wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 26, 2023 – 05:41 PM EDT

PDB ID : 3IUH
Title : Co2+-bound form of Pseudomonas stutzeri L-rhamnose isomerase
Authors : Yoshida, H.; Yamaji, M.; Ishii, T.; Izumori, K.; Kamitori, S.
Deposited on : 2009-08-31
Resolution : 2.00 Å(reported)

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

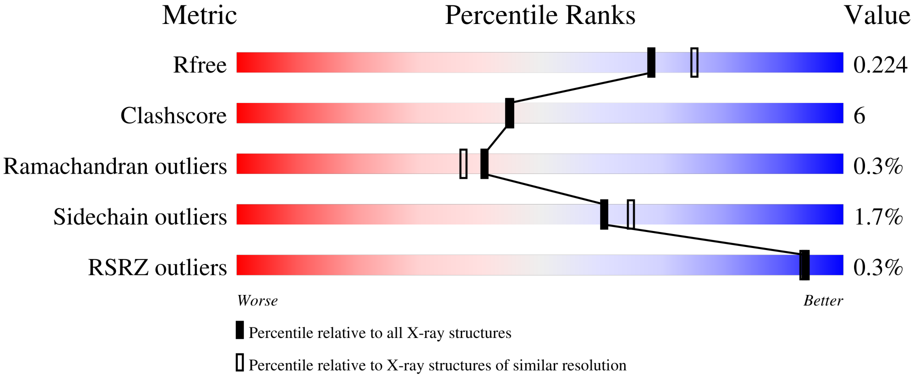
MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	438	
1	B	438	
1	C	438	
1	D	438	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 14306 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-rhamnose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	417	3237	2034	580	614	9	0	0	0
1	B	418	3236	2031	581	615	9	0	0	0
1	C	421	3252	2040	584	619	9	0	0	0
1	D	420	3253	2043	583	618	9	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	ASN	ASP	engineered mutation	UNP Q75WH8
A	431	GLY	-	expression tag	UNP Q75WH8
A	432	SER	-	expression tag	UNP Q75WH8
A	433	HIS	-	expression tag	UNP Q75WH8
A	434	HIS	-	expression tag	UNP Q75WH8
A	435	HIS	-	expression tag	UNP Q75WH8
A	436	HIS	-	expression tag	UNP Q75WH8
A	437	HIS	-	expression tag	UNP Q75WH8
A	438	HIS	-	expression tag	UNP Q75WH8
B	150	ASN	ASP	engineered mutation	UNP Q75WH8
B	431	GLY	-	expression tag	UNP Q75WH8
B	432	SER	-	expression tag	UNP Q75WH8
B	433	HIS	-	expression tag	UNP Q75WH8
B	434	HIS	-	expression tag	UNP Q75WH8
B	435	HIS	-	expression tag	UNP Q75WH8
B	436	HIS	-	expression tag	UNP Q75WH8
B	437	HIS	-	expression tag	UNP Q75WH8
B	438	HIS	-	expression tag	UNP Q75WH8
C	150	ASN	ASP	engineered mutation	UNP Q75WH8
C	431	GLY	-	expression tag	UNP Q75WH8
C	432	SER	-	expression tag	UNP Q75WH8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	433	HIS	-	expression tag	UNP Q75WH8
C	434	HIS	-	expression tag	UNP Q75WH8
C	435	HIS	-	expression tag	UNP Q75WH8
C	436	HIS	-	expression tag	UNP Q75WH8
C	437	HIS	-	expression tag	UNP Q75WH8
C	438	HIS	-	expression tag	UNP Q75WH8
D	150	ASN	ASP	engineered mutation	UNP Q75WH8
D	431	GLY	-	expression tag	UNP Q75WH8
D	432	SER	-	expression tag	UNP Q75WH8
D	433	HIS	-	expression tag	UNP Q75WH8
D	434	HIS	-	expression tag	UNP Q75WH8
D	435	HIS	-	expression tag	UNP Q75WH8
D	436	HIS	-	expression tag	UNP Q75WH8
D	437	HIS	-	expression tag	UNP Q75WH8
D	438	HIS	-	expression tag	UNP Q75WH8

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Co 2 2	0	0
2	B	2	Total Co 2 2	0	0
2	C	2	Total Co 2 2	0	0
2	D	2	Total Co 2 2	0	0

