



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:18 PM UTC

PDB ID : 2VBZ / pdb\_00002vbz  
Title : Feast or famine regulatory protein (Rv3291c) from *M. tuberculosis* complexed with L-Tryptophan  
Authors : Shrivastava, T.; Ramachandran, R.  
Deposited on : 2007-09-18  
Resolution : 2.80 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.

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

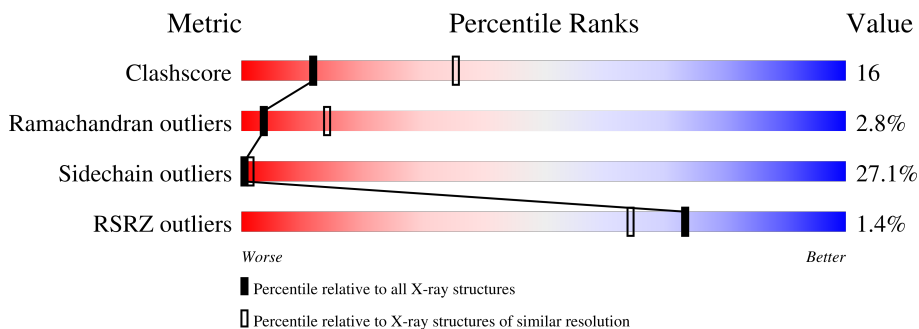
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	150	 16%
1	B	150	 2%

## 2 Entry composition [i](#)

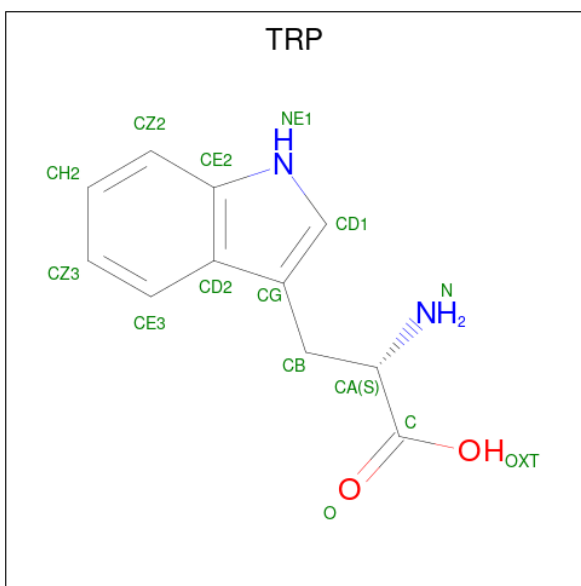
There are 3 unique types of molecules in this entry. The entry contains 2296 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	147	Total 1127	C 697	N 209	O 220	S 1	0	0	0
1	B	147	Total 1111	C 689	N 203	O 218	S 1	0	0	0

- Molecule 2 is TRYPTOPHAN (CCD ID: TRP) (formula:  $C_{11}H_{12}N_2O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 15	C 11	N 2	O 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	23	Total 23	O 23	0

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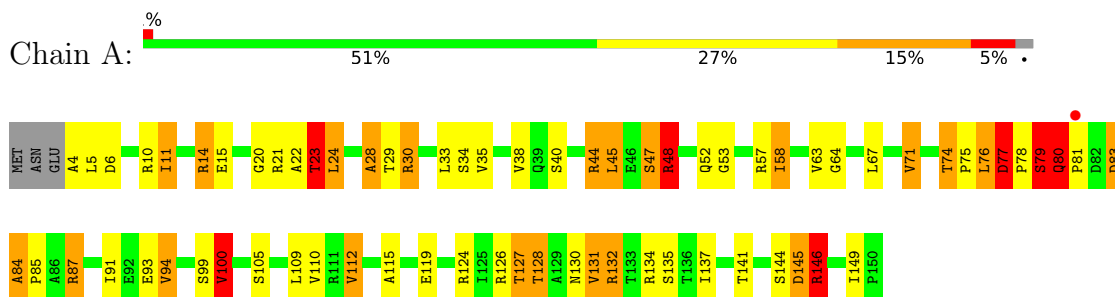
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	B	20	Total	O	0	0
			20	20		

