

wwPDB X-ray Structure Validation Summary Report (i)

Jan 27, 2024 - 08:31 PM EST

PDB ID	:	1DEA
Title	:	STRUCTURE AND CATALYTIC MECHANISM OF GLUCOSAMINE
		6-PHOSPHATE DEAMINASE FROM ESCHERICHIA COLI AT 2.1
		ANGSTROMS RESOLUTION
Authors	:	Oliva, G.; Fontes, M.R.M.; Garratt, R.C.; Altamirano, M.M.; Calcagno, M.L.;
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Deposited on	:	1995-09-13
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:

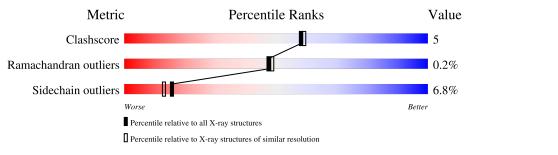
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	А	266	81%	15%	•••
1	В	266	86%	11%	••



1DEA

2 Entry composition (i)

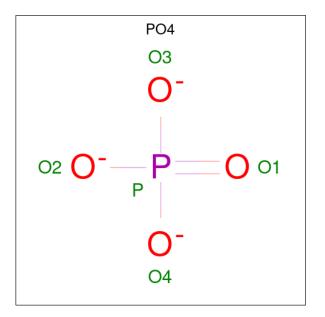
There are 3 unique types of molecules in this entry. The entry contains 4552 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUCOSAMINE 6-PHOSPHATE DEAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	266	Total	С	Ν	0	\mathbf{S}	0	0	0
	200	2092	1328	364	386	14	0	0	0	
1	1 B	266	Total	С	Ν	0	S	0	0	0
			2092	1328	364	386	14	0	0	0

• Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	TotalOP541	0	0
2	А	1	TotalOP541	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0



• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	169	Total O 169 169	0	0
3	В	179	Total O 179 179	0	0

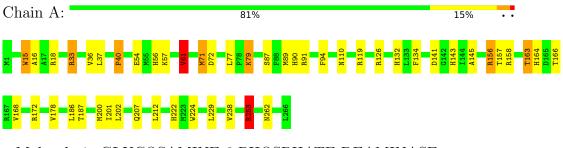


3 Residue-property plots (i)

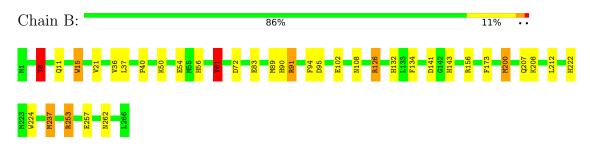
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

Note EDS was not executed.

• Molecule 1: GLUCOSAMINE 6-PHOSPHATE DEAMINASE



• Molecule 1: GLUCOSAMINE 6-PHOSPHATE DEAMINASE





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	H 3 2	Depositor	
Cell constants	125.71Å 125.71Å 222.87Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	6.00 - 2.10	Depositor	
% Data completeness	(Not available) (6.00-2.10)	Depositor	
(in resolution range)			
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	X-PLOR	Depositor	
R, R_{free}	0.174 , (Not available)	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	4552	wwPDB-VP	
Average B, all atoms $(Å^2)$	24.0	wwPDB-VP	



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: PO4

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		
INIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.68	0/2139	1.26	19/2898~(0.7%)	
1	В	0.69	0/2139	1.27	18/2898~(0.6%)	
All	All	0.68	0/4278	1.27	37/5796~(0.6%)	

There are no bond length outliers.

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	156	ARG	NE-CZ-NH2	-12.27	114.16	120.30
1	В	95	ASP	CB-CG-OD1	9.50	126.85	118.30
1	В	91	ARG	NE-CZ-NH2	-9.25	115.67	120.30
1	А	156	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	В	224	TRP	CD1-CG-CD2	7.82	112.55	106.30

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	А	2092	0	2081	28	0
1	В	2092	0	2081	12	0
2	А	10	0	0	0	0
2	В	10	0	0	0	0

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Mol	3	Non-H	1 0	H(added)	Clashes	Symm-Clashes
3	А	169	0	0	5	0
3	В	179	0	0	2	0
All	All	4552	0	4162	40	0

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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 5.

The worst 5 of 40 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:200:MET:HE3	1:A:238:VAL:HG21	1.58	0.85
1:A:36:VAL:H	1:A:132:HIS:HD2	1.34	0.73
1:A:200:MET:SD	3:A:406:HOH:O	2.52	0.66
1:B:36:VAL:H	1:B:132:HIS:HD2	1.40	0.66
1:A:253:ARG:HB2	1:A:253:ARG:HH11	1.64	0.63

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	Percentiles	
1	А	264/266~(99%)	252 (96%)	11 (4%)	1 (0%)	34 32	
1	В	264/266~(99%)	254 (96%)	10 (4%)	0	100 100	
All	All	528/532~(99%)	506 (96%)	21 (4%)	1 (0%)	47 49	

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	40	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 Outliers		Percentiles		
1	А	227/227~(100%)	212~(93%)	15 (7%)	16 14		
1	В	227/227~(100%)	211 (93%)	16 (7%)	15 12		
All	All	454/454~(100%)	423~(93%)	31 (7%)	16 13		

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	253	ARG
1	В	222	HIS
1	В	40	PRO
1	В	253	ARG
1	В	207	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	213	GLN
1	В	132	HIS
1	В	56	HIS
1	В	22	ASN
1	В	90	HIS

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)

4 ligands are modelled in this entry.

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 Ch		Chain	Chain Res	Link	Bond lengths			Bond angles		
	Type	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	PO4	А	268	-	4,4,4	2.57	3 (75%)	6,6,6	0.39	0
2	PO4	В	267	-	4,4,4	2.96	3 (75%)	6,6,6	0.48	0
2	PO4	А	267	-	4,4,4	2.84	3 (75%)	6,6,6	0.52	0
2	PO4	В	268	-	4,4,4	2.57	3 (75%)	6,6,6	0.45	0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
2	В	267	PO4	P-O3	-3.37	1.44	1.54
2	В	267	PO4	P-O2	-3.23	1.44	1.54
2	А	267	PO4	P-O3	-3.22	1.44	1.54
2	В	267	PO4	P-04	-3.08	1.45	1.54
2	А	267	PO4	P-O2	-3.07	1.45	1.54

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 (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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

