



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:30 am GMT

PDB ID : 2XTQ
Title : STRUCTURE OF THE P107A COLICIN M MUTANT FROM E. COLI
Authors : Helbig, S.; Patzer, S.I.; Braun, V.; Zeth, K.
Deposited on : 2010-10-12
Resolution : 2.31 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
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

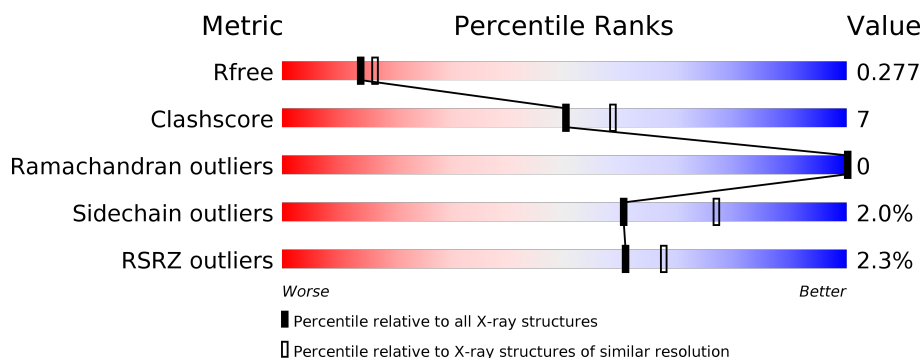
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	4787 (2.34-2.30)
Clashscore	112137	5439 (2.34-2.30)
Ramachandran outliers	110173	5386 (2.34-2.30)
Sidechain outliers	110143	5385 (2.34-2.30)
RSRZ outliers	101464	4814 (2.34-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	271	<div> <div>3%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	B	271	<div> <div>%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	C	271	<div> <div>3%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
1	D	271	<div> <div>2%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	E	271	<div> <div>%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	F	271	<div> <div>2%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	271	<div><div>%</div><div><div></div><div>86%</div><div>14%</div></div></div>
1	H	271	<div><div>4%</div><div><div></div><div>87%</div><div>11%</div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17024 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 COLICIN-M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	3	0	0
			2067	1317	352	390	8			
1	B	270	Total	C	N	O	S	1	2	0
			2078	1325	354	391	8			
1	C	270	Total	C	N	O	S	1	1	0
			2075	1322	355	390	8			
1	D	270	Total	C	N	O	S	4	1	0
			2073	1322	353	390	8			
1	E	270	Total	C	N	O	S	2	2	0
			2079	1325	355	391	8			
1	F	270	Total	C	N	O	S	1	0	0
			2067	1317	352	390	8			
1	G	270	Total	C	N	O	S	1	0	0
			2067	1317	352	390	8			
1	H	270	Total	C	N	O	S	4	0	0
			2067	1317	352	390	8			

There are 8 discrepancies between the modelled and reference sequences:

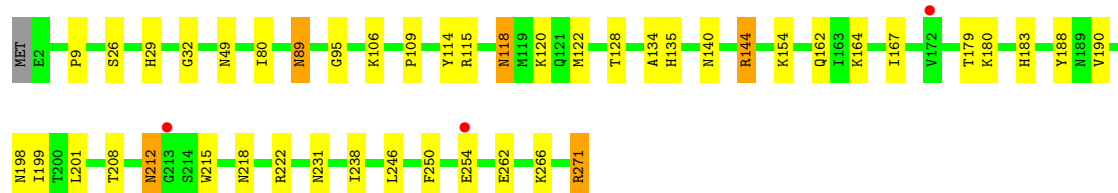
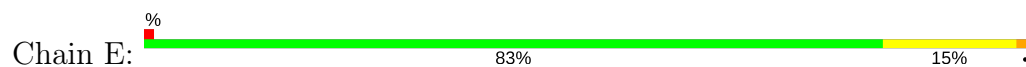
Chain	Residue	Modelled	Actual	Comment	Reference
A	107	ALA	PRO	ENGINEERED MUTATION	UNP P05820
B	107	ALA	PRO	ENGINEERED MUTATION	UNP P05820
C	107	ALA	PRO	ENGINEERED MUTATION	UNP P05820
D	107	ALA	PRO	ENGINEERED MUTATION	UNP P05820
E	107	ALA	PRO	ENGINEERED MUTATION	UNP P05820
F	107	ALA	PRO	ENGINEERED MUTATION	UNP P05820
G	107	ALA	PRO	ENGINEERED MUTATION	UNP P05820
H	107	ALA	PRO	ENGINEERED MUTATION	UNP P05820

- Molecule 2 is water.

