wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 12:28 AM GMT

PDB ID	:	2AJT
Title	:	Crystal structure of L-Arabinose Isomerase from E.coli
Authors	:	Manjasetty, B.A.; Fedorov, E.V.; Almo, S.C.; Chance, M.R.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2005-08-02
Resolution	:	2.60 Å(reported)

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

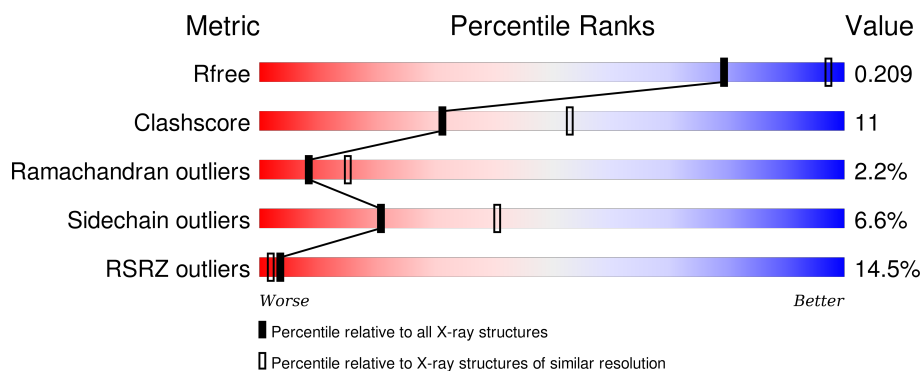|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	Percentile Ranks	Value
Rfree		0.209
Clashscore		11
Ramachandran outliers		2.2%
Sidechain outliers		6.6%
RSRZ outliers		14.5%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 <=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	500	10% — 73% — 24% — ·
1	B	500	7% — 76% — 19% — · ·
1	C	500	27% — 80% — 16% — ·

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11483 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 L-arabinose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total 3833	C 2434	N 663	O 712	S 24	0	0	0
1	B	498	Total 3875	C 2461	N 670	O 719	S 25	0	1	0
1	C	498	Total 3687	C 2335	N 635	O 693	S 24	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	PRO	ARG	SEE REMARK 999	UNP P08202
B	72	PRO	ARG	SEE REMARK 999	UNP P08202
C	72	PRO	ARG	SEE REMARK 999	UNP P08202

- Molecule 2 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	40	Total 40	O 40	0	0
2	B	33	Total 33	O 33	0	0
2	C	15	Total 15	O 15	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
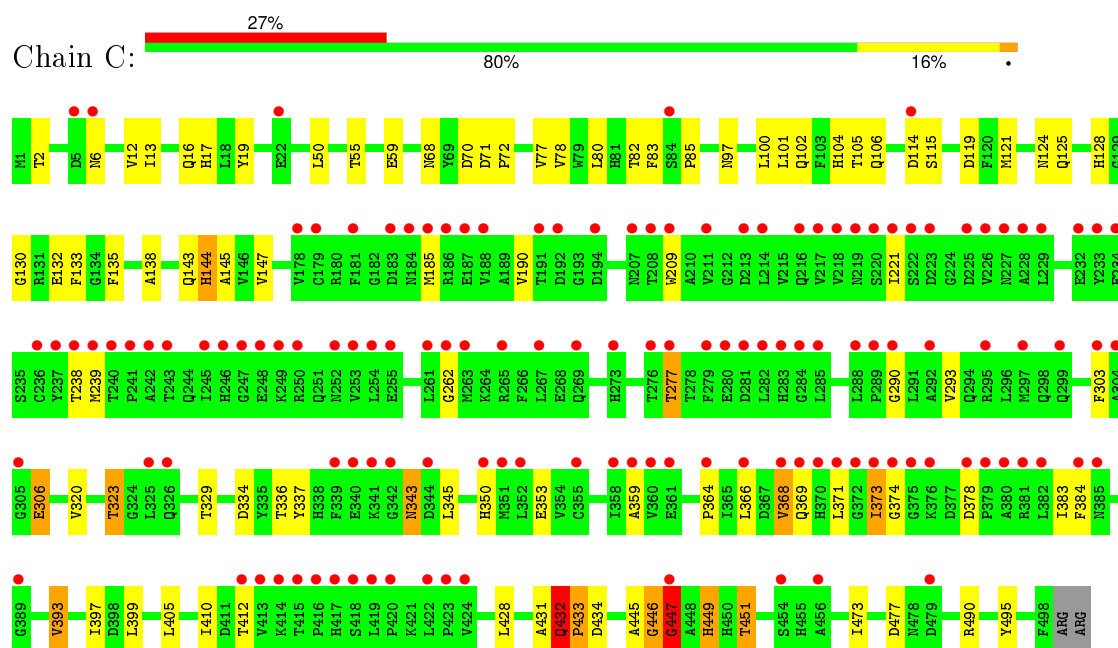
- Molecule 1: L-arabinose isomerase

