

wwPDB X-ray Structure Validation Summary Report (i)

Dec 11, 2022 – 01:59 AM EST

PDB ID : 1DE6

Title : L-RHAMNOSE ISOMERASE

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Deposited on : 1999-11-13

Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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 : 2.31.2

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

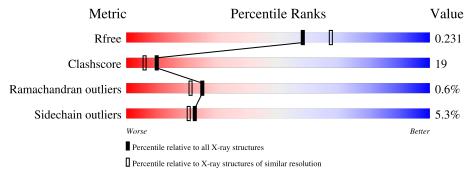
Validation Pipeline (wwPDB-VP) : 2.31.2

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 2.10 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	Similar resolution
14164116	(# Entries)	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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%

Mol	Chain	Length	Quality of cha	ain	
1	A	426	60%	30%	7% •
1	В	426	55%	34%	8% ••
1	С	426	60%	30%	8% ••
1	D	426	56%	34%	7% ••



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14331 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		
1	Λ	416	Total	С	N	О	S	0	0	0
1	A	410	3309	2090	587	619	13	U	0	U
1	В	416	Total	С	N	О	S	0	0	0
1	Б	410	3309	2090	587	619	13	U	U	U
1	С	416	Total	С	N	О	S	0	0	0
1		410	3309	2090	587	619	13	U		
1	D	416	Total	С	N	О	S	0	0	0
1	D	416	3309	2090	587	619	13	U	0 0	

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	-	expression tag	UNP P32170
A	3	HIS	-	expression tag	UNP P32170
A	4	HIS	-	expression tag	UNP P32170
A	5	HIS	-	expression tag	UNP P32170
A	6	HIS	-	expression tag	UNP P32170
A	7	HIS	-	expression tag	UNP P32170
A	8	HIS	-	expression tag	UNP P32170
В	2	GLY	-	expression tag	UNP P32170
В	3	HIS	-	expression tag	UNP P32170
В	4	HIS	-	expression tag	UNP P32170
В	5	HIS	-	expression tag	UNP P32170
В	6	HIS	-	expression tag	UNP P32170
В	7	HIS	-	expression tag	UNP P32170
В	8	HIS	-	expression tag	UNP P32170
С	2	GLY	-	expression tag	UNP P32170
С	3	HIS	-	expression tag	UNP P32170
С	4	HIS	-	expression tag	UNP P32170
С	5	HIS	-	expression tag	UNP P32170
С	6	HIS	-	expression tag	UNP P32170
С	7	HIS	-	expression tag	UNP P32170
С	8	HIS	-	expression tag	UNP P32170

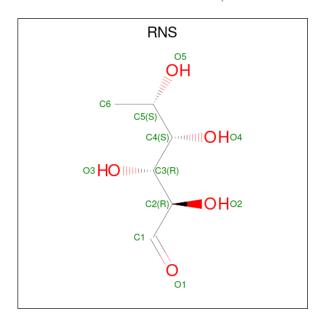
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Chain	Residue	Modelled	Actual	Comment	Reference
D	2	GLY	-	expression tag	UNP P32170
D	3	HIS	-	expression tag	UNP P32170
D	4	HIS	-	expression tag	UNP P32170
D	5	HIS	-	expression tag	UNP P32170
D	6	HIS	-	expression tag	UNP P32170
D	7	HIS	-	expression tag	UNP P32170
D	8	HIS	-	expression tag	UNP P32170

 \bullet Molecule 2 is L-RHAMNOSE (three-letter code: RNS) (formula: $\mathrm{C_6H_{12}O_5}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 11 6 5	0	0
2	В	1	Total C O 11 6 5	0	0
2	С	1	Total C O 11 6 5	0	0
2	D	1	Total C O 11 6 5	0	0

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total Zn 1 1	0	0
3	С	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0

 \bullet Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mn 1 1	0	0
4	В	1	Total Mn 1 1	0	0
4	С	1	Total Mn 1 1	0	0
4	D	1	Total Mn 1 1	0	0

• Molecule 5 is water.

