



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:26 AM GMT

PDB ID : 2QR6  
Title : Crystal structure of IMP dehydrogenase/GMP reductase-like protein (NP\_599840.1) from Corynebacterium glutamicum ATCC 13032 Kitasato at 1.50 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2007-07-27  
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) 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

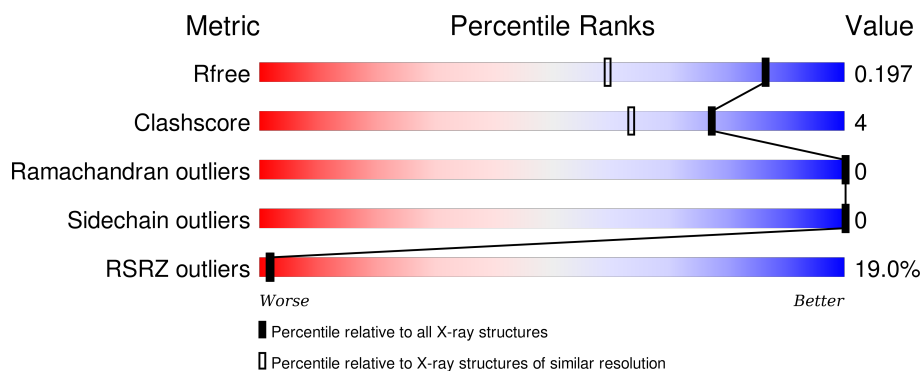
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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))
$R_{free}$	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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. 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  $\leq 5\%$ . 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	393	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3147 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 IMP dehydrogenase/GMP reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	371	2862	1819	491	538	2	12	0	25	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MSE	-	LEADER SEQUENCE	UNP Q8NSR4
A	-17	GLY	-	LEADER SEQUENCE	UNP Q8NSR4
A	-16	SER	-	LEADER SEQUENCE	UNP Q8NSR4
A	-15	ASP	-	LEADER SEQUENCE	UNP Q8NSR4
A	-14	LYS	-	LEADER SEQUENCE	UNP Q8NSR4
A	-13	ILE	-	LEADER SEQUENCE	UNP Q8NSR4
A	-12	HIS	-	LEADER SEQUENCE	UNP Q8NSR4
A	-11	HIS	-	LEADER SEQUENCE	UNP Q8NSR4
A	-10	HIS	-	LEADER SEQUENCE	UNP Q8NSR4
A	-9	HIS	-	LEADER SEQUENCE	UNP Q8NSR4
A	-8	HIS	-	LEADER SEQUENCE	UNP Q8NSR4
A	-7	HIS	-	LEADER SEQUENCE	UNP Q8NSR4
A	-6	GLU	-	LEADER SEQUENCE	UNP Q8NSR4
A	-5	ASN	-	LEADER SEQUENCE	UNP Q8NSR4
A	-4	LEU	-	LEADER SEQUENCE	UNP Q8NSR4
A	-3	TYR	-	LEADER SEQUENCE	UNP Q8NSR4
A	-2	PHE	-	LEADER SEQUENCE	UNP Q8NSR4
A	-1	GLN	-	LEADER SEQUENCE	UNP Q8NSR4
A	0	GLY	-	LEADER SEQUENCE	UNP Q8NSR4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	285	Total	O	0	0
			285	285		



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.13Å 127.13Å 54.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.66 – 1.50 29.66 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.66-1.50) 99.4 (29.66-1.50)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.169 , 0.188 0.176 , 0.197	Depositor DCC
$R_{free}$ test set	3530 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.4	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 57.4	EDS
Estimated twinning fraction	0.028 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 69853 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3147	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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	0.82	0/2978	0.94	8/4028 (0.2%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	A	128	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	A	373[A]	VAL	CB-CA-C	6.26	123.30	111.40
1	A	373[B]	VAL	CB-CA-C	6.26	123.30	111.40
1	A	133	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	353	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	314	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	242	ASP	CB-CG-OD2	-5.04	113.76	118.30

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	2862	0	2860	21	0
2	A	285	0	0	0	0
All	All	3147	0	2860	21	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 4.