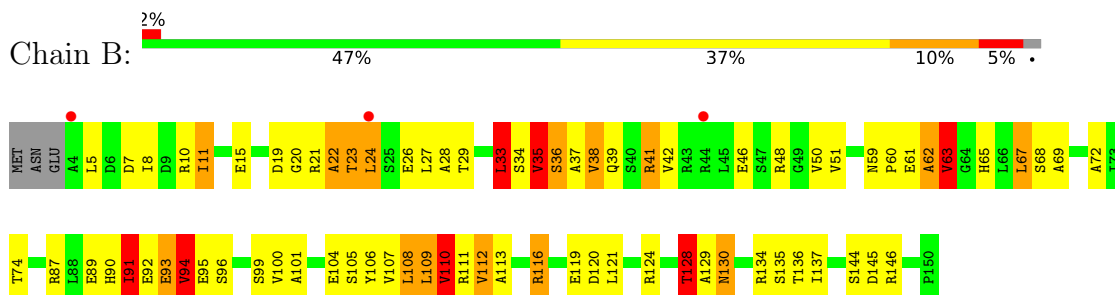
### 3 Residue-property plots [i](#)

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: TRANSCRIPTIONAL REGULATORY PROTEIN



- Molecule 1: TRANSCRIPTIONAL REGULATORY PROTEIN



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.97Å 100.97Å 99.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.43 – 2.80 71.40 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.9 (71.43-2.80) 96.9 (71.40-2.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.205 , 0.253 0.181 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.5	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 33.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for -h,-l,-k 0.011 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2296	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.67% 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	1.87	17/1141 (1.5%)	1.88	28/1552 (1.8%)
1	B	1.97	20/1125 (1.8%)	2.02	41/1533 (2.7%)
All	All	1.92	37/2266 (1.6%)	1.95	69/3085 (2.2%)

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	3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	ASP	N-CA	-14.69	1.25	1.46
1	B	107	VAL	CA-C	9.74	1.64	1.52
1	A	115	ALA	CA-CB	-8.38	1.40	1.53
1	B	112	VAL	C-O	8.19	1.33	1.24
1	B	109	LEU	C-O	7.58	1.32	1.23
1	A	141	THR	CA-CB	-7.37	1.43	1.53
1	B	91	ILE	CA-C	7.32	1.60	1.52
1	B	91	ILE	CA-CB	7.32	1.62	1.53
1	B	101	ALA	CA-CB	-7.26	1.42	1.53
1	B	113	ALA	CA-CB	6.88	1.64	1.53
1	A	74	THR	CA-C	6.86	1.60	1.53
1	B	94	VAL	C-O	-6.64	1.14	1.23
1	B	105	SER	C-N	6.59	1.42	1.33
1	B	29	THR	CA-CB	6.22	1.64	1.53
1	A	135	SER	CA-C	-6.09	1.45	1.52
1	B	94	VAL	CA-C	-5.84	1.47	1.53
1	B	144	SER	N-CA	-5.56	1.39	1.46
1	A	63	VAL	CA-CB	5.48	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	ARG	CA-C	5.45	1.59	1.52
1	B	11	ILE	CA-CB	5.42	1.61	1.54
1	B	107	VAL	C-N	5.39	1.41	1.33
1	A	78	PRO	N-CA	5.37	1.53	1.47
1	A	53	GLY	N-CA	5.36	1.50	1.45
1	A	132	ARG	CB-CG	-5.23	1.36	1.52
1	A	126	ARG	N-CA	5.22	1.52	1.46
1	B	129	ALA	CA-CB	-5.21	1.44	1.53
1	B	106	TYR	C-N	-5.20	1.26	1.33
1	B	72	ALA	CA-CB	-5.20	1.46	1.53
1	A	146	ARG	C-O	-5.20	1.17	1.23
1	A	6	ASP	N-CA	5.18	1.52	1.45
1	B	35	VAL	CA-CB	5.15	1.61	1.54
1	B	107	VAL	C-O	5.15	1.29	1.24
1	A	80	GLN	N-CA	5.10	1.53	1.45
1	A	84	ALA	C-O	-5.09	1.19	1.24
1	A	146	ARG	N-CA	-5.08	1.40	1.46
1	B	69	ALA	CA-CB	-5.05	1.45	1.53
1	A	134	ARG	N-CA	5.04	1.52	1.46

