



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:44 PM GMT

PDB ID : 4FXU
Title : Crystallographic structure of trimeric riboflavin synthase from *Brucella abortus*
Authors : Serer, M.I.; Bonomi, H.R.; Guimaraes, B.G.; Rossi, R.C.; Goldbaum, F.A.; Klinke, S.
Deposited on : 2012-07-03
Resolution : 1.90 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

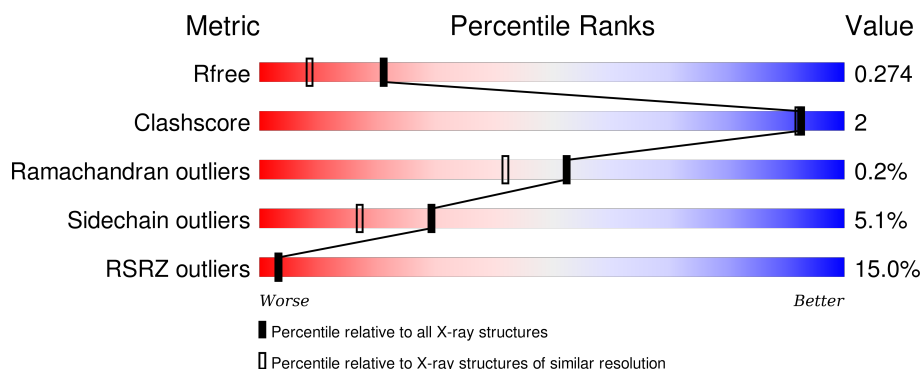
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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. 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	210	<div> <div>7%</div> <div>87%</div> <div>5%</div> <div>8%</div> </div>
1	B	210	<div> <div>24%</div> <div>74%</div> <div>6%</div> <div>20%</div> </div>
1	C	210	<div> <div>9%</div> <div>86%</div> <div>7%</div> <div>6%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4291 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 Riboflavin synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1460	925	253	278	4			
1	B	169	Total	C	N	O	S	0	0	0
			1189	746	206	233	4			
1	C	197	Total	C	N	O	S	0	0	0
			1494	940	260	290	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	LEU	-	EXPRESSION TAG	UNP G8SX20
A	204	GLU	-	EXPRESSION TAG	UNP G8SX20
A	205	HIS	-	EXPRESSION TAG	UNP G8SX20
A	206	HIS	-	EXPRESSION TAG	UNP G8SX20
A	207	HIS	-	EXPRESSION TAG	UNP G8SX20
A	208	HIS	-	EXPRESSION TAG	UNP G8SX20
A	209	HIS	-	EXPRESSION TAG	UNP G8SX20
A	210	HIS	-	EXPRESSION TAG	UNP G8SX20
B	203	LEU	-	EXPRESSION TAG	UNP G8SX20
B	204	GLU	-	EXPRESSION TAG	UNP G8SX20
B	205	HIS	-	EXPRESSION TAG	UNP G8SX20
B	206	HIS	-	EXPRESSION TAG	UNP G8SX20
B	207	HIS	-	EXPRESSION TAG	UNP G8SX20
B	208	HIS	-	EXPRESSION TAG	UNP G8SX20
B	209	HIS	-	EXPRESSION TAG	UNP G8SX20
B	210	HIS	-	EXPRESSION TAG	UNP G8SX20
C	203	LEU	-	EXPRESSION TAG	UNP G8SX20
C	204	GLU	-	EXPRESSION TAG	UNP G8SX20
C	205	HIS	-	EXPRESSION TAG	UNP G8SX20
C	206	HIS	-	EXPRESSION TAG	UNP G8SX20
C	207	HIS	-	EXPRESSION TAG	UNP G8SX20
C	208	HIS	-	EXPRESSION TAG	UNP G8SX20
C	209	HIS	-	EXPRESSION TAG	UNP G8SX20

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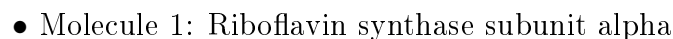
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Chain	Residue	Modelled	Actual	Comment	Reference
C	210	HIS	-	EXPRESSION TAG	UNP G8SX20

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	67	Total O 67 67	0	0
2	B	16	Total O 16 16	0	0
2	C	65	Total O 65 65	0	0

- Molecule 1: Riboflavin synthase subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.42Å 93.48Å 103.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.72 – 1.90 27.72 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (27.72-1.90) 99.9 (27.72-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 1.91Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.232 , 0.264 0.240 , 0.274	Depositor DCC
R_{free} test set	2606 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 52107 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4291	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.50	0/1483	0.69	0/2015
1	B	0.48	0/1200	0.64	0/1631
1	C	0.54	0/1517	0.70	0/2060
All	All	0.51	0/4200	0.68	0/5706

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	1460	0	1435	8	0
1	B	1189	0	1107	5	0
1	C	1494	0	1475	4	0
2	A	67	0	0	0	0
2	B	16	0	0	0	0
2	C	65	0	0	0	0
All	All	4291	0	4017	16	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 2.

