



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2019 – 11:32 AM EDT

PDB ID : 2VC0  
Title : Feast or famine regulatory protein (Rv3291c) from *M. tuberculosis* complexed with L-Leucine  
Authors : Shrivastava, T.; Ramachandran, R.  
Deposited on : 2007-09-18  
Resolution : 2.50 Å (reported)

This is a Full wwPDB X-ray Structure Validation 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.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.4
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)	:	2.4

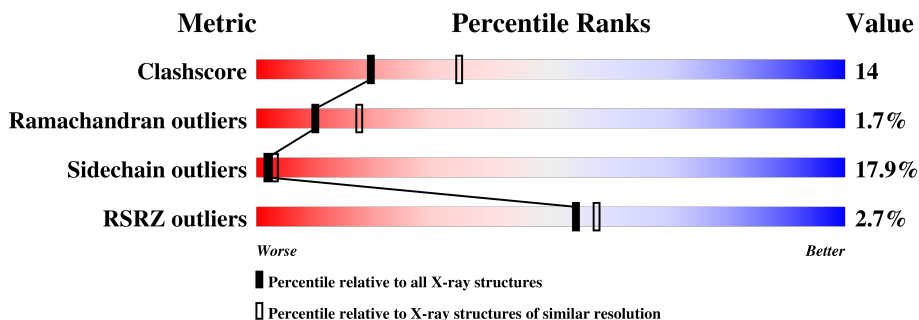
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

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	150	<div> <div>2%</div> <div>69%</div> <div>19%</div> <div>11%</div> <div>.</div> </div>
1	B	150	<div> <div>3%</div> <div>55%</div> <div>33%</div> <div>8%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

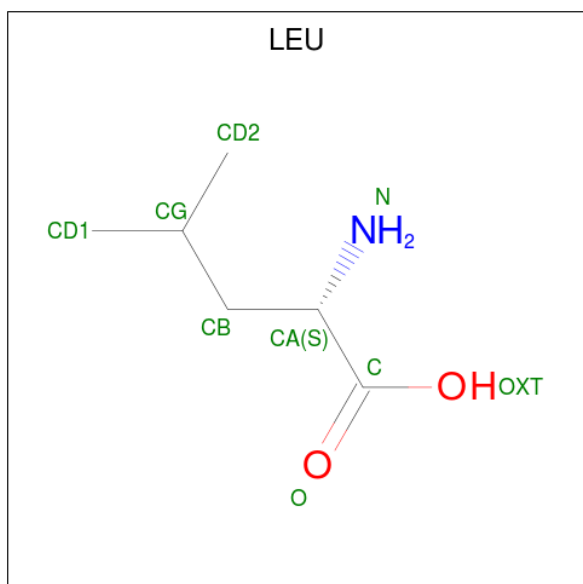
There are 3 unique types of molecules in this entry. The entry contains 2293 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRANSCRIPTIONAL REGULATORY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	0	0
			1127	697	209	220	1			
1	B	147	Total	C	N	O	S	0	0	0
			1111	689	203	218	1			

- Molecule 2 is LEUCINE (three-letter code: LEU) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total	O	0	0
			25	25		

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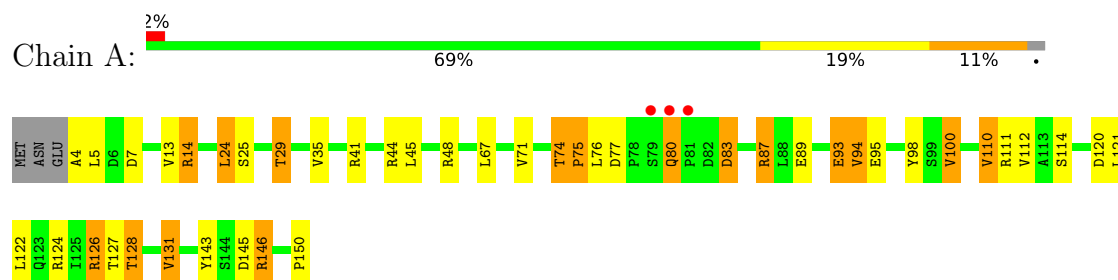
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	21	Total	O	0	0
			21	21		

