	0.67	0/2434
1	G	0.37	0/1795	0.63	0/2434
1	H	0.45	0/1795	0.70	0/2434
1	I	0.49	0/1795	0.71	0/2434
1	J	0.56	0/1795	0.75	0/2434
1	K	0.52	0/1795	0.73	0/2434
1	L	0.48	0/1795	0.71	0/2434
1	M	0.39	0/1795	0.66	0/2434
All	All	0.45	1/23335 (0.0%)	0.68	0/31642

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	0	1
1	I	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	THR	C-N	-14.50	1.00	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	29	THR	Mainchain
1	I	111	TYR	Sidechain

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	1771	0	1774	109	1
1	B	1771	0	1775	105	0
1	C	1771	0	1775	98	0
1	D	1771	0	1775	110	1
1	E	1771	0	1775	102	0
1	F	1771	0	1775	109	0
1	G	1771	0	1775	120	0
1	H	1771	0	1775	109	0
1	I	1771	0	1775	115	0
1	J	1771	0	1775	110	0
1	K	1771	0	1775	120	0
1	L	1771	0	1775	127	0
1	M	1771	0	1775	110	0
2	C	6	0	5	2	0
2	D	6	0	5	0	0
2	E	6	0	5	2	0
2	F	6	0	5	4	0
2	G	6	0	5	1	0
2	H	6	0	5	2	0
2	I	6	0	5	4	0
2	K	6	0	5	3	0
2	L	6	0	5	1	0
3	A	6	0	8	5	0
3	B	6	0	5	3	0
3	J	6	0	5	5	0
3	M	6	0	5	2	0
All	All	23101	0	23142	1365	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 30.

The worst 5 of 1365 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:F:146:GLY:HA3	2:F:361:3GR:O2	1.37	1.24
1:M:70:GLN:HE22	1:M:135:THR:HG23	1.08	1.15
1:A:70:GLN:HE22	1:A:135:THR:HG23	1.18	1.07
1:F:91:GLN:HG2	1:F:95:GLN:HE21	1.21	1.05
1:J:91:GLN:HG2	1:J:95:GLN:HE21	1.16	1.04

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:A:189:ARG:NH2	1:D:194:GLY:O[2_656]	2.19	0.01

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	229/360 (64%)	207 (90%)	21 (9%)	1 (0%)	38	78
1	B	229/360 (64%)	203 (89%)	24 (10%)	2 (1%)	20	62
1	C	229/360 (64%)	209 (91%)	18 (8%)	2 (1%)	20	62
1	D	229/360 (64%)	200 (87%)	24 (10%)	5 (2%)	8	36
1	E	229/360 (64%)	211 (92%)	15 (7%)	3 (1%)	14	51
1	F	229/360 (64%)	209 (91%)	17 (7%)	3 (1%)	14	51
1	G	229/360 (64%)	205 (90%)	20 (9%)	4 (2%)	11	44
1	H	229/360 (64%)	205 (90%)	19 (8%)	5 (2%)	8	36
1	I	229/360 (64%)	210 (92%)	16 (7%)	3 (1%)	14	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	229/360 (64%)	208 (91%)	17 (7%)	4 (2%)	11	44
1	K	229/360 (64%)	205 (90%)	20 (9%)	4 (2%)	11	44
1	L	229/360 (64%)	205 (90%)	20 (9%)	4 (2%)	11	44
1	M	229/360 (64%)	204 (89%)	22 (10%)	3 (1%)	14	51
All	All	2977/4680 (64%)	2681 (90%)	253 (8%)	43 (1%)	13	49

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	ASP
1	B	171	ASP
1	C	171	ASP
1	D	171	ASP
1	E	171	ASP