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	TYR	CA-C-O	-12.22	107.14	121.44
1	B	129	ALA	CA-C-N	-12.13	104.69	123.12
1	B	129	ALA	C-N-CA	-12.13	104.69	123.12
1	B	107	VAL	CA-C-O	-10.33	108.94	120.72
1	B	130	ASN	CB-CA-C	10.04	127.30	111.73
1	B	91	ILE	CB-CA-C	9.72	124.36	111.33
1	B	108	LEU	CA-C-O	-8.99	110.82	120.80
1	A	30	ARG	N-CA-C	8.68	120.82	111.36
1	A	74	THR	CA-C-N	8.37	130.31	119.84
1	A	74	THR	C-N-CA	8.37	130.31	119.84
1	B	106	TYR	O-C-N	8.33	133.98	123.15
1	B	105	SER	CA-C-O	-8.32	109.85	120.00
1	A	58	ILE	N-CA-C	8.28	120.26	109.58
1	A	131	VAL	N-CA-CB	-7.99	100.40	111.19
1	B	109	LEU	N-CA-C	-7.93	96.75	109.76
1	A	79	SER	N-CA-C	7.91	119.69	111.14
1	B	145	ASP	N-CA-C	7.59	121.89	112.47
1	A	48	ARG	N-CA-C	-7.47	100.69	110.33
1	B	108	LEU	N-CA-CB	-7.37	98.36	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	THR	N-CA-C	7.34	120.36	111.40
1	B	99	SER	N-CA-CB	7.18	121.95	110.46
1	B	94	VAL	N-CA-CB	6.75	119.19	111.90
1	B	135	SER	N-CA-C	6.73	120.48	109.72
1	A	71	VAL	CB-CA-C	6.61	120.16	110.77
1	A	146	ARG	NE-CZ-NH1	6.50	128.00	121.50
1	B	33	LEU	N-CA-C	6.40	117.95	108.60
1	A	23	THR	N-CA-C	6.26	120.12	110.42
1	B	91	ILE	CA-CB-CG2	6.25	121.13	110.50
1	B	137	ILE	CB-CA-C	6.22	119.73	111.21
1	B	99	SER	CB-CA-C	-6.19	98.99	109.83
1	B	63	VAL	N-CA-CB	-6.16	104.16	112.16
1	B	48	ARG	N-CA-C	-6.12	101.49	110.42
1	B	15	GLU	N-CA-C	6.08	117.91	111.28
1	A	20	GLY	N-CA-C	-6.04	105.11	115.61
1	A	126	ARG	N-CA-C	-6.03	104.62	111.07
1	B	95	GLU	N-CA-C	6.01	118.79	111.82
1	B	112	VAL	CB-CA-C	5.98	121.10	111.29
1	A	28	ALA	CA-C-N	-5.88	111.36	120.31
1	A	28	ALA	C-N-CA	-5.88	111.36	120.31
1	B	110	VAL	N-CA-CB	-5.79	101.09	111.92
1	A	112	VAL	N-CA-CB	-5.74	103.81	112.35
1	A	64	GLY	N-CA-C	5.71	122.34	114.92
1	A	137	ILE	CA-C-O	-5.70	114.55	121.04
1	B	74	THR	CB-CA-C	-5.69	101.49	110.02
1	A	146	ARG	CB-CA-C	5.69	120.93	111.83
1	B	107	VAL	O-C-N	5.68	128.93	123.14
1	A	77	ASP	CA-C-N	5.59	126.53	120.83
1	A	77	ASP	C-N-CA	5.59	126.53	120.83
1	A	83	ASP	N-CA-CB	-5.57	101.15	110.39
1	A	11	ILE	N-CA-C	5.55	115.75	110.42
1	A	127	THR	N-CA-CB	5.51	118.42	110.20
1	A	100	VAL	CB-CA-C	5.47	121.03	111.18
1	B	129	ALA	O-C-N	-5.45	116.31	122.68
1	A	74	THR	CB-CA-C	5.36	117.28	110.16
1	B	144	SER	N-CA-CB	-5.35	101.52	110.99
1	B	137	ILE	CA-CB-CG1	-5.35	101.31	110.40
1	B	109	LEU	CB-CG-CD2	-5.35	94.66	110.70
1	B	107	VAL	N-CA-CB	-5.27	101.46	111.21
1	B	50	VAL	N-CA-C	5.26	115.53	110.74
1	B	107	VAL	CA-CB-CG2	-5.16	101.62	110.40
1	A	100	VAL	N-CA-CB	-5.16	101.83	111.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	ALA	N-CA-C	-5.12	103.17	110.59
1	B	145	ASP	CB-CA-C	-5.07	103.42	111.48
1	A	127	THR	CA-CB-CG2	5.05	119.08	110.50
1	A	131	VAL	N-CA-C	-5.04	101.61	108.06
1	B	38	VAL	N-CA-C	-5.04	105.41	110.30
1	B	19	ASP	N-CA-C	5.02	115.61	107.23
1	B	134	ARG	CA-C-N	-5.02	114.93	122.81
1	B	134	ARG	C-N-CA	-5.02	114.93	122.81