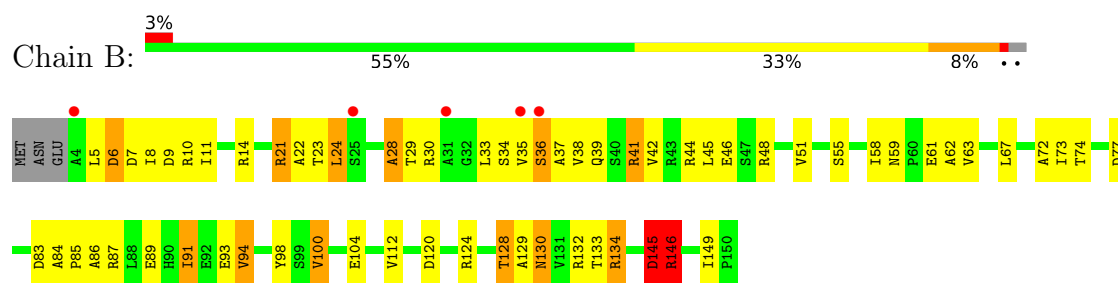
### 3 Residue-property plots [i](#)

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: TRANSCRIPTIONAL REGULATORY PROTEIN



#### • Molecule 1: TRANSCRIPTIONAL REGULATORY PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.88Å 100.88Å 99.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.25 – 2.50 24.47 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.0 (71.25-2.50) 95.1 (24.47-2.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.212 , 0.257 0.191 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.1	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 47.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -h,-l,-k 0.014 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2293	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.80% 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 ⓘ

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	1.36	6/1141 (0.5%)	1.35	18/1552 (1.2%)
1	B	1.26	5/1125 (0.4%)	1.26	7/1533 (0.5%)
All	All	1.31	11/2266 (0.5%)	1.31	25/3085 (0.8%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	ARG	CD-NE	-7.98	1.32	1.46
1	A	146	ARG	CB-CG	-6.21	1.35	1.52
1	B	98	TYR	CD1-CE1	6.13	1.48	1.39
1	B	134	ARG	CG-CD	6.04	1.67	1.51
1	A	98	TYR	CD1-CE1	5.80	1.48	1.39
1	A	143	TYR	CD2-CE2	5.48	1.47	1.39
1	B	55	SER	CA-CB	5.21	1.60	1.52
1	A	114	SER	CB-OG	5.19	1.49	1.42
1	B	86	ALA	CA-CB	5.08	1.63	1.52
1	A	41	ARG	CG-CD	-5.06	1.39	1.51
1	B	98	TYR	CE1-CZ	5.03	1.45	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	ARG	CB-CA-C	7.68	125.77	110.40
1	B	100	VAL	CG1-CB-CG2	7.33	122.63	110.90
1	B	146	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	B	130	ASN	CB-CA-C	7.22	124.83	110.40
1	A	110	VAL	CG1-CB-CG2	6.83	121.83	110.90
1	A	111	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	129	ALA	C-N-CA	-6.54	105.36	121.70
1	A	48	ARG	C-N-CA	-6.53	108.58	122.30
1	A	100	VAL	CG1-CB-CG2	6.29	120.97	110.90
1	A	111	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	B	77	ASP	CB-CG-OD2	-6.13	112.78	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	A	131	VAL	CG1-CB-CG2	5.70	120.02	110.90
1	A	146	ARG	CB-CG-CD	-5.70	96.78	111.60
1	A	146	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	A	146	ARG	N-CA-CB	-5.62	100.49	110.60
1	A	146	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	B	146	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	131	VAL	N-CA-CB	-5.60	99.19	111.50
1	B	21	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	120	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	A	120	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	126	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	A	14	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	A	146	ARG	CA-CB-CG	5.00	124.41	113.40

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	1127	0	1130	24	0
1	B	1111	0	1104	48	0
2	A	9	0	10	0	0
3	A	25	0	0	3	0
3	B	21	0	0	1	0
All	All	2293	0	2244	62	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 14.

