



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 10:48 pm GMT

PDB ID : 3T5M  
Title : Crystal structure of the S112A mutant of mycroicine immunity protein (MccF) with AMP  
Authors : Nocek, B.; Zhou, M.; Gu, M.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2011-07-27  
Resolution : 1.75 Å(reported)

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	trunk31020
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk31020

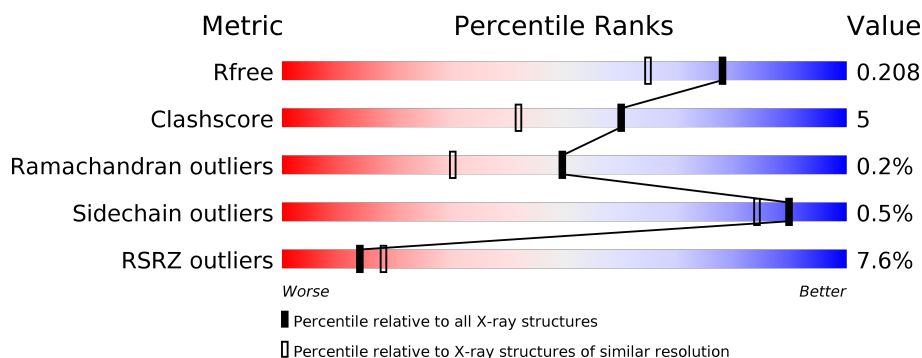
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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))
$R_{free}$	111664	3053 (1.76-1.72)
Clashscore	122126	3201 (1.76-1.72)
Ramachandran outliers	120053	3169 (1.76-1.72)
Sidechain outliers	120020	3169 (1.76-1.72)
RSRZ outliers	108989	2999 (1.76-1.72)

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  $\geq 3$ , 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	336	
1	B	336	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5960 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.

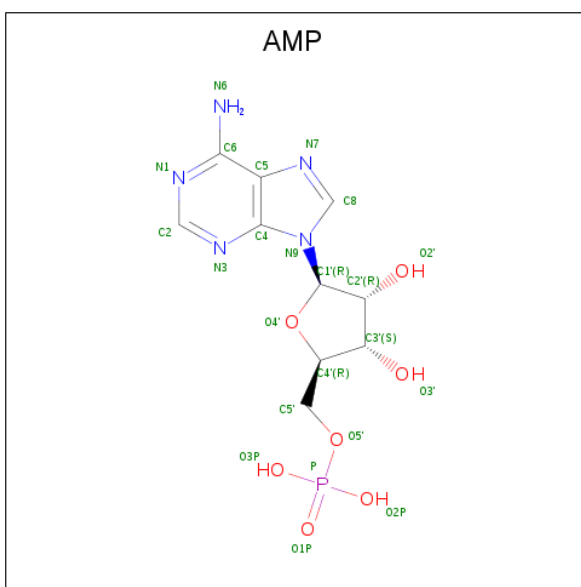
- Molecule 1 is a protein called Microcin immunity protein MccF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	3	0
			2655	1712	431	498	14			
1	B	333	Total	C	N	O	S	0	2	0
			2625	1697	423	491	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q81RT8
A	-1	ASN	-	EXPRESSION TAG	UNP Q81RT8
A	0	ALA	-	EXPRESSION TAG	UNP Q81RT8
A	112	ALA	SER	ENGINEERED MUTATION	UNP Q81RT8
B	-2	SER	-	EXPRESSION TAG	UNP Q81RT8
B	-1	ASN	-	EXPRESSION TAG	UNP Q81RT8
B	0	ALA	-	EXPRESSION TAG	UNP Q81RT8
B	112	ALA	SER	ENGINEERED MUTATION	UNP Q81RT8