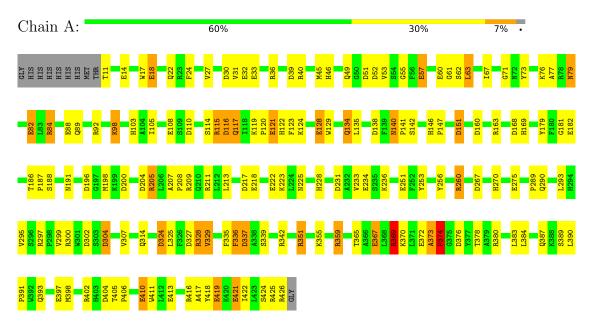
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	250	Total O 250 250	0	0
5	В	286	Total O 286 286	0	0
5	С	263	Total O 263 263	0	0
5	D	244	Total O 244 244	0	0



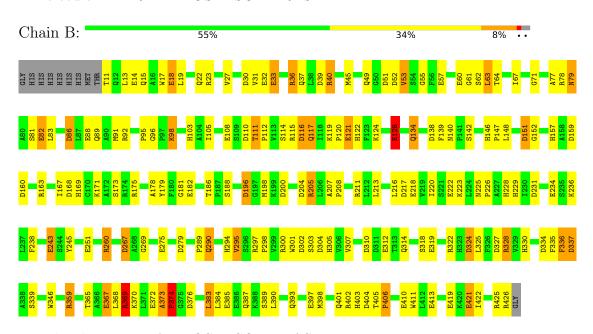
3 Residue-property plots (i)

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.

• Molecule 1: L-RHAMNOSE ISOMERASE

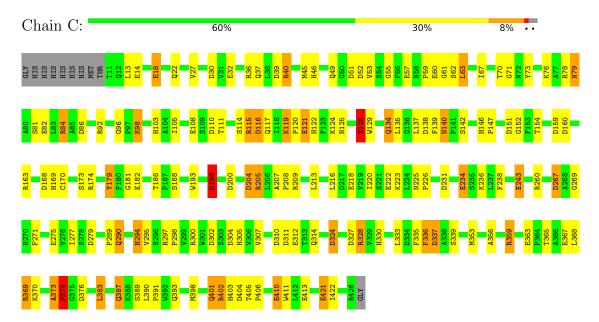


• Molecule 1: L-RHAMNOSE ISOMERASE

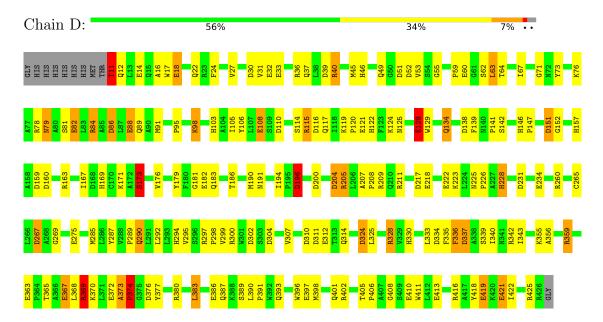


• Molecule 1: L-RHAMNOSE ISOMERASE





• Molecule 1: L-RHAMNOSE ISOMERASE





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	169.18Å 162.44Å 77.73Å	Donositor
a, b, c, α , β , γ	90.00° 109.89° 90.00°	Depositor
Resolution (Å)	30.00 - 2.10	Depositor
Resolution (A)	28.81 - 2.10	EDS
% Data completeness	87.0 (30.00-2.10)	Depositor
(in resolution range)	92.3 (28.81-2.10)	EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.80 (at 2.10Å)	Xtriage
Refinement program	TNT	Depositor
D D.	0.244 , 0.244	Depositor
R, R_{free}	0.172 , 0.231	DCC
R_{free} test set	5391 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32 , 101.9	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14331	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, RNS, MN

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	В	ond lengths	Bond angles		
Moi Chain		RMSZ	77 1		# Z > 5	
1	A	1.28	28/3389~(0.8%)	1.73	73/4602 (1.6%)	
1	В	1.30	29/3389~(0.9%)	1.79	$74/4602 \; (1.6\%)$	
1	С	1.25	20/3389~(0.6%)	1.82	81/4602 (1.8%)	
1	D	1.26	$24/3389 \; (0.7\%)$	1.76	73/4602 (1.6%)	
All	All	1.27	101/13556 (0.7%)	1.78	301/18408 (1.6%)	

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(A)
1	A	32	GLU	CD-OE2	11.09	1.37	1.25
1	D	108	GLU	CD-OE2	9.36	1.35	1.25
1	В	218	GLU	CD-OE2	9.10	1.35	1.25
1	С	18	GLU	CD-OE2	9.01	1.35	1.25
1	D	397	GLU	CD-OE2	8.96	1.35	1.25

The worst 5 of 301 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	С	205	ARG	NE-CZ-NH2	-25.65	107.48	120.30
1	С	205	ARG	NE-CZ-NH1	20.12	130.36	120.30
1	В	359	ARG	NE-CZ-NH2	-19.60	110.50	120.30
1	D	205	ARG	NE-CZ-NH1	18.95	129.78	120.30
1	С	359	ARG	NE-CZ-NH2	-18.36	111.12	120.30