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	ASN	Peptide
1	A	47	SER	Peptide
1	A	76	LEU	Peptide

## 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	1127	0	1130	34	0
1	B	1111	0	1104	41	0
2	A	15	0	9	1	0
3	A	23	0	0	3	0
3	B	20	0	0	2	0
All	All	2296	0	2243	71	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 16.

All (71) 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:80:GLN:H	1:A:80:GLN:CD	1.80	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ARG:HD3	3:A:2016:HOH:O	1.75	0.86
1:B:42:VAL:O	1:B:46:GLU:HG3	1.83	0.78
1:A:57:ARG:CB	3:A:2004:HOH:O	2.34	0.75
1:B:8:ILE:CG2	1:B:41:ARG:HH21	2.02	0.73
1:A:80:GLN:CD	1:A:80:GLN:N	2.45	0.73
1:B:8:ILE:HG22	1:B:41:ARG:HH21	1.55	0.71
1:A:83:ASP:HB3	1:A:87:ARG:HD2	1.73	0.69
1:A:146:ARG:NH2	1:B:89:GLU:O	2.22	0.68
1:A:124:ARG:O	1:A:128:THR:HG23	1.94	0.68
1:B:124:ARG:O	1:B:128:THR:HG23	1.94	0.66
1:A:21:ARG:NH1	1:B:20:GLY:O	2.28	0.66
1:A:83:ASP:HB3	1:A:87:ARG:CD	2.27	0.65
1:A:124:ARG:O	1:A:128:THR:CG2	2.46	0.64
1:B:116:ARG:HH11	1:B:116:ARG:CB	2.11	0.64
1:B:68:SER:OG	1:B:111:ARG:HG2	2.00	0.61
1:B:116:ARG:HH11	1:B:116:ARG:CG	2.14	0.61
1:A:15:GLU:OE1	1:A:30:ARG:NH1	2.35	0.59
1:A:77:ASP:C	1:A:77:ASP:OD1	2.43	0.58
1:B:21:ARG:O	1:B:22:ALA:C	2.47	0.57
1:A:14:ARG:HA	1:A:149:ILE:HD13	1.87	0.56
1:B:33:LEU:CD2	1:B:37:ALA:HB3	2.36	0.56
1:B:109:LEU:HD12	1:B:110:VAL:N	2.21	0.55
1:B:91:ILE:HD11	1:B:93:GLU:HG2	1.90	0.54
1:B:7:ASP:HA	1:B:10:ARG:HB3	1.89	0.54
1:B:59:ASN:HD22	1:B:62:ALA:HB2	1.73	0.54
1:B:109:LEU:HD12	1:B:110:VAL:H	1.72	0.54
1:B:33:LEU:HD23	1:B:34:SER:H	1.71	0.54
1:A:100:VAL:HG22	1:B:136:THR:HG22	1.90	0.52
1:B:91:ILE:C	1:B:91:ILE:HD12	2.35	0.52
1:B:116:ARG:HH11	1:B:116:ARG:HG2	1.75	0.52
1:A:24:LEU:HB3	1:A:35:VAL:HG13	1.92	0.52
