



# wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 01:27 AM GMT

PDB ID : 1F4H  
Title : E. COLI (LACZ) BETA-GALACTOSIDASE (ORTHORHOMBIC)  
Authors : Juers, D.H.; Jacobson, R.H.; Wigley, D.; Zhang, X.J.; Huber, R.E.; Tronrud, D.E.; Matthews, B.W.  
Deposited on : 2000-06-07  
Resolution : 2.80 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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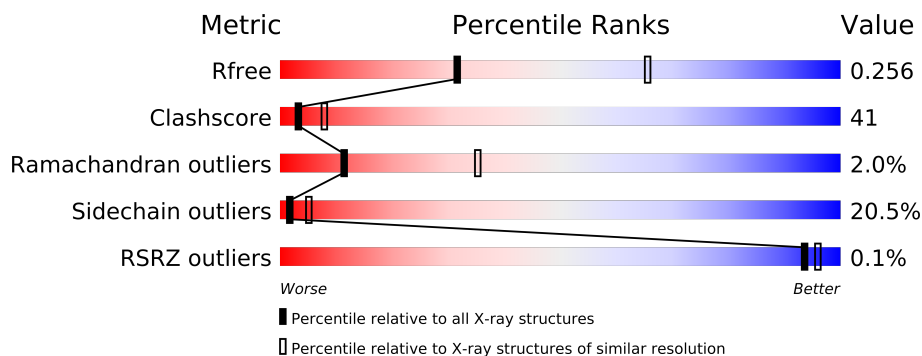
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 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))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1021	
1	B	1021	
1	C	1021	
1	D	1021	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	3002	-	X
2	MG	D	3002	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33805 atoms, of which 0 are hydrogen and 0 are deuterium.

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 BETA-GALACTOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1021	Total	C	N	O	S	84	7	0
			8238	5209	1466	1525	38			
1	B	1021	Total	C	N	O	S	84	7	0
			8238	5209	1466	1525	38			
1	C	1021	Total	C	N	O	S	84	7	0
			8238	5209	1466	1525	38			
1	D	1021	Total	C	N	O	S	84	7	0
			8238	5209	1466	1525	38			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is water.

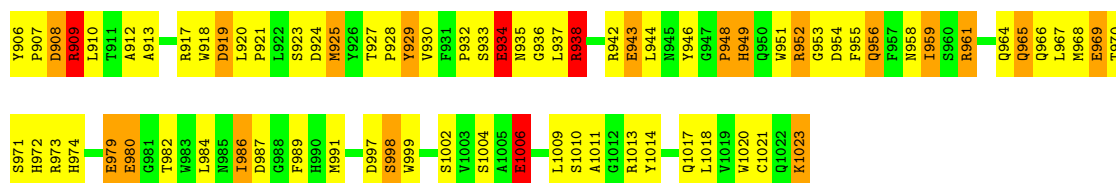
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	211	Total	O	0	0
			211	211		
3	B	202	Total	O	0	0
			202	202		
3	C	220	Total	O	0	0
			220	220		
3	D	212	Total	O	0	0
			212	212		













## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.40Å 173.40Å 204.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.80 24.97 – 2.82	Depositor EDS
% Data completeness (in resolution range)	88.0 (25.00-2.80) 80.5 (24.97-2.82)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 2.80Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, $R_{free}$	0.137 , 0.279 0.124 , 0.256	Depositor DCC
$R_{free}$ test set	1590 reflections (1.53%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.7	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 112.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 105768 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	33805	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.86 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.2179e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	1.11	56/8515 (0.7%)	1.72	186/11615 (1.6%)
1	B	1.09	53/8515 (0.6%)	1.69	174/11615 (1.5%)
1	C	1.08	49/8515 (0.6%)	1.69	187/11615 (1.6%)
1	D	1.10	54/8515 (0.6%)	1.70	183/11615 (1.6%)
All	All	1.09	212/34060 (0.6%)	1.70	730/46460 (1.6%)

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	2	0
1	B	1	0
1	C	4	1
1	D	1	0
All	All	8	1