- Molecule 1: L-arabinose isomerase

- Molecule 1: L-arabinose isomerase

Chain C:

27%

80%

16%
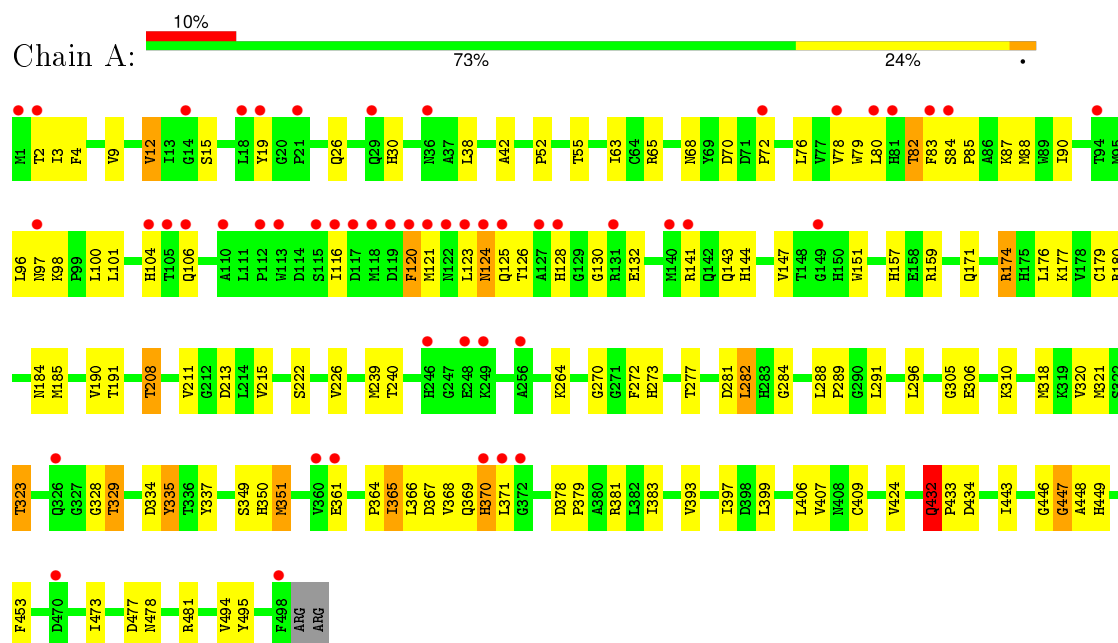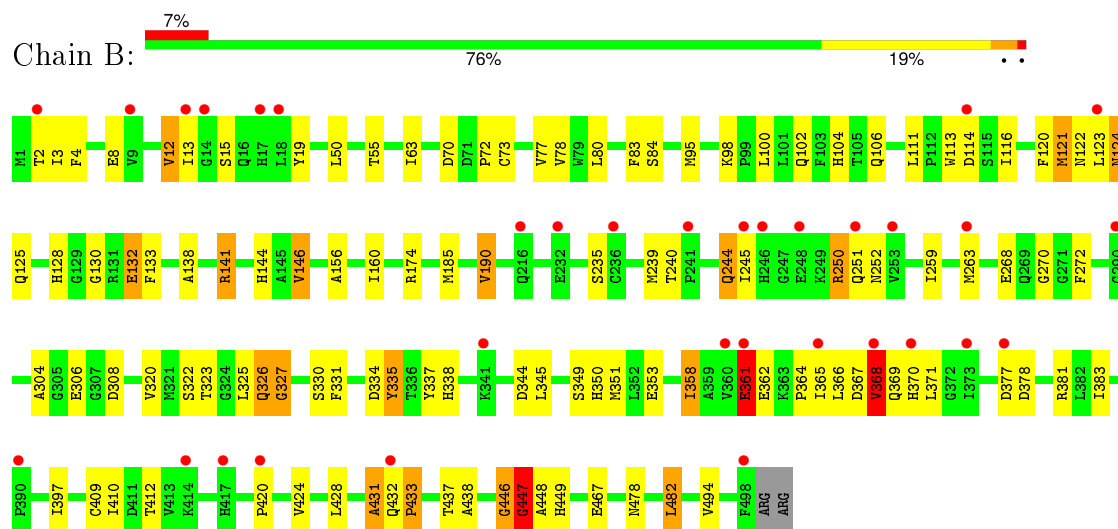
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	116.54Å 116.54Å 214.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.84 – 2.60 19.84 – 2.60	Depositor EDS
% Data completeness (in resolution range)	84.5 (19.84-2.60) 84.5 (19.84-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	71.36 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.217 , 0.278 0.224 , 0.209	Depositor DCC
R_{free} test set	2204 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	51.3	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 67.6	EDS
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 44290 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11483	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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, 0.375 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	0.49	0/3927	0.66	1/5351 (0.0%)
1	B	0.49	1/3976 (0.0%)	0.65	0/5411
1	C	0.44	0/3776	0.60	1/5157 (0.0%)
All	All	0.47	1/11679 (0.0%)	0.64	2/15919 (0.0%)

