Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 08:45 PM EDT

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PDB ID	:	5IDX
Title	:	Crystal structure of an oxidoreductase from Burkholderia vietnamiensis
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2016-02-24
Resolution	:	1.95 Å(reported)

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 1.95 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.
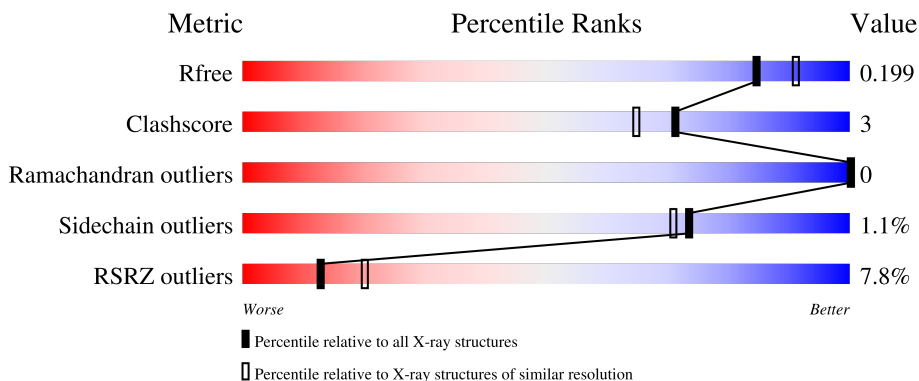
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 >=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% 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	267	9% ▕ 90% 8% ·
1	B	267	7% ▕ 91% 7% ·

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4238 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 Short-chain dehydrogenase/reductase SDR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	3	0
			1858	1158	341	350	9			
1	B	263	Total	C	N	O	S	0	2	0
			1898	1177	354	358	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP A4JGH3
A	-6	ALA	-	expression tag	UNP A4JGH3
A	-5	HIS	-	expression tag	UNP A4JGH3
A	-4	HIS	-	expression tag	UNP A4JGH3
A	-3	HIS	-	expression tag	UNP A4JGH3
A	-2	HIS	-	expression tag	UNP A4JGH3
A	-1	HIS	-	expression tag	UNP A4JGH3
A	0	HIS	-	expression tag	UNP A4JGH3
B	-7	MET	-	initiating methionine	UNP A4JGH3
B	-6	ALA	-	expression tag	UNP A4JGH3
B	-5	HIS	-	expression tag	UNP A4JGH3
B	-4	HIS	-	expression tag	UNP A4JGH3
B	-3	HIS	-	expression tag	UNP A4JGH3
B	-2	HIS	-	expression tag	UNP A4JGH3
B	-1	HIS	-	expression tag	UNP A4JGH3
B	0	HIS	-	expression tag	UNP A4JGH3

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	198	Total 198	O 198	0	0
3	B	249	Total 249	O 249	0	0