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	A	3309	0	3231	116	0
1	В	3309	0	3231	137	0
1	С	3309	0	3231	126	0
1	D	3309	0	3231	142	0
2	A	11	0	11	4	0
2	В	11	0	12	0	0
2	С	11	0	12	2	0
2	D	11	0	12	0	0
3	A	1	0	0	0	0
3	В	1	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	В	1	0	0	0	0
4	С	1	0	0	0	0
4	D	1	0	0	0	0
5	A	250	0	0	11	0
5	В	286	0	0	15	0
5	С	263	0	0	9	0
5	D	244	0	0	8	0
All	All	14331	0	12971	499	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 19.

The worst 5 of 499 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ (\rm \mathring{A}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:C:398:MET:HE2	1:C:402:ARG:HE	1.02	1.17
1:B:398:MET:HE2	1:B:402:ARG:HE	1.02	1.16
1:A:421:GLU:HG3	1:A:422:ILE:HG12	1.31	1.13
1:A:398:MET:HE2	1:A:402:ARG:HE	1.12	1.06
1:A:393:GLN:NE2	1:D:393:GLN:HE22	1.53	1.05

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	Perce	\mathbf{ntiles}
1	A	414/426 (97%)	397 (96%)	15 (4%)	2 (0%)	29	26
1	В	414/426 (97%)	397 (96%)	14 (3%)	3 (1%)	22	18
1	С	414/426 (97%)	394 (95%)	17 (4%)	3 (1%)	22	18
1	D	414/426 (97%)	395 (95%)	17 (4%)	2 (0%)	29	26
All	All	1656/1704 (97%)	1583 (96%)	63 (4%)	10 (1%)	25	21

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	SER
1	В	62	SER
1	С	62	SER
1	D	62	SER
1	С	59	PRO

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 Outlie		Percentiles		
1	A	351/359~(98%)	334 (95%)	17 (5%)	25 24		
1	В	351/359 (98%)	331 (94%)	20 (6%)	20 18		
1	С	351/359 (98%)	332 (95%)	19 (5%)	22 20		
1	D	351/359 (98%)	332 (95%)	19 (5%)	22 20		
All	All	1404/1436 (98%)	1329 (95%)	75 (5%)	22 20		



5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	53	VAL
1	D	374	PRO
1	D	79	ASN
1	D	196	ASP
1	В	128	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	С	393	GLN
1	D	314	GLN
1	D	49	GLN
1	D	125	ASN
1	В	79	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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).



Mal	Mol Type Chain Re			Link	Bond lengths			Bond angles		
MIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	RNS	С	3462	-	8,10,10	1.14	1 (12%)	9,13,13	1.15	1 (11%)
2	RNS	A	1462	4	8,10,10	1.00	1 (12%)	9,13,13	1.84	3 (33%)
2	RNS	D	4462	-	8,10,10	0.87	0	9,13,13	1.00	0
2	RNS	В	2462	-	8,10,10	1.31	2 (25%)	9,13,13	1.27	1 (11%)

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	RNS	С	3462	-	-	7/12/14/14	-
2	RNS	A	1462	4	-	5/12/14/14	-
2	RNS	D	4462	-	-	8/12/14/14	-
2	RNS	В	2462	-	-	5/12/14/14	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z}$	$\operatorname{Observed}(\mathring{A})$	Ideal(A)
2	С	3462	RNS	O5-C5	2.55	1.50	1.43
2	В	2462	RNS	O3-C3	2.14	1.48	1.43
2	В	2462	RNS	O5-C5	2.11	1.48	1.43
2	A	1462	RNS	O5-C5	2.00	1.48	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	1462	RNS	O3-C3-C2	3.39	115.38	109.17
2	A	1462	RNS	O3-C3-C4	2.73	115.83	109.47
2	В	2462	RNS	C4-C3-C2	-2.72	108.79	113.54
2	С	3462	RNS	C4-C3-C2	-2.47	109.23	113.54
2	A	1462	RNS	C3-C2-C1	-2.11	104.45	111.10

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1462	RNS	C3-C4-C5-O5
2	В	2462	RNS	C3-C4-C5-C6
2	В	2462	RNS	C3-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
2	В	2462	RNS	O4-C4-C5-O5
2	С	3462	RNS	C3-C4-C5-C6

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3462	RNS	2	0
2	A	1462	RNS	4	0

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

