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Full wwPDB X-ray Structure Validation Report (i)

Sep 27, 2017 – 04:49 AM EDT

PDB ID	:	1FSF
Title	:	GLUCOSAMINE-6-PHOSPHATE DEAMINASE FROM E.COLI, T CONFORMER, AT 1.9A RESOLUTION
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Deposited on	:	unknown
Resolution	:	1.90 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

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 1.90 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.

| Percentile relative to all X-ray structures |
| Percentile relative to X-ray structures of similar resolution |
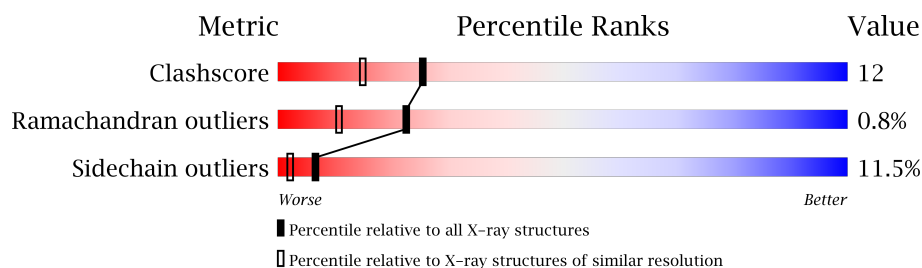
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)

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 >=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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	266	77% 16% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2390 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	A	266	Total	C	N	O	S	0	0	0
			2092	1328	364	386	14			

- Molecule 2 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	298	Total	O	0	0
			298	298		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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

Chain A:
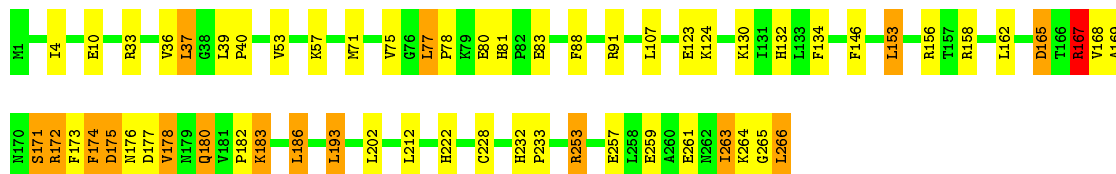
4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	126.68Å 126.68Å 139.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.90	Depositor
% Data completeness (in resolution range)	92.1 (50.00-1.90)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, SHELXL-97	Depositor
R, R_{free}	0.183 , 0.232	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2390	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	0.57	1/2139 (0.0%)	1.10	10/2898 (0.3%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	LEU	C-OXT	17.80	1.57	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	ARG	NE-CZ-NH2	-8.69	115.96	120.30
1	A	88	PHE	CB-CG-CD1	8.55	126.78	120.80
1	A	33	ARG	NE-CZ-NH1	8.19	124.40	120.30
1	A	167	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	88	PHE	CB-CG-CD2	-6.59	116.19	120.80
1	A	167	ARG	CD-NE-CZ	6.14	132.20	123.60
1	A	91	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	158	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	A	193	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	156	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	PHE	Peptide

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	2092	0	2081	50	0
2	A	298	0	0	2	0
All	All	2390	0	2081	50	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 12.