All (62) 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:145:ASP:HB3	3:A:2024:HOH:O	1.47	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ARG:HB3	1:B:44:ARG:HH11	1.16	1.04
1:B:72:ALA:HB1	1:B:104:GLU:HG3	1.51	0.91
1:B:104:GLU:HG2	1:B:134:ARG:NH2	1.85	0.89
1:B:44:ARG:HB3	1:B:44:ARG:NH1	1.89	0.87
1:A:124:ARG:O	1:A:128:THR:HG23	1.81	0.80
1:B:33:LEU:HD22	1:B:37:ALA:CB	2.14	0.78
1:B:91:ILE:HD12	1:B:93:GLU:OE1	1.87	0.75
1:B:6:ASP:O	1:B:9:ASP:HB2	1.90	0.71
1:A:146:ARG:NH2	1:B:89:GLU:O	2.24	0.70
1:B:63:VAL:HG12	1:B:63:VAL:O	1.95	0.67
1:A:94:VAL:O	1:B:146:ARG:NH1	2.29	0.66
1:B:124:ARG:O	1:B:128:THR:HG23	1.95	0.65
1:B:42:VAL:O	1:B:46:GLU:HG3	1.98	0.63
1:B:8:ILE:HG21	1:B:41:ARG:HH21	1.63	0.63
1:B:104:GLU:HG2	1:B:134:ARG:HH21	1.62	0.62
1:B:91:ILE:HD11	1:B:93:GLU:HG2	1.82	0.62
1:B:91:ILE:CD1	1:B:93:GLU:OE1	2.49	0.61
1:A:24:LEU:HB3	1:A:35:VAL:HG13	1.83	0.60
1:B:72:ALA:CB	1:B:104:GLU:HG3	2.31	0.60
1:B:44:ARG:CB	1:B:44:ARG:HH11	2.04	0.59
1:A:146:ARG:NH1	1:B:94:VAL:O	2.35	0.59
1:B:124:ARG:O	1:B:128:THR:CG2	2.50	0.59
1:B:28:ALA:HA	1:B:38:VAL:HG21	1.85	0.59
1:A:4:ALA:N	3:A:2001:HOH:O	2.36	0.57
1:B:104:GLU:CG	1:B:134:ARG:NH2	2.65	0.57
1:B:33:LEU:HD22	1:B:37:ALA:HB3	1.85	0.56
1:B:6:ASP:OD2	1:B:41:ARG:NH1	2.39	0.56
1:B:33:LEU:HD22	1:B:37:ALA:HB1	1.86	0.56
1:B:7:ASP:HA	1:B:10:ARG:HG3	1.87	0.56
1:B:45:LEU:O	1:B:48:ARG:O	2.23	0.55
1:B:59:ASN:HD22	1:B:62:ALA:HB2	1.70	0.55
1:A:89:GLU:O	1:B:146:ARG:NH2	2.40	0.55
1:A:83:ASP:OD2	1:A:83:ASP:N	2.37	0.53
1:A:13:VAL:HB	1:B:58:ILE:HD12	1.91	0.53
1:A:25:SER:O	1:A:29:THR:HG23	2.08	0.53
1:B:34:SER:C	1:B:36:SER:H	2.12	0.52
1:A:80:GLN:HE21	1:A:80:GLN:CA	2.22	0.52
1:A:93:GLU:HG2	1:A:121:LEU:HD13	1.92	0.51
1:B:74:THR:OG1	1:B:104:GLU:OE2	2.21	0.50
1:B:8:ILE:HG21	1:B:41:ARG:NH2	2.27	0.50
1:A:150:PRO:HD2	1:B:63:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:O	1:A:126:ARG:HG3	2.12	0.49
1:B:146:ARG:HH11	1:B:146:ARG:CG	2.26	0.48
1:B:28:ALA:CA	1:B:38:VAL:HG21	2.43	0.47
1:A:150:PRO:HD2	1:B:63:VAL:CG1	2.44	0.47
1:B:83:ASP:N	1:B:83:ASP:OD2	2.38	0.46
1:A:14:ARG:HD2	3:A:2003:HOH:O	2.16	0.46
1:B:124:ARG:HD3	3:B:2013:HOH:O	2.17	0.45
1:A:95:GLU:CG	1:B:145:ASP:HA	2.48	0.44
1:B:24:LEU:HG	1:B:39:GLN:HG3	2.00	0.44
1:A:95:GLU:HG3	1:B:145:ASP:HA	1.99	0.43
1:A:146:ARG:NH2	1:B:89:GLU:HG3	2.33	0.43
1:B:14:ARG:HA	1:B:149:ILE:HD13	1.99	0.43
1:A:74:THR:HA	1:A:75:PRO:HD3	1.93	0.42
1:A:124:ARG:O	1:A:128:THR:CG2	2.58	0.42
1:B:21:ARG:O	1:B:22:ALA:C	2.57	0.42
1:A:76:LEU:HD23	1:A:76:LEU:HA	1.72	0.42
1:A:83:ASP:O	1:A:87:ARG:HG3	2.20	0.42
1:B:34:SER:O	1:B:36:SER:N	2.53	0.41
1:B:84:ALA:N	1:B:85:PRO:CD	2.83	0.41
1:B:73:ILE:HG22	1:B:133:THR:HG22	2.04	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	145/150 (97%)	142 (98%)	3 (2%)	0	100	100
1	B	145/150 (97%)	124 (86%)	16 (11%)	5 (3%)	4	5
All	All	290/300 (97%)	266 (92%)	19 (7%)	5 (2%)	10	17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	28	ALA
1	B	145	ASP
1	B	30	ARG
1	B	35	VAL
1	B	29	THR