3 Residue-property plots ⓘ

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: Short-chain dehydrogenase/reductase SDR
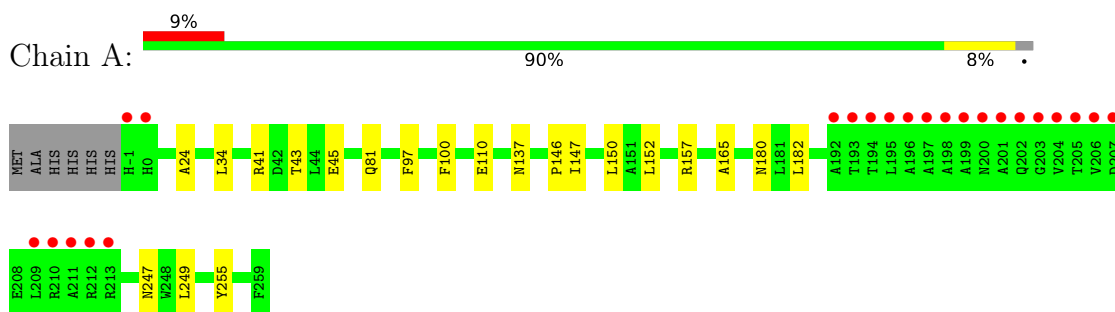
• Molecule 1: Short-chain dehydrogenase/reductase SDR
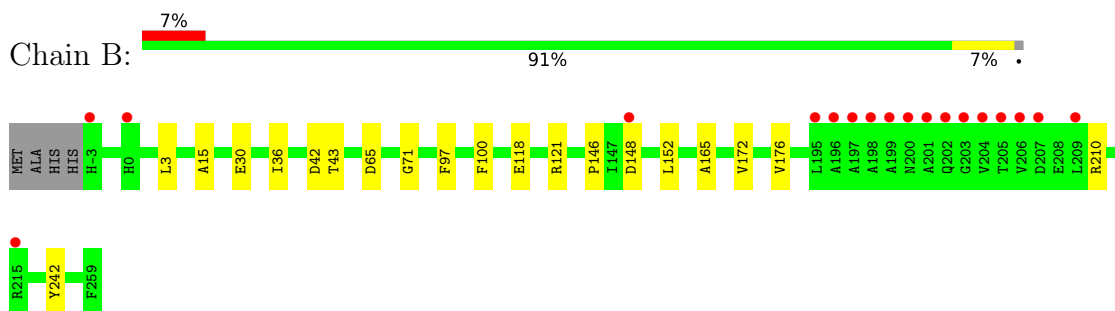
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	110.75Å 110.75Å 110.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.16 – 1.95 45.17 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.16-1.95) 100.0 (45.17-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.15 (at 1.95Å)	Xtriage
Refinement program	PHENIX dev_2313	Depositor
R, R_{free}	0.161 , 0.199 0.161 , 0.199	Depositor DCC
R_{free} test set	1955 reflections (3.88%)	wwPDB-VP
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.7	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.033 for -h,-l,-k 0.018 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4238	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4

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	0.32	0/1895	0.51	0/2581
1	B	0.33	0/1933	0.51	0/2630
All	All	0.33	0/3828	0.51	0/5211

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	1858	0	1849	15	0
1	B	1898	0	1887	11	0
2	A	10	0	0	1	0
2	B	25	0	0	1	0
3	A	198	0	0	6	1
3	B	249	0	0	2	1
All	All	4238	0	3736	26	1

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 3.

All (26) 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:118[A]:GLU:OE2	1:B:121:ARG:NH2	2.25	0.68
1:A:110:GLU:OE2	3:A:401:HOH:O	2.13	0.66
2:A:302:SO4:O4	3:A:402:HOH:O	2.14	0.64
1:A:81:GLN:NE2	3:A:403:HOH:O	2.28	0.64
1:B:148:ASP:OD2	3:B:401:HOH:O	2.17	0.57
1:A:137:ASN:HD22	1:A:180:ASN:ND2	2.06	0.54
1:B:97:PHE:HA	1:B:100:PHE:CD2	2.42	0.54
1:B:3:LEU:HD12	1:B:30:GLU:HG3	1.95	0.49
1:A:97:PHE:HA	1:A:100:PHE:CD2	2.48	0.48
1:B:42:ASP:OD1	1:B:43:THR:N	2.47	0.46
1:B:15:ALA:HB3	1:B:36:ILE:HB	1.98	0.46
1:A:249:LEU:HD21	1:A:255:TYR:HB3	1.97	0.46
1:A:146:PRO:HG2	1:B:165:ALA:HB3	1.97	0.46
1:A:165:ALA:HB3	1:B:146:PRO:HG2	1.98	0.45
1:A:157:ARG:NH1	3:A:415:HOH:O	2.50	0.44
1:A:24:ALA:HB1	1:A:34:LEU:HD13	2.00	0.44
1:B:65:ASP:O	1:B:71:GLY:HA3	2.18	0.44
1:A:137:ASN:HB2	1:A:180:ASN:HD22	1.84	0.43
1:A:157:ARG:NE	3:A:405:HOH:O	2.32	0.42
1:B:100:PHE:CE2	1:B:152:LEU:HG	2.54	0.42
1:B:172:VAL:HA	1:B:176:VAL:O	2.19	0.42
2:B:303:SO4:O2	3:B:402:HOH:O	2.21	0.42
1:A:147:ILE:HD12	1:A:150:LEU:HD12	2.01	0.42
1:A:43:THR:HB	3:A:437:HOH:O	2.20	0.41
1:A:182:LEU:HD11	1:A:247:ASN:HD22	1.85	0.41
1:A:100:PHE:CE2	1:A:152:LEU:HG	2.56	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:521:HOH:O	3:B:465:HOH:O[3_554]	2.10	0.10