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

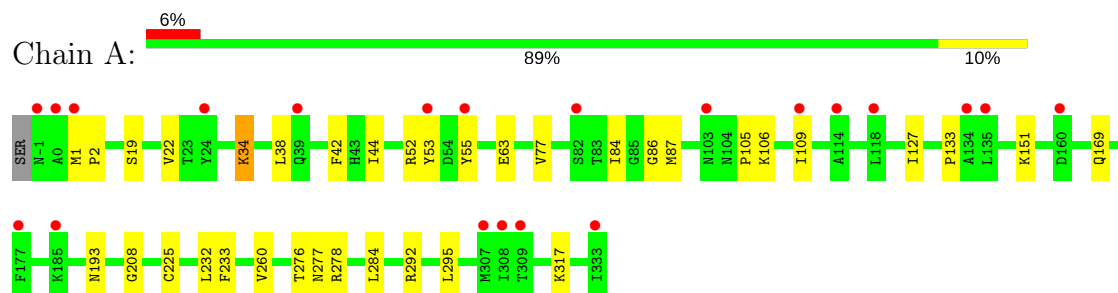
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	332	Total 332	O 332	0	0
4	B	296	Total 296	O 296	0	0

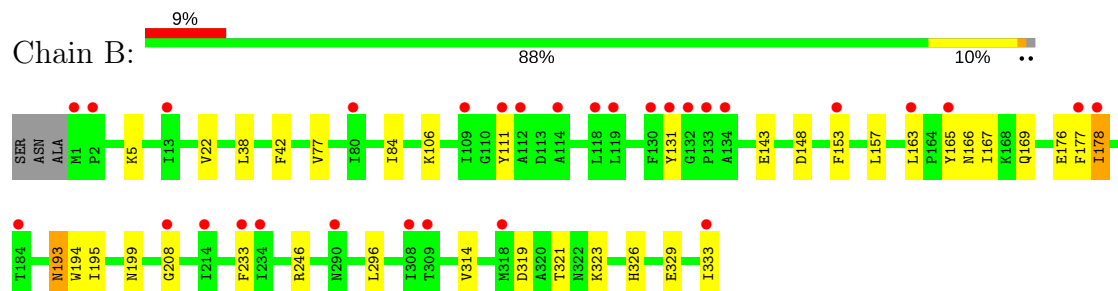
### 3 Residue-property plots [i](#)

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: Microcin immunity protein MccF



#### • Molecule 1: Microcin immunity protein MccF



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.39Å 118.39Å 55.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.71 – 1.75 32.21 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.1 (28.71-1.75) 98.9 (32.21-1.75)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.00 (at 1.75Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.185 , 0.202 0.191 , 0.208	Depositor DCC
$R_{free}$ test set	3911 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.2	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5960	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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

### 5.1 Standard geometry

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

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	0.27	0/2732	0.46	0/3711
1	B	0.28	0/2700	0.48	0/3671
All	All	0.27	0/5432	0.47	0/7382

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2655	0	2612	26	0
1	B	2625	0	2565	27	0
2	A	23	0	12	1	0
2	B	23	0	12	1	0
3	A	6	0	8	2	0
4	A	332	0	0	6	0
4	B	296	0	0	2	0
All	All	5960	0	5209	53	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.