The worst 5 of 212 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	249	GLU	CD-OE2	8.77	1.35	1.25
1	B	241	GLU	CD-OE2	8.07	1.34	1.25
1	C	508	GLU	CD-OE2	8.02	1.34	1.25
1	D	181	GLU	CD-OE2	7.94	1.34	1.25
1	A	198	GLU	CD-OE2	7.86	1.34	1.25

The worst 5 of 730 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	251	ARG	NE-CZ-NH2	-13.90	113.35	120.30
1	D	210	ARG	NE-CZ-NH1	13.54	127.07	120.30
1	D	425	ARG	NE-CZ-NH1	13.14	126.87	120.30
1	D	668	VAL	C-N-CD	-13.14	91.69	120.60
1	A	356	ARG	NE-CZ-NH1	13.13	126.87	120.30

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	166	ARG	CA
1	A	187	MET	CA
1	B	118	ASN	CA
1	C	291	LEU	CA
1	C	503	TYR	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	352	ARG	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8238	0	7824	643	0
1	B	8238	0	7824	695	0
1	C	8238	0	7824	667	0
1	D	8238	0	7823	632	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	211	0	0	13	0
3	B	202	0	0	12	0
3	C	220	0	0	24	0
3	D	212	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	33805	0	31295	2582	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 41.

The worst 5 of 2582 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:173:LEU:HB3	1:A:177:LEU:HD21	1.21	1.17
1:B:427:THR:HA	1:B:436:MET:HE1	1.26	1.14
1:B:734:SER:HB3	1:B:860:GLY:HA3	1.24	1.12
1:D:427:THR:HA	1:D:436:MET:HE1	1.32	1.11
1:A:777:LEU:HD21	1:A:889:ALA:HB2	1.28	1.10

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	1026/1021 (100%)	923 (90%)	86 (8%)	17 (2%)	14	42
1	B	1026/1021 (100%)	917 (89%)	89 (9%)	20 (2%)	12	37
1	C	1026/1021 (100%)	918 (90%)	82 (8%)	26 (2%)	9	28
1	D	1026/1021 (100%)	921 (90%)	85 (8%)	20 (2%)	12	37
All	All	4104/4084 (100%)	3679 (90%)	342 (8%)	83 (2%)	11	35

5 of 83 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	647	SER
1	A	733	ALA
1	A	734	SER
1	A	1005	ALA
1	B	79	PRO

### 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	880/873 (101%)	700 (80%)	180 (20%)	2	5
1	B	880/873 (101%)	690 (78%)	190 (22%)	1	4
1	C	880/873 (101%)	703 (80%)	177 (20%)	2	5
1	D	880/873 (101%)	709 (81%)	171 (19%)	2	6
All	All	3520/3492 (101%)	2802 (80%)	718 (20%)	2	5

5 of 718 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	789	LEU
1	C	165	SER
1	D	746	ASP
1	B	843	GLN
1	B	1004	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	597	ASN
1	C	221	GLN
1	D	693	GLN
1	B	622	HIS
1	B	965	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1021/1021 (100%)	-1.31	2 (0%) 93 95	2, 26, 68, 100	19 (1%)
1	B	1021/1021 (100%)	-1.21	0 100 100	4, 31, 72, 100	19 (1%)
1	C	1021/1021 (100%)	-1.25	1 (0%) 93 96	6, 28, 65, 100	19 (1%)
1	D	1021/1021 (100%)	-1.29	0 100 100	3, 26, 65, 100	19 (1%)
All	All	4084/4084 (100%)	-1.27	3 (0%) 93 96	2, 28, 68, 100	76 (1%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	733	ALA	2.6
1	C	732	ALA	2.2
1	A	734	SER	2.0

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	3002	1/1	0.12	4.87	31,31,31,31	0
2	MG	D	3002	1/1	0.10	2.13	25,25,25,25	0
2	MG	A	3001	1/1	0.10	0.33	28,28,28,28	0
2	MG	B	3002	1/1	0.07	-0.18	36,36,36,36	0
2	MG	C	3002	1/1	0.07	-0.43	31,31,31,31	0
2	MG	D	3001	1/1	0.07	-0.67	40,40,40,40	0
2	MG	B	3001	1/1	0.04	-1.66	20,20,20,20	0
2	MG	C	3001	1/1	0.03	-2.11	15,15,15,15	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.