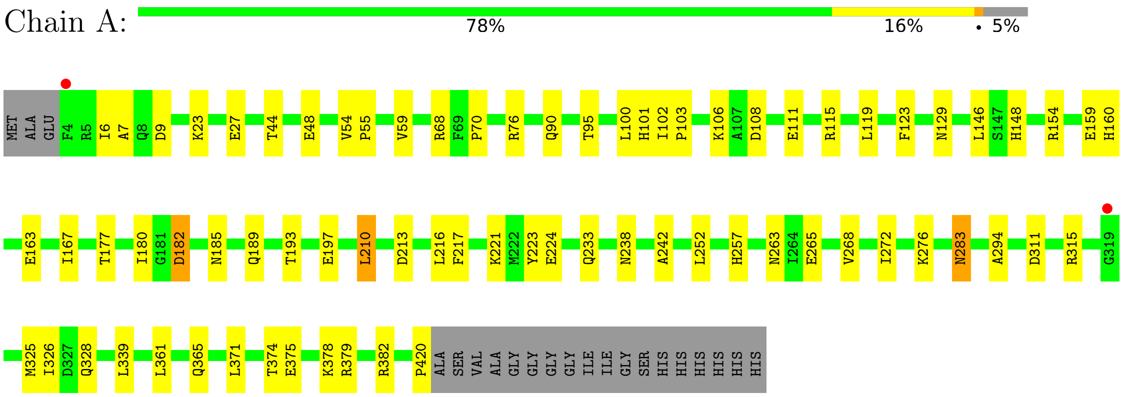
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	328	Total O 328 328	0	0
3	B	290	Total O 290 290	0	0
3	C	324	Total O 324 324	0	0
3	D	378	Total O 378 378	0	0

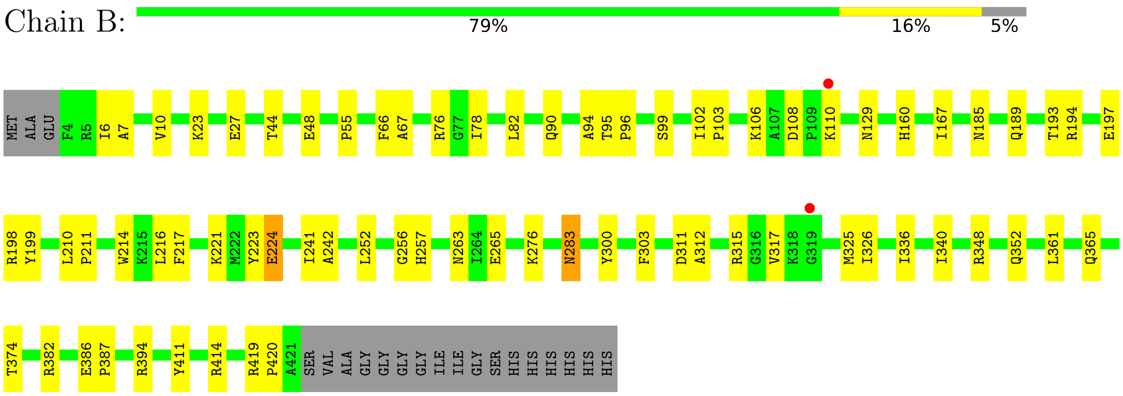
3 Residue-property plots ⓘ

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.

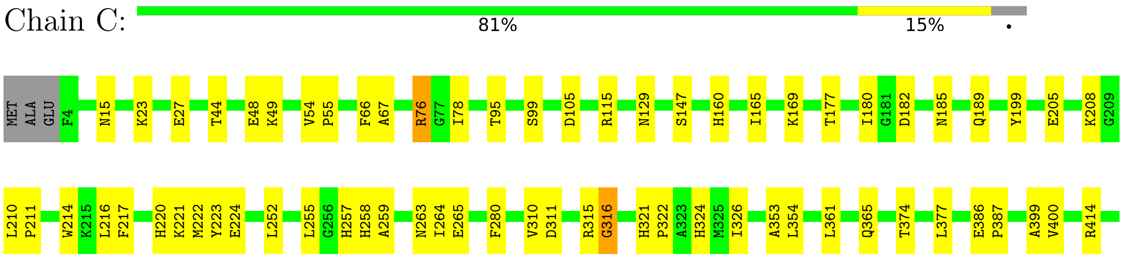
- Molecule 1: L-rhamnose isomerase

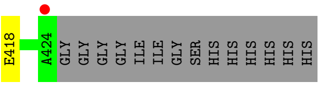


- Molecule 1: L-rhamnose isomerase



- Molecule 1: L-rhamnose isomerase





- Molecule 1: L-rhamnose isomerase

Chain D:

