

Full wwPDB X-ray Structure Validation Report (i)

Sep 13, 2020 - 10:37 AM BST

PDB ID	:	2VBW
Title	:	Feast or famine regulatory protein (Rv3291c)from M. tuberculosis complexed
		with L-Phenylalanine
Authors	:	Shrivastava, T.; Ramachandran, R.
Deposited on	:	2007-09-18
$\operatorname{Resolution}$:	2.20 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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	$2.14.4.\mathrm{dev1}$

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	Percent	tile Ranks V	/alue
Clashscore 📕			14
Wa	orse	Better	
P	ercentile relative to all X-ray stru	uctures	
0 P	ercentile relative to X-ray structu	ures of similar resolution	
Motrio	Whole archive	Similar resolut	tion

Metric	Whole archive	Similar resolution
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
Clashscore	141614	5594(2.20-2.20)

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 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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain		
1	А	150	75%	21%	•••
1	В	150	77%	20%	•••



$2 \mathrm{VBW}$

2 Entry composition (i)

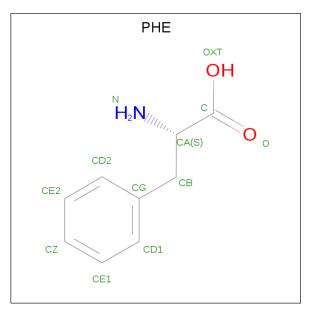
There are 3 unique types of molecules in this entry. The entry contains 2356 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	Δ	147	Total	С	Ν	Ο	S	0	0	0
	147	1128	697	209	221	1	0	0	0	
1	р	147	Total	С	Ν	Ο	S	0	0	0
	D	141	1111	689	203	218	1		0	0

• Molecule 2 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total C N O 12 9 1 2	0	0

• Molecule 3 is water.

Mol	Chain	ain Residues Atoms		ZeroOcc	AltConf
3	А	54	$\begin{array}{cc} \text{Total} & \text{O} \\ 54 & 54 \end{array}$	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	51	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 51 & 51 \end{array}$	0	0



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. 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. 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.

Note EDS failed to run properly.

• Molecule 1: TRANSCRIPTIONAL REGULATORY PROTEIN



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants	100.95\AA 100.95\AA 99.31\AA	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.43 - 2.20	Depositor
% Data completeness	99.9 (71.43-2.20)	Depositor
(in resolution range)		-
R _{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.06 ({ m at}2.20{ m \AA})$	Xtriage
Refinement program	REFMAC $5.2.0005$	Depositor
R, R_{free}	0.211 , 0.254	Depositor
Wilson B-factor $(Å^2)$	35.5	Xtriage
Anisotropy	0.081	Xtriage
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-l,-k	Xtriage
Estimated twinning fraction	0.010 for l,-k,h	Aurage
Total number of atoms	2356	wwPDB-VP
Average B, all atoms $(Å^2)$	40.0	wwPDB-VP

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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	Bo	nd lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	1.05	3/1142~(0.3%)	1.07	8/1553~(0.5%)	
1	В	0.96	3/1125~(0.3%)	1.01	4/1533~(0.3%)	
All	All	1.00	6/2267~(0.3%)	1.04	12/3086~(0.4%)	

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	А	126	ARG	C-N	9.00	1.54	1.34
1	В	55	SER	CA-CB	8.39	1.65	1.52
1	А	125	ILE	C-N	6.18	1.48	1.34
1	А	119	GLU	CB-CG	-6.09	1.40	1.52
1	В	104	GLU	CG-CD	5.74	1.60	1.51
1	В	97	CYS	CB-SG	-5.53	1.72	1.81

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	100	VAL	CG1-CB-CG2	7.38	122.71	110.90
1	В	100	VAL	CG1-CB-CG2	7.28	122.54	110.90
1	А	146	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	А	125	ILE	O-C-N	-6.40	112.46	122.70
1	А	131	VAL	CG1-CB-CG2	6.09	120.64	110.90
1	А	146	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	А	110	VAL	CG1-CB-CG2	5.70	120.02	110.90
1	В	137	ILE	CG1-CB-CG2	-5.65	98.97	111.40
1	В	146	ARG	CG-CD-NE	5.59	123.54	111.80
1	В	110	VAL	CG1-CB-CG2	5.20	119.23	110.90
1	А	126	ARG	C-N-CA	-5.12	108.91	121.70
1	А	10	ARG	NE-CZ-NH1	5.02	122.81	120.30

All (12) bond angle outliers are listed below:

There are no chirality outliers.

There are no planarity outliers.