### 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	121/126 (96%)	100 (83%)	21 (17%)	2	3
1	B	118/126 (94%)	97 (82%)	21 (18%)	2	3
All	All	239/252 (95%)	197 (82%)	42 (18%)	2	3

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	7	ASP
1	A	24	LEU
1	A	29	THR
1	A	44	ARG
1	A	45	LEU
1	A	67	LEU
1	A	71	VAL
1	A	74	THR
1	A	75	PRO
1	A	80	GLN
1	A	83	ASP
1	A	87	ARG
1	A	93	GLU
1	A	94	VAL
1	A	100	VAL
1	A	110	VAL
1	A	112	VAL
1	A	127	THR

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Mol	Chain	Res	Type
1	A	128	THR
1	A	131	VAL
1	B	5	LEU
1	B	6	ASP
1	B	11	ILE
1	B	23	THR
1	B	24	LEU
1	B	36	SER
1	B	41	ARG
1	B	51	VAL
1	B	61	GLU
1	B	67	LEU
1	B	87	ARG
1	B	91	ILE
1	B	94	VAL
1	B	100	VAL
1	B	112	VAL
1	B	120	ASP
1	B	128	THR
1	B	130	ASN
1	B	132	ARG
1	B	145	ASP
1	B	146	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	80	GLN
1	B	59	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

1 ligand is modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	147/150 (98%)	-0.39	3 (2%) 65 67	19, 38, 64, 82	0
1	B	147/150 (98%)	-0.11	5 (3%) 45 48	19, 43, 92, 97	0
All	All	294/300 (98%)	-0.25	8 (2%) 54 58	19, 40, 91, 97	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	35	VAL	3.9
1	B	36	SER	3.7
1	A	80	GLN	3.0
1	B	4	ALA	3.0
1	A	81	PRO	2.8
1	A	79	SER	2.6
1	B	25	SER	2.2
1	B	31	ALA	2.1

### 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	LEU	A	1151	9/9	0.90	0.24	68,71,73,75	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.