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	186/287 (65%)	176 (95%)	10 (5%)	26	64
1	B	186/287 (65%)	175 (94%)	11 (6%)	23	60
1	C	186/287 (65%)	176 (95%)	10 (5%)	26	64
1	D	186/287 (65%)	173 (93%)	13 (7%)	18	53
1	E	186/287 (65%)	170 (91%)	16 (9%)	12	42
1	F	186/287 (65%)	173 (93%)	13 (7%)	18	53
1	G	186/287 (65%)	175 (94%)	11 (6%)	23	60
1	H	186/287 (65%)	174 (94%)	12 (6%)	20	56
1	I	186/287 (65%)	176 (95%)	10 (5%)	26	64
1	J	186/287 (65%)	171 (92%)	15 (8%)	14	45
1	K	186/287 (65%)	171 (92%)	15 (8%)	14	45
1	L	186/287 (65%)	174 (94%)	12 (6%)	20	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	186/287 (65%)	177 (95%)	9 (5%)	30	69
All	All	2418/3731 (65%)	2261 (94%)	157 (6%)	20	56

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	189	ARG
1	H	103	ASP
1	L	186	ARG
1	G	34	ARG
1	G	145	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	84	GLN
1	H	95	GLN
1	M	70	GLN
1	G	110	GLN
1	G	169	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	A	361	-	5,5,5	0.19	0	5,5,5	0.45	0
3	GOL	B	361	-	5,5,5	4.77	1 (20%)	5,5,5	4.02	1 (20%)
2	3GR	C	361	-	5,5,5	2.41	1 (20%)	4,5,5	6.43	1 (25%)
2	3GR	D	361	-	5,5,5	2.41	1 (20%)	4,5,5	6.42	1 (25%)
2	3GR	E	361	-	5,5,5	2.41	1 (20%)	4,5,5	6.42	1 (25%)
2	3GR	F	361	-	5,5,5	2.40	1 (20%)	4,5,5	6.42	1 (25%)
2	3GR	G	361	-	5,5,5	2.41	1 (20%)	4,5,5	6.41	1 (25%)
2	3GR	H	361	-	5,5,5	2.41	1 (20%)	4,5,5	6.42	1 (25%)
2	3GR	I	361	-	5,5,5	2.41	1 (20%)	4,5,5	6.41	1 (25%)
3	GOL	J	361	1	5,5,5	4.77	1 (20%)	5,5,5	4.03	1 (20%)
2	3GR	K	361	-	5,5,5	2.40	1 (20%)	4,5,5	6.43	1 (25%)
2	3GR	L	361	-	5,5,5	2.41	1 (20%)	4,5,5	6.43	1 (25%)
3	GOL	M	361	1	5,5,5	4.77	1 (20%)	5,5,5	4.03	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	361	-	-	0/4/4/4	0/0/0/0
3	GOL	B	361	-	-	0/4/4/4	0/0/0/0
2	3GR	C	361	-	1/1/1/2	0/2/4/4	0/0/0/0
2	3GR	D	361	-	1/1/1/2	0/2/4/4	0/0/0/0
2	3GR	E	361	-	1/1/1/2	0/2/4/4	0/0/0/0
2	3GR	F	361	-	1/1/1/2	0/2/4/4	0/0/0/0
2	3GR	G	361	-	1/1/1/2	0/2/4/4	0/0/0/0
2	3GR	H	361	-	1/1/1/2	0/2/4/4	0/0/0/0
2	3GR	I	361	-	1/1/1/2	0/2/4/4	0/0/0/0
3	GOL	J	361	1	-	0/4/4/4	0/0/0/0
2	3GR	K	361	-	1/1/1/2	0/2/4/4	0/0/0/0
2	3GR	L	361	-	1/1/1/2	0/2/4/4	0/0/0/0
3	GOL	M	361	1	-	0/4/4/4	0/0/0/0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	361	GOL	O3-C3	-10.60	0.97	1.42
3	B	361	GOL	O3-C3	-10.60	0.97	1.42
3	J	361	GOL	O3-C3	-10.60	0.97	1.42
2	G	361	3GR	O3-C3	-5.25	0.97	1.19
2	I	361	3GR	O3-C3	-5.25	0.97	1.19