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	А	1128	0	1133	29	0
1	В	1111	0	1104	38	0
2	А	12	0	8	0	0
3	А	54	0	0	5	0
3	В	51	0	0	7	0
All	All	2356	0	2245	65	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 (65) 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:124:ARG:O	1:B:128:THR:HG23	1.49	1.10
1:B:14:ARG:HG3	1:B:14:ARG:HH11	1.45	1.10
1:B:146:ARG:HH11	1:B:146:ARG:HB2	1.18	1.06
1:A:44:ARG:HB3	1:A:44:ARG:HH21	0.89	1.04
1:A:44:ARG:HB3	1:A:44:ARG:NH2	1.74	1.02
1:A:44:ARG:CB	1:A:44:ARG:HH21	1.76	0.98
1:B:65:HIS:HD2	3:B:2009:HOH:O	1.47	0.96
1:B:146:ARG:HH11	1:B:146:ARG:CB	1.86	0.88
1:B:24:LEU:H	1:B:24:LEU:HD12	1.40	0.87
1:A:124:ARG:O	1:A:128:THR:HG23	1.82	0.79
1:B:14:ARG:HG3	1:B:14:ARG:NH1	1.79	0.79
1:B:8:ILE:HB	1:B:41:ARG:NH2	1.99	0.77
1:B:65:HIS:CD2	3:B:2009:HOH:O	2.28	0.76
1:B:146:ARG:HB2	1:B:146:ARG:NH1	2.00	0.75
1:B:61:GLU:HG2	3:B:2007:HOH:O	1.86	0.74
1:B:124:ARG:O	1:B:128:THR:CG2	2.32	0.74
1:B:48:ARG:CB	3:B:2006:HOH:O	2.36	0.73
1:A:65:HIS:HD2	3:B:2051:HOH:O	1.71	0.72
1:B:48:ARG:O	1:B:50:VAL:N	2.25	0.68
1:A:94:VAL:O	1:B:146:ARG:NH1	2.28	0.67
1:A:145:ASP:HB3	3:A:2050:HOH:O	1.96	0.65
1:B:126:ARG:HG2	1:B:131:VAL:O	1.99	0.62

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Continued from prev		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å) 0.62	
1:A:65:HIS:CD2	3:B:2051:HOH:O	2.50		
1:B:73:ILE:HG22	1:B:133:THR:HG22	1.84	0.60	
1:B:14:ARG:HA	1:B:149:ILE:HD13	1.84	0.58	
1:B:8:ILE:HB	1:B:41:ARG:HH22	1.69	0.58	
1:A:116:ARG:HG2	3:A:2030:HOH:O	2.03	0.57	
1:A:123:GLN:O	1:A:127:THR:HG23	2.04	0.57	
1:B:24:LEU:H	1:B:24:LEU:CD1	2.15	0.57	
1:B:10:ARG:O	1:B:14:ARG:HB2	2.04	0.57	
1:A:25:SER:O	1:A:29:THR:HG22	2.06	0.55	
1:A:9:ASP:OD1	1:A:44:ARG:NH1	2.38	0.55	
1:B:6:ASP:O	1:B:8:ILE:N	2.40	0.54	
1:A:57:ARG:CB	3:A:2009:HOH:O	2.56	0.53	
1:A:41:ARG:O	1:A:44:ARG:NH2	2.41	0.52	
1:B:146:ARG:HH11	1:B:146:ARG:CG	2.22	0.52	
1:B:72:ALA:HB1	1:B:104:GLU:HG3	1.92	0.51	
1:A:146:ARG:HG2	1:A:146:ARG:O	2.09	0.51	
1:B:59:ASN:HD22	1:B:59:ASN:C	2.15	0.51	
1:A:80:GLN:CG	1:A:81:PRO:HD2	2.41	0.50	
1:A:24:LEU:HB3	1:A:35:VAL:HG13	1.94	0.50	
1:A:116:ARG:NH1	1:A:119:GLU:OE2	2.45	0.49	
1:B:44:ARG:HB3	1:B:44:ARG:NH1	2.29	0.48	
1:B:126:ARG:HG3	1:B:126:ARG:NH1	2.30	0.47	
1:A:74:THR:HG23	3:A:2011:HOH:O	2.14	0.47	
1:B:124:ARG:HD3	3:B:2041:HOH:O	2.14	0.46	
1:A:80:GLN:CD	1:A:81:PRO:HD2	2.35	0.46	
1:A:74:THR:CG2	3:A:2011:HOH:O	2.64	0.46	
1:A:80:GLN:HG3	1:A:81:PRO:HD2	1.97	0.46	
1:B:6:ASP:O	1:B:9:ASP:N	2.46	0.46	
1:B:44:ARG:HB3	1:B:44:ARG:HH11	1.83	0.44	
1:B:45:LEU:O	1:B:48:ARG:O	2.35	0.44	
1:B:126:ARG:HG3	1:B:126:ARG:HH11	1.83	0.44	
1:A:9:ASP:OD2	1:A:44:ARG:NH1	2.52	0.43	
1:A:150:PRO:HD2	1:B:63:VAL:HG13	2.00	0.43	
1:B:14:ARG:CG	1:B:14:ARG:NH1	2.62	0.43	
1:B:14:ARG:HG2	1:B:149:ILE:HD13	2.01	0.42	
1:A:25:SER:O	1:A:29:THR:CG2	2.68	0.42	
1:A:74:THR:HG22	1:A:104:GLU:HG2	2.01	0.41	
1:A:28:ALA:HA	1:A:38:VAL:HG21	2.02	0.41	
1:B:9:ASP:OD2	1:B:44:ARG:NH2	2.47	0.41	
1:A:28:ALA:HB1	1:A:33:LEU:O	2.20	0.40	
1:A:93:GLU:HG2	1:A:121:LEU:HD13	2.04	0.40	

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e e		$r \sim j \sim \cdots$

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:B:14:ARG:CG	1:B:14:ARG:HH11	2.01	0.40	
1:B:93:GLU:CG	1:B:121:LEU:HD13	2.51	0.40	

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides 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		B	ond leng	gths	B	ond ang	les
				nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
	2	PHE	А	1153	-	$9,\!12,\!12$	1.43	2 (22%)	$10,\!15,\!15$	0.41	0

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	PHE	А	1153	-	-	0/4/8/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	А	1153	PHE	CZ-CE2	2.79	1.45	1.38
2	А	1153	PHE	CE1-CD1	2.38	1.43	1.38

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)

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

