



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:40 PM UTC

PDB ID : 4DK1 / pdb\_00004dk1  
Title : Crystal Structure of MacA-MexA chimeric protein, containing the Pseudomonas aeruginosa MexA alpha-hairpin domain.  
Authors : Xu, Y.; Ha, N.C.  
Deposited on : 2012-02-03  
Resolution : 3.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

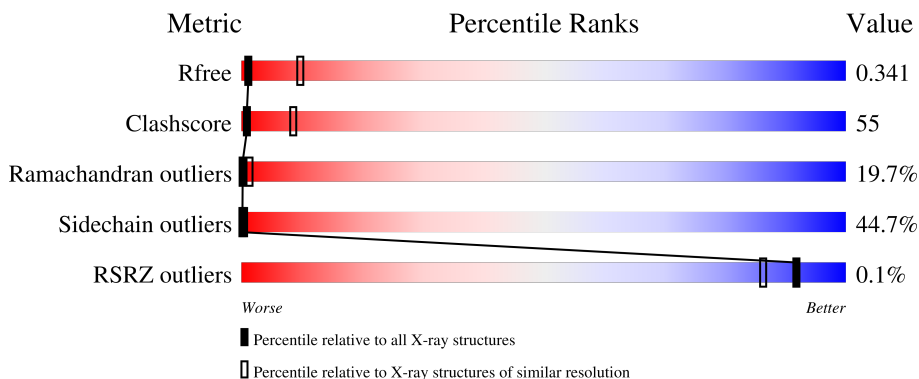
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	341	 13% 28% 23% 17% 19%
1	B	341	 12% 29% 27% 16% 16%
1	C	341	 16% 27% 27% 12% 18%
1	D	341	 16% 26% 27% 12% 18%

## 2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 8568 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Putative MacA, Multidrug resistance protein mexA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	276	2108	1316	355	435	2	4	0	0
1	B	285	2191	1369	369	451	2	4	0	0
1	C	278	2135	1336	358	439	2	4	0	0
1	D	278	2134	1334	359	439	2	4	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	expression tag	UNP Q2EHL9
A	27	ALA	-	expression tag	UNP Q2EHL9
A	28	MSE	-	expression tag	UNP Q2EHL9
A	29	ASP	-	expression tag	UNP Q2EHL9
A	68	ILE	VAL	SEE REMARK 999	UNP Q2EHL9
A	85	LEU	ILE	SEE REMARK 999	UNP Q2EHL9
B	26	GLY	-	expression tag	UNP Q2EHL9
B	27	ALA	-	expression tag	UNP Q2EHL9
B	28	MSE	-	expression tag	UNP Q2EHL9
B	29	ASP	-	expression tag	UNP Q2EHL9
B	68	ILE	VAL	SEE REMARK 999	UNP Q2EHL9
B	85	LEU	ILE	SEE REMARK 999	UNP Q2EHL9
C	26	GLY	-	expression tag	UNP Q2EHL9
C	27	ALA	-	expression tag	UNP Q2EHL9
C	28	MSE	-	expression tag	UNP Q2EHL9
C	29	ASP	-	expression tag	UNP Q2EHL9
C	68	ILE	VAL	SEE REMARK 999	UNP Q2EHL9
C	85	LEU	ILE	SEE REMARK 999	UNP Q2EHL9
D	26	GLY	-	expression tag	UNP Q2EHL9
D	27	ALA	-	expression tag	UNP Q2EHL9
D	28	MSE	-	expression tag	UNP Q2EHL9