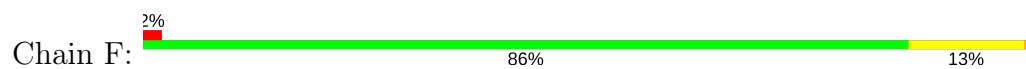
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	67	Total 67	O 67	0	0
2	B	59	Total 59	O 59	0	0
2	C	61	Total 61	O 61	0	0
2	D	60	Total 60	O 60	0	0
2	E	50	Total 50	O 50	0	0
2	F	52	Total 52	O 52	0	0
2	G	49	Total 49	O 49	0	0
2	H	53	Total 53	O 53	0	0



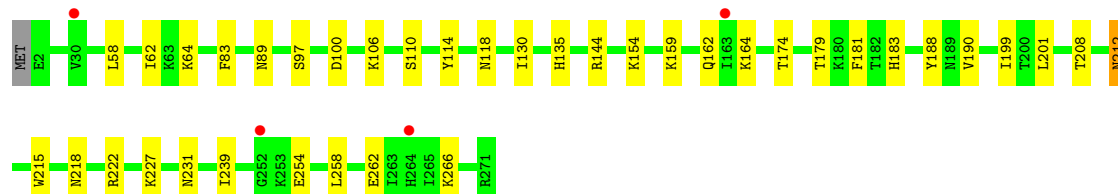
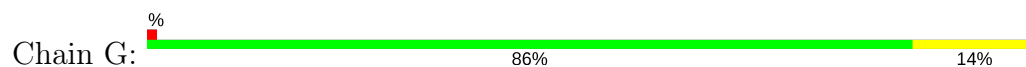
• Molecule 1: COLICIN-M



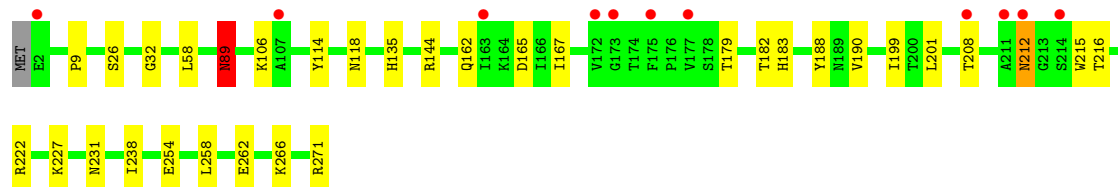
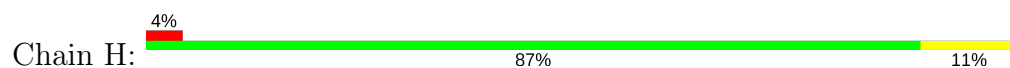
• Molecule 1: COLICIN-M



• Molecule 1: COLICIN-M



• Molecule 1: COLICIN-M



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.85Å 63.11Å 189.34Å 87.59° 82.17° 65.65°	Depositor
Resolution (Å)	48.68 – 2.31 48.68 – 2.31	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.68-2.31) 90.6 (48.68-2.31)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.240 , 0.273 0.242 , 0.277	Depositor DCC
R_{free} test set	4514 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 11.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.419 for h,h-k,h-l 0.167 for -h,-h+k,-l 0.167 for -h,-k,-h+l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	17024	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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 [i](#)

5.1 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	1.63	3/2117 (0.1%)	0.88	4/2879 (0.1%)
1	B	0.97	7/2134 (0.3%)	0.83	2/2901 (0.1%)
1	C	1.25	2/2127 (0.1%)	1.03	2/2890 (0.1%)
1	D	1.85	5/2126 (0.2%)	1.20	6/2890 (0.2%)
1	E	1.24	3/2136 (0.1%)	0.93	7/2905 (0.2%)
1	F	0.94	2/2117 (0.1%)	0.84	2/2879 (0.1%)
1	G	0.81	1/2117 (0.0%)	0.74	2/2879 (0.1%)
1	H	1.02	4/2117 (0.2%)	0.77	3/2879 (0.1%)
All	All	1.26	27/16991 (0.2%)	0.91	28/23102 (0.1%)

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	C	0	1
1	D	0	1
1	E	0	1
1	H	0	1
All	All	0	5

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	140	ASN	CG-ND2	72.25	3.13	1.32
1	A	266	LYS	CG-CD	62.30	3.64	1.52
1	C	89	ASN	CG-OD1	43.80	2.20	1.24
1	E	89	ASN	CG-OD1	35.46	2.02	1.24
1	H	266	LYS	CG-CD	26.88	2.43	1.52