All (16) 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:124:ARG:HH22	1:A:153:ASN:ND2	1.52	1.06
1:A:124:ARG:NH2	1:A:153:ASN:ND2	2.30	0.77
1:A:124:ARG:NH2	1:A:153:ASN:HD22	1.91	0.67
1:A:124:ARG:HH22	1:A:153:ASN:HD22	1.37	0.63
1:C:3:THR:HB	1:C:5:ILE:HD12	1.80	0.63
1:B:26:ILE:HG12	1:B:86:ILE:HD11	1.85	0.58
1:B:32:PRO:HA	1:B:35:ILE:HD12	1.88	0.56
1:B:196:ARG:HA	1:B:199:GLN:HG2	1.89	0.55
1:C:5:ILE:HD11	1:C:100:GLY:N	2.24	0.53
1:A:1:MET:HE3	1:B:98:MET:HB3	1.96	0.48
1:A:124:ARG:HH22	1:A:153:ASN:HD21	1.53	0.46
1:C:6:ILE:HD12	1:C:87:ASN:HB3	1.98	0.45
1:A:13:ASP:CG	1:A:25:ARG:HH21	2.20	0.44
1:A:21:GLY:H	1:A:72:LEU:HD13	1.84	0.43
1:B:134:ALA:HA	1:B:137:ILE:HD12	2.00	0.42
1:C:4:GLY:HA2	1:C:147:GLY:O	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	190/210 (90%)	185 (97%)	4 (2%)	1 (0%)	34	21
1	B	159/210 (76%)	155 (98%)	4 (2%)	0	100	100
1	C	195/210 (93%)	191 (98%)	4 (2%)	0	100	100
All	All	544/630 (86%)	531 (98%)	12 (2%)	1 (0%)	52	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	GLN

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	148/173 (86%)	143 (97%)	5 (3%)	44	33
1	B	111/173 (64%)	105 (95%)	6 (5%)	27	15
1	C	155/173 (90%)	145 (94%)	10 (6%)	21	10
All	All	414/519 (80%)	393 (95%)	21 (5%)	29	17

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	48	LEU
1	A	93	LYS
1	A	124	ARG
1	A	155	VAL
1	B	44	SER
1	B	48	LEU
1	B	93	LYS
1	B	133	LEU
1	B	164	LEU
1	B	199	GLN
1	C	1	MET
1	C	3	THR
1	C	13	ASP
1	C	18	LEU
1	C	84	ARG
1	C	91	SER
1	C	132	GLU
1	C	163	LEU
1	C	164	LEU
1	C	197	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	ASN
1	B	139	GLN
1	B	189	GLN
1	C	158	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 carbohydrates 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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	194/210 (92%)	0.56	14 (7%) 18 20	31, 45, 64, 91	0
1	B	169/210 (80%)	1.57	51 (30%) 1 0	39, 63, 93, 107	0
1	C	197/210 (93%)	0.69	19 (9%) 10 11	28, 42, 60, 91	0
All	All	560/630 (88%)	0.91	84 (15%) 3 3	28, 48, 79, 107	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	134	ALA	5.5
1	B	12	VAL	5.1
1	B	175	GLY	4.6
1	B	49	THR	4.5
1	B	155	VAL	4.5
1	B	123	VAL	4.3
1	B	50	VAL	4.3
1	B	71	ALA	4.2
1	B	179	ALA	4.1
1	B	26	ILE	4.0
1	B	125	PHE	4.0
1	B	74	LEU	4.0
1	C	94	LEU	3.8
1	B	35	ILE	3.8
1	C	57	GLY	3.7
1	B	171	VAL	3.6
1	B	41	ILE	3.6
1	B	34	THR	3.6
1	B	163	LEU	3.5
1	B	30	TYR	3.5
1	B	39	ALA	3.5
1	B	13	ASP	3.5
1	B	156	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	102	LEU	3.4
1	A	145	LEU	3.3
1	A	68	TRP	3.3
1	C	145	LEU	3.2
1	A	111	ALA	3.2
1	C	143	VAL	3.2
1	B	36	GLU	3.2
1	B	4	GLY	3.2
1	C	144	ALA	3.2
1	C	196	ARG	3.2
1	C	136	PHE	3.1
1	B	24	LEU	3.0
1	B	37	LEU	3.0
1	B	9	ILE	3.0
1	B	86	ILE	3.0
1	B	23	LEU	2.9
1	B	176	GLU	2.9
1	A	144	ALA	2.9
1	B	111	ALA	2.9
1	B	21	GLY	2.8
1	B	29	ALA	2.8
1	B	153	ASN	2.7
1	B	104	PHE	2.7
1	A	183	VAL	2.7
1	B	122	ALA	2.7
1	B	73	ARG	2.7
1	C	148	THR	2.6
1	A	76	THR	2.6
1	C	33	GLU	2.6
1	B	200	TYR	2.6
1	B	116	ARG	2.5
1	B	157	ALA	2.5
1	B	197	LEU	2.5
1	B	38	GLY	2.5
1	B	199	GLN	2.5
1	A	32	PRO	2.4
1	C	51	VAL	2.4
1	B	170	GLU	2.4
1	B	6	ILE	2.3
1	A	101	HIS	2.3
1	A	95	GLY	2.3
1	C	189	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	143	VAL	2.3
1	B	14	ARG	2.3
1	A	107	VAL	2.2
1	B	198	ALA	2.2
1	A	190	LEU	2.2
1	C	42	ALA	2.2
1	B	22	VAL	2.2
1	C	183	VAL	2.2
1	B	11	LYS	2.2
1	B	169	LEU	2.2
1	B	25	ARG	2.1
1	A	200	TYR	2.1
1	C	43	CYS	2.1
1	C	185	ILE	2.1
1	A	18	LEU	2.1
1	C	174	TRP	2.1
1	C	121	ASP	2.1
1	A	61	ARG	2.0
1	C	86	ILE	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.