All (53) 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:5:LYS:HA	1:B:333:ILE:HG13	1.57	0.84
1:A:87:MET:O	1:B:246:ARG:HD3	1.82	0.80
1:B:166:ASN:OD1	1:B:326:HIS:CE1	2.41	0.73
1:B:194:TRP:HB3	1:B:296:LEU:HD11	1.74	0.69
1:A:34:LYS:HG3	1:A:44:ILE:HD13	1.85	0.58
1:B:176:GLU:HG2	1:B:178:ILE:HG12	1.84	0.58
1:A:169:GLN:NE2	1:A:193:ASN:HA	2.20	0.57
1:B:143:GLU:HG3	4:B:348:HOH:O	2.05	0.56
1:A:1:MET:HB2	1:A:2:PRO:HD2	1.89	0.54
1:B:5:LYS:HA	1:B:333:ILE:CG1	2.34	0.54
1:A:34:LYS:CG	1:A:44:ILE:HD13	2.38	0.53
1:B:333:ILE:O	1:B:333:ILE:HD12	2.09	0.53
1:B:177:PHE:CE1	2:B:801:AMP:C2	2.96	0.53
1:B:314:VAL:HB	1:B:329:GLU:HG2	1.88	0.53
1:A:105:PRO:HB3	1:A:127:ILE:HD13	1.89	0.52
1:A:225[A]:CYS:HA	3:A:501:GOL:H32	1.91	0.52
1:B:153:PHE:CE1	1:B:157:LEU:HD12	2.45	0.52
1:A:225[B]:CYS:HA	3:A:501:GOL:H32	1.92	0.52
2:A:801:AMP:N1	4:A:505:HOH:O	2.34	0.51
1:A:169:GLN:NE2	4:A:590:HOH:O	2.43	0.51
1:B:165:TYR:CE2	1:B:167:ILE:CD1	2.94	0.51
1:A:284:LEU:HD23	1:A:295:LEU:HD11	1.94	0.49
1:A:22:VAL:HB	1:A:84:ILE:HG21	1.96	0.48
1:B:77:VAL:O	1:B:106:LYS:HE3	2.13	0.48
1:B:208:GLY:HA3	1:B:233:PHE:O	2.13	0.47
1:B:323:LYS:HB3	1:B:323:LYS:HZ2	1.79	0.47
1:A:208:GLY:HA3	1:A:233:PHE:O	2.15	0.47
1:A:292:ARG:NH1	4:A:570:HOH:O	2.48	0.47
1:B:148:ASP:OD1	4:B:383:HOH:O	2.20	0.47
1:B:177:PHE:O	1:B:178:ILE:HG23	2.15	0.47
1:A:77:VAL:O	1:A:106:LYS:HE3	2.15	0.46
1:A:151:LYS:NZ	4:A:407:HOH:O	2.43	0.46
1:B:169:GLN:OE1	1:B:193:ASN:HA	2.16	0.46
1:A:53:TYR:CZ	1:A:55:TYR:HA	2.50	0.46
1:A:109:ILE:HD11	1:A:133:PRO:HD2	1.98	0.46
1:A:278:ARG:HD3	4:A:586:HOH:O	2.15	0.45
1:A:232:LEU:HB2	1:A:260:VAL:HG11	1.98	0.45
1:B:319:ASP:O	1:B:323:LYS:N	2.50	0.45
1:A:317:LYS:HD3	4:A:665:HOH:O	2.17	0.44
1:B:199:ASN:HB3	1:B:321:THR:OG1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ARG:NH2	1:A:63:GLU:OE2	2.50	0.44
1:A:38:LEU:HD23	1:A:42:PHE:O	2.17	0.43
1:B:165:TYR:CE2	1:B:167:ILE:HD13	2.53	0.43
1:A:169:GLN:HE22	1:A:193:ASN:HA	1.80	0.43
1:B:166:ASN:OD1	1:B:326:HIS:NE2	2.52	0.43
1:A:19:SER:OG	1:A:86:GLY:HA3	2.19	0.42
1:B:111:TYR:HB2	1:B:131:TYR:CZ	2.54	0.42
1:B:195:ILE:O	1:B:296:LEU:HD12	2.20	0.42
1:B:333:ILE:HD12	1:B:333:ILE:C	2.39	0.42
1:B:22:VAL:HB	1:B:84:ILE:HG21	2.02	0.41
1:B:38:LEU:HD23	1:B:42:PHE:O	2.21	0.41
1:A:34:LYS:HG2	1:A:44:ILE:CD1	2.50	0.41
1:A:276:THR:O	1:A:277:ASN:HB2	2.22	0.40

There are no symmetry-related clashes.

