



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:42 PM GMT

PDB ID : 4A8R  
Title : PROTEIN CRYSTALLIZATION AND MICROGRAVITY: GLUCOSE ISOMERASE CRYSTALS GROWN DURING THE PCDF-PROTEIN MISSION  
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Deposited on : 2011-11-21  
Resolution : 1.42 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](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.

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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 : 1.7 (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

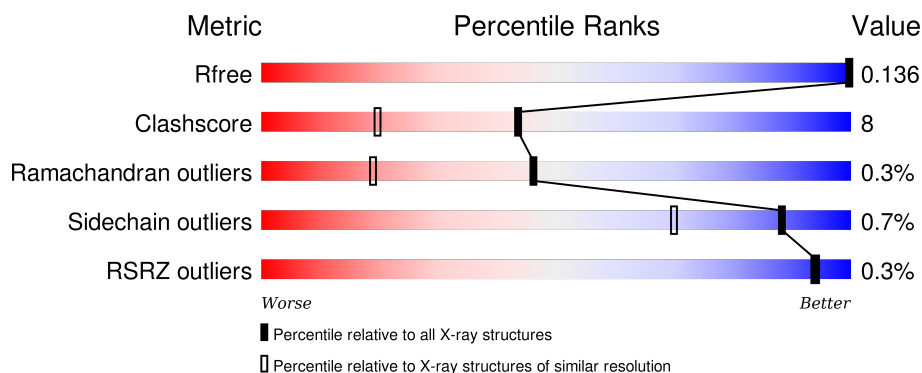
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 1.42 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	1632 (1.44-1.40)
Clashscore	102246	1743 (1.44-1.40)
Ramachandran outliers	100387	1698 (1.44-1.40)
Sidechain outliers	100360	1697 (1.44-1.40)
RSRZ outliers	91569	1632 (1.44-1.40)

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	388	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	1388[A]	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	1388[B]	-	-	-	X
3	CO	A	1390	-	-	-	X
3	CO	A	1391	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3655 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 XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	26	0
			3166	2008	558	591	9			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	1
			12	6	6		
2	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Co	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	457	Total 471	O 471	0	14



- Molecule 1: XYLOSE ISOMERASE

MET  
 N2  
 Y3  
 Q4  
 D24  
 P25  
 F26  
 R31  
 E38  
 R42  
 H49  
 G50  
 V51  
 D65  
 R68  
 E69  
 E70  
 R76  
 M84  
 K85  
 Y86  
 P87  
 D110  
 R121  
 E128  
 E132  
 M158  
 V169  
 R177  
 E181  
 P184  
 N185  
 E186  
 P187  
 R188  
 E204  
 E207  
 R208  
 Y012

M250  
 K253  
 Y254  
 D255  
 Q256  
 D257  
 R266  
 Y280  
 R284  
 D297  
 P324  
 E325  
 E328  
 E337  
 R340  
 E358  
 V362  
 R368  
 R374  
 G385  
 A386  
 R387  
 GLY

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.53Å 98.22Å 102.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.77 – 1.42 24.55 – 1.42	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.77-1.42) 100.0 (24.55-1.42)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.77 (at 1.42Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.103 , 0.130 0.111 , 0.136	Depositor DCC
$R_{free}$ test set	4334 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	6.9	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 50.7	EDS
Estimated twinning fraction	0.013 for -h,-l,-k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 87039 reflections	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	3655	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.87% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	1.26	18/3305 (0.5%)	1.14	19/4472 (0.4%)

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	2

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	358	GLU	CB-CG	8.62	1.68	1.52
1	A	280	TYR	CD1-CE1	7.83	1.51	1.39
1	A	280	TYR	CE2-CZ	-7.22	1.29	1.38
1	A	266	ARG	CZ-NH2	-6.65	1.24	1.33
1	A	358	GLU	CD-OE1	-6.64	1.18	1.25

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	ARG	NE-CZ-NH1	-10.22	115.19	120.30
1	A	255	ASP	CB-CG-OD1	9.42	126.78	118.30
1	A	374	ARG	NE-CZ-NH2	8.31	124.45	120.30
1	A	208	ARG	NE-CZ-NH1	-7.21	116.70	120.30
1	A	257	ASP	CB-CG-OD1	7.19	124.77	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	250	ASN	Mainchain
1	A	76	ARG	Sidechain

## 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	3166	0	3076	44	0
2	A	16	0	19	7	0
3	A	2	0	0	0	0
4	A	471	0	0	32	2
All	All	3655	0	3095	51	2

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 8.

The worst 5 of 51 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:368[B]:ARG:HH11	1:A:368[B]:ARG:CB	0.98	1.59
2:A:1388[A]:GOL:H32	4:A:2318:HOH:O	1.18	1.31
1:A:368[B]:ARG:HB3	1:A:368[B]:ARG:NH1	1.00	1.30
1:A:368[B]:ARG:HH11	1:A:368[B]:ARG:CG	1.64	1.10
1:A:358:GLU:OE1	4:A:2422[B]:HOH:O	1.68	1.10

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2082:HOH:O	4:A:2341:HOH:O[4_555]	2.12	0.08
4:A:2273:HOH:O	4:A:2314:HOH:O[3_555]	2.18	0.02

## 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	410/388 (106%)	394 (96%)	14 (3%)	2 (0%)	34	9

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186[A]	GLU
1	A	186[B]	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	321/304 (106%)	318 (99%)	3 (1%)	84	62

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51[A]	VAL
1	A	51[B]	VAL
1	A	185	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	ASN

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Mol	Chain	Res	Type
1	A	348	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](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GOL	A	1388[A]	-	5,5,5	0.81	0	5,5,5	1.11	0
2	GOL	A	1388[B]	-	5,5,5	0.89	0	5,5,5	0.81	0
2	GOL	A	1389	3	3,3,5	0.96	0	2,2,5	0.98	0

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	GOL	A	1388[A]	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1388[B]	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	1389	3	-	0/1/1/4	0/0/0/0

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.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1388[A]	GOL	3	0
2	A	1388[B]	GOL	2	0
2	A	1389	GOL	2	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](#)

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	386/388 (99%)	-0.69	1 (0%) 94 94	4, 8, 17, 27	19 (4%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ASN	3.4

### 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](#)

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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CO	A	1391	1/1	1.00	0.22	29.84	21,21,21,21	0
3	CO	A	1390	1/1	1.00	0.16	23.12	14,14,14,14	0
2	GOL	A	1388[A]	6/6	0.95	0.10	2.58	9,10,16,17	6
2	GOL	A	1388[B]	6/6	0.95	0.10	2.39	11,16,18,19	6
2	GOL	A	1389	4/6	0.97	0.06	1.71	9,9,12,16	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.