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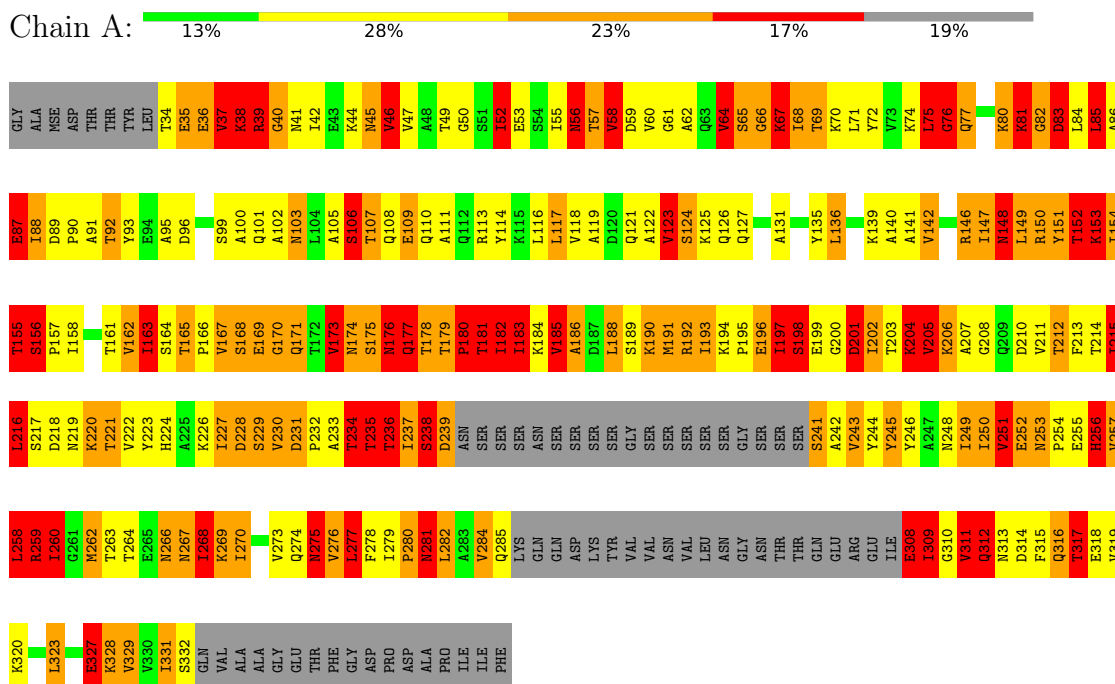
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Chain	Residue	Modelled	Actual	Comment	Reference
D	29	ASP	-	expression tag	UNP Q2EHL9
D	68	ILE	VAL	SEE REMARK 999	UNP Q2EHL9
D	85	LEU	ILE	SEE REMARK 999	UNP Q2EHL9

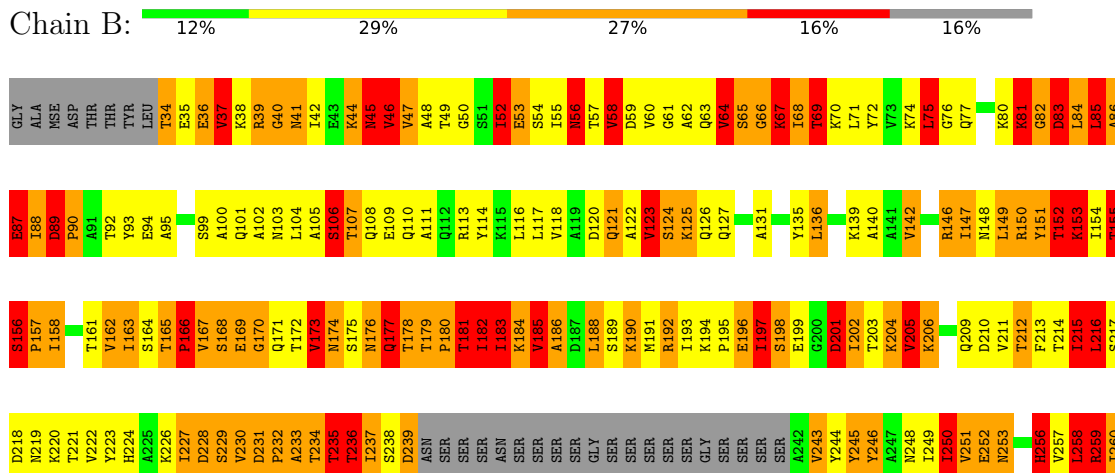
### 3 Residue-property plots

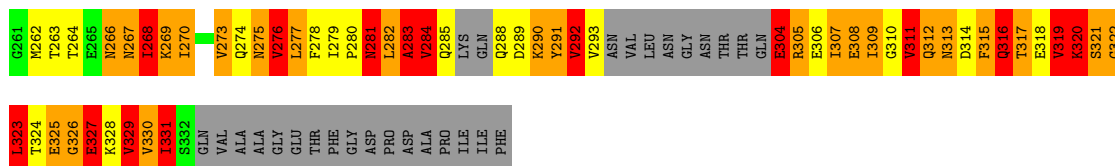
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Putative MacA, Multidrug resistance protein mexA