1:B:37:ALA:O	1:B:41:ARG:HG2	2.09	0.51
1:A:83:ASP:O	1:A:87:ARG:HG3	2.11	0.51
1:B:124:ARG:HD3	3:B:2015:HOH:O	2.10	0.51
1:A:105:SER:HB3	2:A:1151:TRP:CE2	2.46	0.50
1:B:59:ASN:ND2	1:B:62:ALA:HB2	2.26	0.50
1:A:84:ALA:HB3	1:A:85:PRO:HD3	1.94	0.49
1:B:116:ARG:HG2	1:B:116:ARG:NH1	2.27	0.48
1:B:96:SER:O	1:B:108:LEU:HA	2.14	0.48
1:A:77:ASP:O	1:A:77:ASP:CG	2.51	0.48
1:B:41:ARG:HG2	1:B:41:ARG:H	1.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LEU:HD22	1:B:37:ALA:HB3	1.97	0.47
1:B:116:ARG:CG	1:B:116:ARG:NH1	2.76	0.46
1:B:34:SER:C	1:B:36:SER:H	2.22	0.46
1:A:4:ALA:HA	3:A:2001:HOH:O	2.16	0.46
1:B:33:LEU:HD21	1:B:37:ALA:HB3	1.97	0.45
1:B:63:VAL:HG13	1:B:63:VAL:O	2.17	0.45
1:B:93:GLU:CD	1:B:93:GLU:H	2.26	0.43
1:B:23:THR:O	1:B:24:LEU:C	2.61	0.43
1:A:45:LEU:HD12	1:A:45:LEU:HA	1.59	0.43
1:B:91:ILE:CD1	1:B:93:GLU:HG2	2.48	0.43
1:A:76:LEU:HD23	1:A:76:LEU:HA	1.80	0.42
1:B:91:ILE:HD11	1:B:121:LEU:HD11	2.01	0.42
1:A:11:ILE:O	1:A:15:GLU:HG2	2.19	0.42
1:A:94:VAL:O	1:A:94:VAL:HG22	2.18	0.42
1:B:60:PRO:O	1:B:65:HIS:HB2	2.18	0.42
1:A:23:THR:O	1:A:24:LEU:C	2.61	0.41
1:A:124:ARG:O	1:A:128:THR:HG22	2.18	0.41
1:A:47:SER:C	1:A:48:ARG:O	2.60	0.41
1:A:99:SER:HA	1:A:105:SER:O	2.21	0.41
1:A:14:ARG:NH2	1:A:149:ILE:O	2.53	0.41
1:A:28:ALA:HB1	1:A:33:LEU:O	2.20	0.41
1:A:144:SER:O	1:A:145:ASP:C	2.64	0.41
1:A:146:ARG:NH1	1:B:94:VAL:O	2.54	0.41
1:A:83:ASP:CB	1:A:87:ARG:HD2	2.44	0.41
1:B:90:HIS:HE1	3:B:2014:HOH:O	2.04	0.41
1:B:8:ILE:HD13	1:B:8:ILE:HA	1.98	0.40
1:A:77:ASP:OD1	1:A:79:SER:OG	2.38	0.40
1:B:37:ALA:O	1:B:41:ARG:CG	2.70	0.40
1:B:67:LEU:HD23	1:B:67:LEU:HA	1.94	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%)	134 (92%)	9 (6%)	2 (1%)	9	30
1	B	145/150 (97%)	123 (85%)	16 (11%)	6 (4%)	2	8
All	All	290/300 (97%)	257 (89%)	25 (9%)	8 (3%)	4	14