All (50) 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:36:VAL:H	1:A:132:HIS:HD2	1.20	0.89
1:A:81:HIS:HD2	1:A:83:GLU:H	1.32	0.76
1:A:162:LEU:HB2	1:A:167:ARG:HH11	1.50	0.74
1:A:162:LEU:HB2	1:A:167:ARG:HD3	1.73	0.70
1:A:174:PHE:O	1:A:177:ASP:HB3	1.91	0.70
1:A:171:SER:OG	1:A:178:VAL:HG13	1.94	0.67
1:A:77:LEU:HD22	1:A:78:PRO:HD2	1.76	0.66
1:A:167:ARG:HH21	1:A:183:LYS:HE3	1.64	0.62
1:A:81:HIS:CD2	1:A:83:GLU:H	2.15	0.61
1:A:172:ARG:HA	1:A:176:ASN:HA	1.83	0.59
1:A:265:GLY:O	1:A:266:LEU:HB2	2.05	0.57
1:A:107:LEU:HD13	1:A:186:LEU:HB3	1.89	0.54
1:A:53:VAL:O	1:A:57:LYS:HG3	2.10	0.52
1:A:81:HIS:CD2	1:A:83:GLU:HB2	2.44	0.52
1:A:162:LEU:CB	1:A:167:ARG:HH11	2.19	0.50
1:A:83:GLU:HG3	1:A:173:PHE:HB3	1.93	0.50
1:A:172:ARG:HG3	1:A:173:PHE:N	2.27	0.49
1:A:174:PHE:CZ	1:A:182:PRO:HD3	2.47	0.49
1:A:36:VAL:H	1:A:132:HIS:CD2	2.13	0.49
1:A:172:ARG:HG3	1:A:173:PHE:CD2	2.48	0.48
1:A:259:GLU:O	1:A:263:ILE:HD13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LEU:HD13	1:A:39:LEU:HD21	1.93	0.48
1:A:180:GLN:HA	1:A:180:GLN:NE2	2.28	0.47
1:A:171:SER:CB	1:A:178:VAL:HG22	2.45	0.46
1:A:165:ASP:OD1	1:A:165:ASP:N	2.49	0.46
1:A:162:LEU:O	1:A:167:ARG:NH1	2.49	0.46
1:A:167:ARG:NH2	1:A:183:LYS:HG3	2.31	0.45
1:A:171:SER:HB3	1:A:178:VAL:CA	2.45	0.45
1:A:172:ARG:HG3	1:A:173:PHE:H	1.82	0.45
1:A:172:ARG:HA	1:A:176:ASN:CA	2.46	0.45
1:A:171:SER:CB	1:A:178:VAL:HG13	2.47	0.45
1:A:162:LEU:HB2	1:A:167:ARG:NH1	2.26	0.44
1:A:183:LYS:HA	1:A:183:LYS:HD2	1.58	0.44
1:A:232:HIS:CG	1:A:233:PRO:HD2	2.53	0.44
1:A:171:SER:HB3	1:A:178:VAL:HA	2.00	0.44
1:A:162:LEU:CA	1:A:167:ARG:HH11	2.31	0.44
1:A:168:VAL:HG12	1:A:169:ALA:N	2.32	0.44
1:A:57:LYS:HE2	2:A:555:HOH:O	2.18	0.44
1:A:146:PHE:CE1	1:A:162:LEU:HD22	2.53	0.43
1:A:172:ARG:HA	1:A:176:ASN:ND2	2.33	0.43
1:A:75:VAL:CG2	1:A:186:LEU:HD13	2.49	0.43
1:A:253:ARG:O	1:A:257:GLU:HG3	2.19	0.42
1:A:167:ARG:HH21	1:A:183:LYS:HG3	1.85	0.42
1:A:153:LEU:HD21	1:A:228:CYS:SG	2.60	0.41
1:A:71:MET:HE1	2:A:313:HOH:O	2.20	0.41
1:A:77:LEU:HD22	1:A:78:PRO:CD	2.48	0.41
1:A:4:ILE:HD12	1:A:259:GLU:HG2	2.03	0.41
1:A:172:ARG:HA	1:A:176:ASN:HD22	1.85	0.41
1:A:162:LEU:N	1:A:167:ARG:NH1	2.69	0.40
1:A:183:LYS:N	1:A:183:LYS:HD2	2.30	0.40

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	A	264/266 (99%)	254 (96%)	8 (3%)	2 (1%)	22	11

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	ASP
1	A	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	A	227/227 (100%)	201 (88%)	26 (12%)	6	2

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	37	LEU
1	A	77	LEU
1	A	80	GLU
1	A	123	GLU
1	A	124	LYS
1	A	130	LYS
1	A	134	PHE
1	A	153	LEU
1	A	165	ASP
1	A	167	ARG
1	A	171	SER
1	A	172	ARG
1	A	175	ASP
1	A	178	VAL
1	A	180	GLN
1	A	183	LYS
1	A	186	LEU
1	A	193	LEU

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Mol	Chain	Res	Type
1	A	202	LEU
1	A	212	LEU
1	A	222	HIS
1	A	253	ARG
1	A	261	GLU
1	A	263	ILE
1	A	264	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	60	GLN
1	A	81	HIS
1	A	132	HIS
1	A	176	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 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 (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.