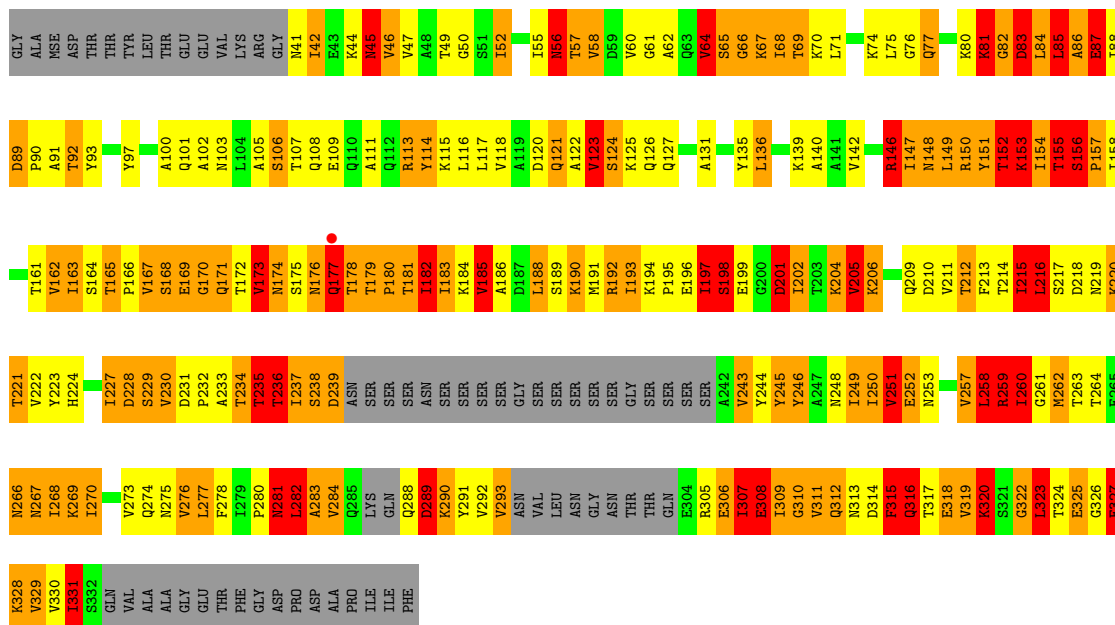
- Molecule 1: Putative MacA, Multidrug resistance protein mexA





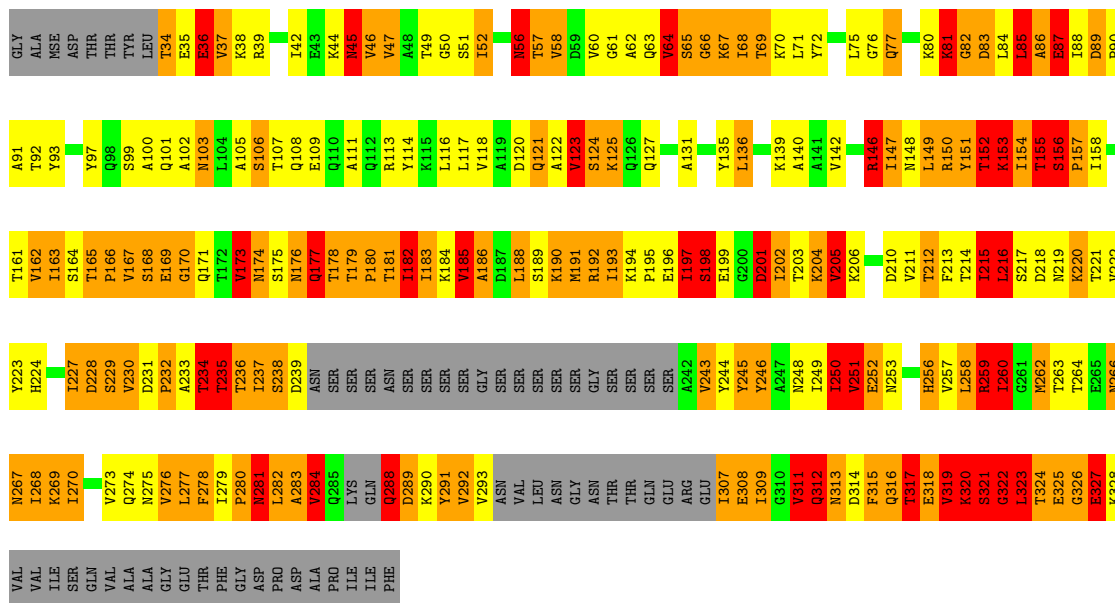
● Molecule 1: Putative MacA, Multidrug resistance protein mexA