All (21) 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:A:267:ILE:HD13	1:A:284[A]:VAL:HG13	1.73	0.70
1:A:267:ILE:HD13	1:A:284[A]:VAL:CG1	2.23	0.68
1:A:340[A]:MSE:HE2	1:A:342[A]:TRP:CZ3	2.33	0.64
1:A:197:ALA:HB1	1:A:209[B]:MSE:HE1	1.79	0.63
1:A:162[A]:LEU:HD23	1:A:194:PRO:HG2	1.83	0.59
1:A:220:GLY:HA3	1:A:236[B]:MSE:HE1	1.88	0.56
1:A:236[A]:MSE:HE2	1:A:265:GLY:O	2.06	0.55
1:A:170:ILE:HG23	1:A:209[A]:MSE:HE3	1.90	0.54
1:A:-5:ASN:O	1:A:-1:GLN:HG3	2.09	0.53
1:A:52[A]:MSE:HE3	1:A:76:VAL:HG21	1.94	0.50
1:A:22:ILE:HG22	1:A:373[B]:VAL:HG22	1.97	0.47
1:A:340[A]:MSE:HE2	1:A:342[A]:TRP:CE3	2.50	0.47
1:A:197:ALA:HB1	1:A:209[B]:MSE:CE	2.46	0.46
1:A:340[A]:MSE:HE2	1:A:342[A]:TRP:HZ3	1.77	0.45
1:A:142:ARG:HA	1:A:164:VAL:O	2.17	0.45
1:A:143:VAL:HG21	1:A:148:VAL:HG23	1.97	0.45
1:A:122:THR:HG21	1:A:154:ILE:HD13	1.99	0.44
1:A:170:ILE:CG2	1:A:209[B]:MSE:HE2	2.48	0.44
1:A:170:ILE:HG23	1:A:209[B]:MSE:HE2	2.01	0.42
1:A:105:GLN:NE2	1:A:317:VAL:O	2.53	0.42
1:A:172:ALA:HA	1:A:209[B]:MSE:SE	2.70	0.41

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	390/393 (99%)	389 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

### 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	293/297 (99%)	293 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	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

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	363/393 (92%)	1.23	69 (19%) <b>2</b> <b>2</b>	21, 31, 51, 75	5 (1%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	177	THR	15.2
1	A	-3	TYR	12.6
1	A	321	VAL	11.0
1	A	183	ASN	8.2
1	A	326	ALA	7.5
1	A	176	ASN	7.0
1	A	-2	PHE	5.3
1	A	98	ALA	5.1
1	A	106	ALA	4.9
1	A	175	VAL	4.7
1	A	-4	LEU	4.6
1	A	-1	GLN	4.4
1	A	342[A]	TRP	4.2
1	A	87	ALA	4.2
1	A	284[A]	VAL	3.9
1	A	77	ILE	3.9
1	A	262	ILE	3.7
1	A	110	ARG	3.7
1	A	2	ARG	3.7
1	A	218	ILE	3.5
1	A	150[A]	GLU	3.5
1	A	97	ILE	3.5
1	A	320	SER	3.4
1	A	162[A]	LEU	3.3
1	A	186	GLU	3.3
1	A	286	LEU	3.3
1	A	101[A]	GLU	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	105	GLN	3.2
1	A	88	ASP	3.2
1	A	102	GLU	3.1
1	A	196	ILE	3.1
1	A	76	VAL	3.1
1	A	91	GLU	3.0
1	A	339	THR	2.9
1	A	189	GLY	2.9
1	A	219	VAL	2.9
1	A	374	ASN	2.9
1	A	104	ASP	2.8
1	A	4	HIS	2.7
1	A	192	ASP	2.7
1	A	99	ALA	2.7
1	A	267	ILE	2.7
1	A	230	LEU	2.7
1	A	276	ALA	2.7
1	A	184	LEU	2.6
1	A	243	VAL	2.6
1	A	-5	ASN	2.6
1	A	154	ILE	2.5
1	A	107	ALA	2.4
1	A	148	VAL	2.4
1	A	164	VAL	2.4
1	A	187	PHE	2.4
1	A	174	HIS	2.4
1	A	74	LEU	2.4
1	A	100	TYR	2.4
1	A	316	VAL	2.4
1	A	301	TYR	2.3
1	A	221	GLY	2.3
1	A	302	PHE	2.3
1	A	27	SER	2.3
1	A	3	ASP	2.3
1	A	310	PRO	2.3
1	A	103	GLY	2.3
1	A	240	ILE	2.3
1	A	94	ALA	2.2
1	A	327	ALA	2.2
1	A	40	TRP	2.1
1	A	59	LEU	2.1
1	A	330	LEU	2.1

## 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.