4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.07Å 104.96Å 113.37Å 90.00° 108.23° 90.00°	Depositor
Resolution (Å)	39.02 – 2.00 39.01 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.2 (39.02-2.00) 92.2 (39.01-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.08 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.183 , 0.225 0.182 , 0.224	Depositor DCC
R_{free} test set	10803 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å^2)	17.7	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.4	EDS
L-test for twinning[2]	$< \|L\| >$ = 0.47, $< L^2 >$ = 0.30	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14306	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: CO

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	0.33	0/3309	0.54	1/4486 (0.0%)
1	B	0.31	0/3307	0.53	0/4484
1	C	0.32	0/3323	0.55	0/4506
1	D	0.33	0/3325	0.55	0/4508
All	All	0.32	0/13264	0.54	1/17984 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	210	LEU	CA-CB-CG	5.16	127.17	115.30

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	3237	0	3141	46	0
1	B	3236	0	3139	45	0
1	C	3252	0	3151	42	0
1	D	3253	0	3153	33	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	328	0	0	3	0
3	B	290	0	0	1	0
3	C	324	0	0	1	0
3	D	378	0	0	5	0
All	All	14306	0	12584	166	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 6.

The worst 5 of 166 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:129:ASN:H	1:B:160:HIS:HE1	1.11	0.97
1:D:129:ASN:H	1:D:160:HIS:HE1	1.14	0.91
1:A:210:LEU:HD11	1:A:216:LEU:HB2	1.58	0.85
1:D:318:LYS:HA	1:D:318:LYS:HE2	1.63	0.79
1:D:129:ASN:H	1:D:160:HIS:CE1	2.02	0.78

There are no symmetry-related clashes.

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	415/438 (95%)	403 (97%)	11 (3%)	1 (0%)	47	44
1	B	416/438 (95%)	406 (98%)	9 (2%)	1 (0%)	47	44
1	C	419/438 (96%)	403 (96%)	14 (3%)	2 (0%)	29	23
1	D	418/438 (95%)	408 (98%)	9 (2%)	1 (0%)	47	44
All	All	1668/1752 (95%)	1620 (97%)	43 (3%)	5 (0%)	41	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	316	GLY
1	A	224	GLU
1	B	224	GLU
1	C	224	GLU
1	D	224	GLU

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	328/341 (96%)	321 (98%)	7 (2%)	53	57
1	B	327/341 (96%)	324 (99%)	3 (1%)	78	83
1	C	328/341 (96%)	323 (98%)	5 (2%)	65	69
1	D	329/341 (96%)	322 (98%)	7 (2%)	53	57
All	All	1312/1364 (96%)	1290 (98%)	22 (2%)	60	65

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	377	LEU
1	D	124	ASP
1	D	99	SER
1	D	354	LEU
1	A	374	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	8	GLN
1	D	344	ASN
1	C	189	GLN
1	D	189	GLN
1	C	160	HIS

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 ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	417/438 (95%)	-0.24	2 (0%)	91	90	11, 20, 36, 44	0
1	B	418/438 (95%)	-0.18	2 (0%)	91	90	9, 21, 38, 45	0
1	C	421/438 (96%)	-0.32	1 (0%)	95	94	10, 19, 32, 52	0
1	D	420/438 (95%)	-0.50	0	100	100	8, 14, 27, 37	0
All	All	1676/1752 (95%)	-0.31	5 (0%)	94	93	8, 18, 34, 52	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	PHE	3.3
1	B	319	GLY	3.3
1	A	319	GLY	2.7
1	B	110	LYS	2.1
1	C	424	ALA	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, 95^{th} 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	CO	C	506	1/1	0.90	0.10	46,46,46,46	1
2	CO	D	508	1/1	0.91	0.09	45,45,45,45	1
2	CO	B	504	1/1	0.94	0.15	36,36,36,36	1
2	CO	A	502	1/1	0.96	0.07	34,34,34,34	1
2	CO	A	501	1/1	0.97	0.13	49,49,49,49	0
2	CO	C	505	1/1	0.97	0.13	50,50,50,50	0
2	CO	D	507	1/1	0.98	0.12	45,45,45,45	0
2	CO	B	503	1/1	0.98	0.07	53,53,53,53	0

6.5 Other polymers

There are no such residues in this entry.