Chain C: 16% 27% 27% 12% 18%



● Molecule 1: Putative MacA, Multidrug resistance protein mexA

Chain D: 16% 26% 27% 12% 18%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.71Å 151.71Å 216.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 3.50 19.95 – 3.50	Depositor EDS
% Data completeness (in resolution range)	91.3 (19.95-3.50) 91.4 (19.95-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.60 (at 3.52Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.314 , 0.368 0.287 , 0.341	Depositor DCC
$R_{free}$ test set	1709 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.6	Xtrriage
Anisotropy	0.398	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.12 , 0.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.31$ , $\langle L^2 \rangle = 0.15$	Xtrriage
Estimated twinning fraction	0.277 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	8568	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	1.60	29/2127 (1.4%)	2.02	79/2884 (2.7%)
1	B	1.59	30/2210 (1.4%)	1.96	79/2994 (2.6%)
1	C	1.26	7/2154 (0.3%)	1.81	53/2920 (1.8%)
1	D	1.28	11/2153 (0.5%)	1.83	63/2917 (2.2%)
All	All	1.44	77/8644 (0.9%)	1.91	274/11715 (2.3%)

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	23
1	B	0	25
1	C	0	22
1	D	0	24
All	All	0	94

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	58	VAL	CA-CB	-13.43	1.41	1.55
1	A	179	THR	C-O	-9.52	1.12	1.24
1	B	45	ASN	CG-ND2	-8.33	1.15	1.33
1	B	121	GLN	CD-NE2	-7.99	1.16	1.33
1	A	58	VAL	CA-CB	-7.66	1.47	1.55

The worst 5 of 274 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	179	THR	CA-C-N	-18.67	102.02	120.31
1	C	179	THR	C-N-CA	-18.67	102.02	120.31
1	B	179	THR	CA-C-N	-17.13	103.52	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	THR	C-N-CA	-17.13	103.52	120.31
1	D	179	THR	CA-C-N	-16.29	102.88	120.14

There are no chirality outliers.

5 of 94 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	37	VAL	Peptide
1	A	39	ARG	Peptide
1	A	56	ASN	Peptide
1	A	75	LEU	Peptide
1	A	85	LEU	Mainchain

## 5.2 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	2108	0	2133	247	2
1	B	2191	0	2215	272	2
1	C	2135	0	2158	225	1
1	D	2134	0	2156	232	1
All	All	8568	0	8662	940	3

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 55.

The worst 5 of 940 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:A:277:LEU:HB2	1:A:319:VAL:HB	1.29	1.15
1:A:67:LYS:NZ	1:A:68:ILE:O	1.89	1.05
1:C:67:LYS:NZ	1:C:68:ILE:O	1.89	1.05
1:D:67:LYS:NZ	1:D:68:ILE:O	1.89	1.05
1:D:197:ILE:HD11	1:D:202:ILE:HD13	1.42	1.01

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:ASN:O	1:D:174:ASN:ND2[3_565]	1.97	0.23
1:A:199:GLU:O	1:B:217:SER:OG[2_665]	2.11	0.09
1:A:176:ASN:O	1:B:174:ASN:ND2[2_665]	2.12	0.08

## 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	270/341 (79%)	163 (60%)	51 (19%)	56 (21%)	0	1
1	B	277/341 (81%)	170 (61%)	56 (20%)	51 (18%)	0	1
1	C	270/341 (79%)	164 (61%)	49 (18%)	57 (21%)	0	1
1	D	270/341 (79%)	161 (60%)	59 (22%)	50 (18%)	0	1
All	All	1087/1364 (80%)	658 (60%)	215 (20%)	214 (20%)	0	1

5 of 214 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	LYS
1	A	75	LEU
1	A	82	GLY
1	A	121	GLN
1	A	122	ALA

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	236/288 (82%)	129 (55%)	107 (45%)	0	0
1	B	245/288 (85%)	136 (56%)	109 (44%)	0	0
1	C	239/288 (83%)	133 (56%)	106 (44%)	0	0
1	D	238/288 (83%)	132 (56%)	106 (44%)	0	0
All	All	958/1152 (83%)	530 (55%)	428 (45%)	0	0

5 of 428 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	81	LYS
1	C	234	THR
1	D	250	ILE
1	C	109	GLU
1	C	176	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	281	ASN
1	D	63	GLN
1	D	285	GLN
1	D	177	GLN
1	D	45	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 oligosaccharides 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	274/341 (80%)	-0.58	0 <a href="#">100</a> <a href="#">100</a>	7, 60, 178, 245	1 (0%)
1	B	283/341 (82%)	-0.53	0 <a href="#">100</a> <a href="#">100</a>	7, 63, 166, 285	1 (0%)
1	C	276/341 (80%)	-0.32	1 (0%) <a href="#">88</a> <a href="#">72</a>	27, 99, 200, 277	1 (0%)
1	D	276/341 (80%)	-0.37	0 <a href="#">100</a> <a href="#">100</a>	27, 93, 190, 275	1 (0%)
All	All	1109/1364 (81%)	-0.45	1 (0%) <a href="#">92</a> <a href="#">86</a>	7, 82, 185, 285	4 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	177	GLN	2.6

### 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 oligosaccharides 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.