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	89	ASN	OD1-CG-ND2	-41.60	26.21	121.90
1	C	89	ASN	OD1-CG-ND2	-37.72	35.13	121.90
1	D	140	ASN	OD1-CG-ND2	-23.32	68.26	121.90
1	E	89	ASN	CB-CG-OD1	-21.57	78.45	121.60
1	F	266	LYS	CD-CE-NZ	-21.14	63.07	111.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	ASN	Sidechain
1	C	89	ASN	Sidechain
1	D	89	ASN	Sidechain
1	E	89	ASN	Sidechain
1	H	89	ASN	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	2067	0	2049	29	3
1	B	2078	0	2068	25	0
1	C	2075	0	2062	36	2
1	D	2073	0	2062	28	0
1	E	2079	0	2062	34	1
1	F	2067	0	2049	27	1
1	G	2067	0	2049	24	1
1	H	2067	0	2049	20	1
2	A	67	0	0	6	0
2	B	59	0	0	7	0
2	C	61	0	0	11	0
2	D	60	0	0	6	0
2	E	50	0	0	11	1
2	F	52	0	0	9	0
2	G	49	0	0	3	0
2	H	53	0	0	2	0
All	All	17024	0	16450	219	7

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 219 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:B:89:ASN:ND2	2:B:2015:HOH:O	1.74	1.16
1:A:137:LEU:HG	2:A:2031:HOH:O	1.49	1.09
1:E:250:PHE:CD2	2:E:2046:HOH:O	2.24	0.91
1:E:198:ASN:O	2:E:2040:HOH:O	1.88	0.90
1:C:140:ASN:HB3	2:C:2032:HOH:O	1.71	0.90

The worst 5 of 7 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:C:212:ASN:ND2	1:G:262:GLU:CB[1_664]	1.89	0.31
1:E:32:GLY:O	1:E:222:ARG:NH1[1_455]	1.91	0.29
1:C:32:GLY:O	1:C:222:ARG:NH1[1_655]	1.97	0.23
1:A:32:GLY:O	1:A:222:ARG:NH1[1_655]	2.01	0.19
1:H:32:GLY:O	1:H:222:ARG:NH1[1_455]	2.10	0.10

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	268/271 (99%)	262 (98%)	6 (2%)	0	100	100
1	B	270/271 (100%)	264 (98%)	6 (2%)	0	100	100
1	C	268/271 (99%)	264 (98%)	4 (2%)	0	100	100
1	D	269/271 (99%)	264 (98%)	5 (2%)	0	100	100
1	E	270/271 (100%)	264 (98%)	6 (2%)	0	100	100
1	F	268/271 (99%)	262 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	268/271 (99%)	264 (98%)	4 (2%)	0	100	100
1	H	268/271 (99%)	264 (98%)	4 (2%)	0	100	100
All	All	2149/2168 (99%)	2108 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	225/226 (100%)	221 (98%)	4 (2%)	64	79
1	B	227/226 (100%)	223 (98%)	4 (2%)	64	79
1	C	226/226 (100%)	221 (98%)	5 (2%)	57	74
1	D	226/226 (100%)	222 (98%)	4 (2%)	64	79
1	E	227/226 (100%)	222 (98%)	5 (2%)	57	74
1	F	225/226 (100%)	219 (97%)	6 (3%)	50	67
1	G	225/226 (100%)	221 (98%)	4 (2%)	64	79
1	H	225/226 (100%)	221 (98%)	4 (2%)	64	79
All	All	1806/1808 (100%)	1770 (98%)	36 (2%)	60	77

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	266	LYS
1	E	212	ASN
1	H	89	ASN
1	E	106	LYS
1	E	271	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	162	GLN
1	E	118	ASN
1	H	118	ASN
1	D	183	HIS
1	E	49	ASN

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](#)

There are no ligands in this entry.

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 ⓘ

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	270/271 (99%)	0.18	8 (2%)	51	58	8, 18, 40, 67	7 (2%)
1	B	270/271 (99%)	0.16	4 (1%)	74	79	9, 19, 37, 94	6 (2%)
1	C	270/271 (99%)	0.20	9 (3%)	47	54	9, 19, 42, 72	6 (2%)
1	D	270/271 (99%)	0.13	5 (1%)	67	73	9, 19, 37, 81	6 (2%)
1	E	270/271 (99%)	0.15	3 (1%)	80	84	8, 19, 40, 67	3 (1%)
1	F	270/271 (99%)	0.20	6 (2%)	62	69	8, 19, 39, 90	5 (1%)
1	G	270/271 (99%)	0.17	4 (1%)	74	79	9, 20, 39, 89	5 (1%)
1	H	270/271 (99%)	0.24	11 (4%)	38	45	10, 20, 44, 72	6 (2%)
All	All	2160/2168 (99%)	0.18	50 (2%)	61	67	8, 19, 41, 94	44 (2%)

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	GLU	7.8
1	F	30	VAL	7.6
1	A	172	VAL	6.8
1	H	172	VAL	6.4
1	H	107	ALA	4.3

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.