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	28	ALA
1	A	22	ALA
1	B	22	ALA
1	B	27	LEU
1	B	62	ALA
1	B	26	GLU
1	B	35	VAL
1	A	81	PRO

### 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	121/126 (96%)	85 (70%)	36 (30%)	0	1
1	B	118/126 (94%)	89 (75%)	29 (25%)	1	2
All	All	239/252 (95%)	174 (73%)	65 (27%)	0	1

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	10	ARG
1	A	14	ARG
1	A	23	THR
1	A	24	LEU
1	A	29	THR
1	A	34	SER
1	A	38	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	40	SER
1	A	44	ARG
1	A	45	LEU
1	A	48	ARG
1	A	52	GLN
1	A	58	ILE
1	A	67	LEU
1	A	71	VAL
1	A	74	THR
1	A	75	PRO
1	A	77	ASP
1	A	79	SER
1	A	80	GLN
1	A	87	ARG
1	A	91	ILE
1	A	93	GLU
1	A	94	VAL
1	A	100	VAL
1	A	109	LEU
1	A	110	VAL
1	A	112	VAL
1	A	119	GLU
1	A	127	THR
1	A	128	THR
1	A	131	VAL
1	A	132	ARG
1	A	145	ASP
1	A	146	ARG
1	B	5	LEU
1	B	11	ILE
1	B	23	THR
1	B	24	LEU
1	B	33	LEU
1	B	35	VAL
1	B	36	SER
1	B	38	VAL
1	B	39	GLN
1	B	41	ARG
1	B	51	VAL
1	B	61	GLU
1	B	63	VAL
1	B	67	LEU

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Mol	Chain	Res	Type
1	B	87	ARG
1	B	91	ILE
1	B	92	GLU
1	B	93	GLU
1	B	94	VAL
1	B	100	VAL
1	B	104	GLU
1	B	110	VAL
1	B	112	VAL
1	B	116	ARG
1	B	119	GLU
1	B	120	ASP
1	B	128	THR
1	B	130	ASN
1	B	146	ARG

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

Mol	Chain	Res	Type
1	A	90	HIS
1	B	147	GLN
1	B	148	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

1 ligand is 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
2	TRP	A	1151	-	15,16,16	2.25	5 (33%)	18,22,22	1.11	2 (11%)

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
2	TRP	A	1151	-	-	2/8/8/8	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1151	TRP	CZ3-CE3	5.84	1.48	1.38
2	A	1151	TRP	CZ2-CE2	3.72	1.45	1.39
2	A	1151	TRP	CE3-CD2	2.77	1.44	1.39
2	A	1151	TRP	CH2-CZ3	2.33	1.43	1.38
2	A	1151	TRP	OXT-C	-2.10	1.24	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1151	TRP	OXT-C-O	-3.13	116.97	124.08
2	A	1151	TRP	CA-CB-CG	2.75	118.71	113.49

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1151	TRP	CA-CB-CG-CD2
2	A	1151	TRP	CA-CB-CG-CD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1151	TRP	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 [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%)	-0.59	1 (0%) 84 77	21, 40, 68, 87	0
1	B	147/150 (98%)	-0.24	3 (2%) 65 56	18, 44, 95, 98	0
All	All	294/300 (98%)	-0.42	4 (1%) 73 64	18, 42, 91, 98	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	ALA	4.2
1	B	44	ARG	3.3
1	B	24	LEU	2.7
1	A	81	PRO	2.4

### 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](#)

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(Å <sup>2</sup> )	Q<0.9
2	TRP	A	1151	15/15	0.92	0.12	47,60,69,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.