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	1
1	B	0	6
1	C	0	2
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	361	GLU	CB-CG	5.09	1.61	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	432	GLN	C-N-CD	7.85	144.88	128.40
1	C	447	GLY	N-CA-C	7.12	130.89	113.10

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	447	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	B	361	GLU	Peptide
1	B	362	GLU	Peptide
1	B	368	VAL	Peptide
1	B	431	ALA	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	3833	0	3662	100	0
1	B	3875	0	3727	93	0
1	C	3687	0	3407	70	0
2	A	40	0	0	0	0
2	B	33	0	0	0	0
2	C	15	0	0	1	0
All	All	11483	0	10796	240	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 11.

The worst 5 of 240 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:190:VAL:HG11	1:B:448:ALA:HB2	1.38	1.04
1:A:190:VAL:HG11	1:A:448:ALA:HB2	1.41	1.02
1:B:337:TYR:H	1:C:106:GLN:HE22	1.10	0.98
1:A:432:GLN:O	1:A:433:PRO:C	2.04	0.88
1:B:364:PRO:HD2	1:B:383:ILE:O	1.75	0.87

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	496/500 (99%)	456 (92%)	30 (6%)	10 (2%)	9	18
1	B	497/500 (99%)	465 (94%)	22 (4%)	10 (2%)	9	18
1	C	496/500 (99%)	467 (94%)	17 (3%)	12 (2%)	7	13
All	All	1489/1500 (99%)	1388 (93%)	69 (5%)	32 (2%)	8	16

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	326	GLN
1	B	361	GLU
1	B	368	VAL
1	B	447	GLY
1	C	306	GLU

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	396/419 (94%)	366 (92%)	30 (8%)	16	32
1	B	406/419 (97%)	378 (93%)	28 (7%)	19	38
1	C	363/419 (87%)	343 (94%)	20 (6%)	27	51
All	All	1165/1257 (93%)	1087 (93%)	78 (7%)	21	40

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	95[B]	MET
1	B	190	VAL
1	C	393	VAL
1	B	121	MET
1	B	132	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	125	GLN
1	B	269	GLN
1	C	287	GLN
1	B	128	HIS
1	B	142	GLN

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 (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, 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	498/500 (99%)	0.51	51 (10%)	9	5	58, 66, 72, 81	0
1	B	498/500 (99%)	0.43	33 (6%)	22	16	59, 66, 72, 82	0
1	C	498/500 (99%)	1.50	133 (26%)	1	0	58, 68, 71, 76	0
All	All	1494/1500 (99%)	0.81	217 (14%)	3	2	58, 67, 71, 82	0

The worst 5 of 217 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	233	TYR	14.8
1	C	245	ILE	10.9
1	C	236	CYS	10.3
1	C	241	PRO	9.5
1	C	237	TYR	9.3

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.