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	361	GOL	O3-C3-C2	8.98	155.32	110.07
3	J	361	GOL	O3-C3-C2	8.99	155.34	110.07
3	M	361	GOL	O3-C3-C2	8.99	155.36	110.07
2	I	361	3GR	O3-C3-C2	12.63	155.28	125.06
2	F	361	3GR	O3-C3-C2	12.64	155.28	125.06

5 of 9 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	361	3GR	C2
2	I	361	3GR	C2
2	C	361	3GR	C2
2	G	361	3GR	C2
2	H	361	3GR	C2

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	361	GOL	5	0
3	B	361	GOL	3	0
2	C	361	3GR	2	0
2	E	361	3GR	2	0
2	F	361	3GR	4	0
2	G	361	3GR	1	0
2	H	361	3GR	2	0
2	I	361	3GR	4	0
3	J	361	GOL	5	0
2	K	361	3GR	3	0
2	L	361	3GR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	361	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 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	231/360 (64%)	0.47	19 (8%) 12 5	56, 93, 132, 143	2 (0%)
1	B	231/360 (64%)	0.08	0 100 100	37, 80, 110, 123	2 (0%)
1	C	231/360 (64%)	0.06	2 (0%) 84 61	39, 77, 111, 116	2 (0%)
1	D	231/360 (64%)	0.09	0 100 100	30, 82, 109, 123	2 (0%)
1	E	231/360 (64%)	0.00	0 100 100	22, 61, 95, 111	2 (0%)
1	F	231/360 (64%)	0.07	2 (0%) 84 61	53, 80, 106, 111	2 (0%)
1	G	231/360 (64%)	0.15	7 (3%) 51 23	51, 86, 118, 126	2 (0%)
1	H	231/360 (64%)	0.10	2 (0%) 84 61	28, 64, 98, 109	2 (0%)
1	I	231/360 (64%)	0.15	1 (0%) 92 77	24, 62, 96, 109	2 (0%)
1	J	231/360 (64%)	0.06	0 100 100	15, 48, 84, 100	2 (0%)
1	K	231/360 (64%)	0.02	1 (0%) 92 77	20, 59, 92, 107	2 (0%)
1	L	231/360 (64%)	0.03	0 100 100	25, 63, 102, 115	2 (0%)
1	M	231/360 (64%)	0.22	4 (1%) 70 42	40, 93, 117, 130	2 (0%)
All	All	3003/4680 (64%)	0.12	38 (1%) 77 51	15, 75, 114, 143	26 (0%)

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	GLY	4.7
1	M	227	VAL	4.6
1	A	29	THR	3.6
1	A	231	GLU	3.5
1	A	31	LEU	3.2

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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	3GR	K	361	6/6	0.82	0.36	4.83	79,80,83,84	0
2	3GR	L	361	6/6	0.86	0.35	3.18	81,82,83,86	0
2	3GR	C	361	6/6	0.79	0.30	2.60	100,100,101,102	0
2	3GR	D	361	6/6	0.89	0.32	1.95	93,93,94,95	0
3	GOL	A	361	6/6	0.66	0.33	1.88	97,98,99,102	0
2	3GR	I	361	6/6	0.86	0.30	1.13	87,87,88,88	0
3	GOL	B	361	6/6	0.78	0.30	1.10	95,96,96,96	0
3	GOL	M	361	6/6	0.82	0.26	0.74	99,100,101,101	0
2	3GR	E	361	6/6	0.77	0.37	-	93,95,98,102	0
2	3GR	G	361	6/6	0.81	0.21	-	103,104,105,106	0
2	3GR	F	361	6/6	0.69	0.27	-	99,100,101,103	0
2	3GR	H	361	6/6	0.80	0.32	-	87,88,89,90	0
3	GOL	J	361	6/6	0.71	0.40	-	92,94,94,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.