## 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	336/336 (100%)	324 (96%)	12 (4%)	0	100	100
1	B	333/336 (99%)	324 (97%)	8 (2%)	1 (0%)	43	24
All	All	669/672 (100%)	648 (97%)	20 (3%)	1 (0%)	49	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	178	ILE

### 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	290/295 (98%)	289 (100%)	1 (0%)	93	89
1	B	284/295 (96%)	282 (99%)	2 (1%)	85	76
All	All	574/590 (97%)	571 (100%)	3 (0%)	90	84

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	B	163	LEU
1	B	193	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	104	ASN
1	B	326	HIS

### 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

3 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	501	-	5,5,5	0.30	0	5,5,5	0.60	0
2	AMP	A	801	-	22,25,25	0.98	1 (4%)	23,38,38	1.91	4 (17%)
2	AMP	B	801	-	22,25,25	0.99	1 (4%)	23,38,38	1.91	4 (17%)

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	501	-	-	0/4/4/4	0/0/0/0
2	AMP	A	801	-	-	0/6/26/26	0/3/3/3
2	AMP	B	801	-	-	0/6/26/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	AMP	C5-C4	3.07	1.47	1.40
2	A	801	AMP	C5-C4	3.09	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	AMP	N3-C2-N1	-7.29	122.62	128.86
2	B	801	AMP	N3-C2-N1	-7.09	122.80	128.86
2	B	801	AMP	C4-C5-N7	-2.96	106.55	109.41
2	B	801	AMP	O3P-P-O5'	-2.79	99.31	106.73
2	A	801	AMP	C4-C5-N7	-2.70	106.80	109.41
2	A	801	AMP	O3P-P-O5'	-2.61	99.78	106.73
2	B	801	AMP	C2-N1-C6	2.05	122.24	118.75
2	A	801	AMP	C2-N1-C6	2.29	122.65	118.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	GOL	2	0
2	A	801	AMP	1	0
2	B	801	AMP	1	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

### 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, 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	335/336 (99%)	0.26	21 (6%) 20 25	19, 32, 52, 73	0
1	B	333/336 (99%)	0.47	30 (9%) 9 11	18, 33, 59, 84	0
All	All	668/672 (99%)	0.36	51 (7%) 14 18	18, 32, 56, 84	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	7.3
1	B	177	PHE	5.8
1	B	333	ILE	4.3
1	B	111	TYR	3.7
1	B	109	ILE	3.6
1	A	333	ILE	3.6
1	A	109	ILE	3.5
1	A	135	LEU	3.4
1	B	178	ILE	3.4
1	A	134	ALA	3.3
1	A	308	ILE	3.2
1	A	-1	ASN	3.2
1	B	165	TYR	3.0
1	B	2	PRO	3.0
1	A	309	THR	2.9
1	B	131	TYR	2.8
1	B	234	ILE	2.7
1	B	309	THR	2.7
1	B	112	ALA	2.7
1	B	133	PRO	2.7
1	A	24	TYR	2.7
1	B	290	ASN	2.6
1	A	177	PHE	2.5
1	B	118	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	114	ALA	2.4
1	A	55	TYR	2.4
1	B	163	LEU	2.4
1	A	53	TYR	2.3
1	B	13	ILE	2.3
1	B	130	PHE	2.3
1	B	153	PHE	2.3
1	B	132	GLY	2.3
1	B	184	THR	2.2
1	B	119	LEU	2.2
1	B	214	ILE	2.2
1	A	82	SER	2.2
1	A	1	MET	2.1
1	A	0	ALA	2.1
1	A	307	MET	2.1
1	A	39	GLN	2.1
1	A	118	LEU	2.1
1	B	308	ILE	2.1
1	B	318	MET	2.1
1	B	233	PHE	2.1
1	A	103	ASN	2.1
1	B	134	ALA	2.1
1	A	160	ASP	2.1
1	A	185	LYS	2.0
1	B	80	ILE	2.0
1	B	114	ALA	2.0
1	B	208	GLY	2.0

## 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. The B-factors column lists the minimum,

median, 95<sup>th</sup> 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	AMP	A	801	23/23	0.69	0.23	46,63,72,74	23
2	AMP	B	801	23/23	0.75	0.22	40,69,74,77	23
3	GOL	A	501	6/6	0.82	0.38	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.