5.3　Torsion angles ⓘ

5.3.1　Protein backbone ⓘ

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	262/267 (98%)	255 (97%)	7 (3%)	0	100	100
1	B	263/267 (98%)	257 (98%)	6 (2%)	0	100	100
All	All	525/534 (98%)	512 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	179/194 (92%)	177 (99%)	2 (1%)	73	71
1	B	185/194 (95%)	183 (99%)	2 (1%)	73	71
All	All	364/388 (94%)	360 (99%)	4 (1%)	73	71

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	45	GLU
1	B	210	ARG
1	B	242	TYR

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	180	ASN
1	A	247	ASN
1	B	56	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 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	$\#|Z| > 2$
2	SO4	B	301	-	4,4,4	0.18	0	6,6,6	0.12	0
2	SO4	B	302	-	4,4,4	0.18	0	6,6,6	0.11	0
2	SO4	A	302	-	4,4,4	0.12	0	6,6,6	0.13	0
2	SO4	B	303	-	4,4,4	0.12	0	6,6,6	0.12	0
2	SO4	A	301	-	4,4,4	0.10	0	6,6,6	0.11	0
2	SO4	B	304	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	B	305	-	4,4,4	0.15	0	6,6,6	0.06	0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	SO4	1	0
2	B	303	SO4	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	261/267 (97%)	0.36	23 (8%)	10	16	16, 26, 73, 100	0
1	B	263/267 (98%)	0.06	18 (6%)	17	25	15, 24, 59, 79	0
All	All	524/534 (98%)	0.21	41 (7%)	13	20	15, 25, 63, 100	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	199	ALA	7.5
1	A	201	ALA	6.7
1	A	204	VAL	6.4
1	A	196	ALA	6.3
1	A	197	ALA	6.1
1	A	206	VAL	5.9
1	A	203	GLY	5.8
1	A	200	ASN	5.7
1	A	202	GLN	5.6
1	A	195	LEU	5.6
1	B	203	GLY	4.9
1	B	199	ALA	4.6
1	A	209	LEU	4.6
1	B	198	ALA	4.6
1	A	198	ALA	4.5
1	B	197	ALA	4.4
1	A	-1	HIS	4.3
1	B	200	ASN	4.2
1	A	212	ARG	4.2
1	B	201	ALA	3.9
1	B	202	GLN	3.5
1	B	148	ASP	3.5
1	A	205	THR	3.3
1	A	207	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	195	LEU	3.2
1	A	211	ALA	3.2
1	B	204	VAL	3.2
1	B	209	LEU	3.0
1	B	205	THR	3.0
1	A	213	ARG	3.0
1	B	207	ASP	2.9
1	B	196	ALA	2.9
1	B	206	VAL	2.6
1	B	-3	HIS	2.5
1	A	0	HIS	2.5
1	A	192	ALA	2.2
1	B	215	ARG	2.2
1	B	0	HIS	2.2
1	A	193	THR	2.1
1	A	194	THR	2.1
1	A	210	ARG	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th 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($Å^2$)	Q<0.9
2	SO4	B	305	5/5	0.80	0.19	113,115,117,118	0
2	SO4	B	303	5/5	0.88	0.14	96,101,101,102	0
2	SO4	B	304	5/5	0.94	0.28	95,100,102,103	0
2	SO4	A	302	5/5	0.97	0.12	27,51,55,63	0
2	SO4	A	301	5/5	0.97	0.13	42,44,54,60	0
2	SO4	B	301	5/5	0.98	0.11	29,37,47,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	302	5/5	0.99	0.08	31,32,40,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.