

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	7XHL
Title	:	Complex structure of a Glucose 6-Phosphate Dehydrogenase from Zymomonas
		mobilis
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Deposited on	:	2022-04-08
Resolution	:	3.25 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)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
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 3.25 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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% 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	Quali	ity of chain	
1	А	487	41%	47%	11% •
1	В	487	4%	43%	12% •
1	С	487	3% 56%	34%	5% 5%
1	D	487	^{2%} 46%	45%	7% •
1	Е	487	44%	45%	9% •
1	F	487	46%	40%	8% 5%



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Mol	Chain	Length	Qua	ality of chain	
1	G	487	.% • 44%	49%	7%
1	Н	487	.% • 44%	46%	9% •

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	NMN	А	501	-	-	Х	-
2	NMN	В	501	-	-	Х	Х



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 28376 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	489	Total	С	Ν	0	\mathbf{S}	0	0	0
	A	402	3712	2357	647	698	10	0	0	0
1	В	470	Total	С	Ν	0	S	0	0	0
1	D	419	3625	2294	633	689	9	0	0	0
1	С	463	Total	С	Ν	0	S	0	Ο	0
1	U	405	3027	1896	552	573	6	0	0	0
1	л	470	Total	С	Ν	Ο	\mathbf{S}	0	0	0
L	D	415	3545	2250	606	679	10	0	0	0
1	F	476	Total	С	Ν	Ο	\mathbf{S}	0	0	0
L	Ľ	470	3587	2276	621	681	9	0	0	0
1	F	469	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
L	Ľ	402	3378	2135	600	634	9	0	0	0
1	C	485	Total	С	Ν	0	\mathbf{S}	0	0	0
	G	405	3735	2366	649	710	10	0	0	0
1	Ц	481	Total	С	Ν	0	S	0	0	0
	11	401	3679	2336	634	699	10	0	0	

• Molecule 1 is a protein called Glucose 6-Phosphate Dehydrogenase.

• Molecule 2 is BETA-NICOTINAMIDE RIBOSE MONOPHOSPHATE (three-letter code: NMN) (formula: $C_{11}H_{16}N_2O_8P$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
9	Δ	1	Total	С	Ν	0	Р	0	0	
	Л	L	22	11	2	8	1	0	0	
0	р	1	1 Total C N O P		0					
	D	1	22	11	2	8	1	0	0	
0	F	1	Total	С	Ν	0	Р	0	0	
		L	22	11	2	8	1	0	0	
0	C	1	Total	С	Ν	Ο	Р	0	0	
2	G		22	11	2	8	1	0	U	



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 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.



• Molecule 1: Glucose 6-Phosphate Dehydrogenase



















• Molecule 1: Glucose 6-Phosphate Dehydrogenase









• Molecule 1: Glucose 6-Phosphate Dehydrogenase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	80.32Å 342.33Å 103.36Å	Deperitor
a, b, c, α , β , γ	90.00° 92.66° 90.00°	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	78.11 - 3.25	Depositor
Resolution (A)	88.41 - 3.25	EDS
% Data completeness	98.8 (78.11-3.25)	Depositor
(in resolution range)	83.3 (88.41-3.25)	EDS
R _{merge}	0.15	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.80 (at 3.26 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D	0.237 , 0.297	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.250 , 0.283	DCC
R_{free} test set	4294 reflections $(4.98%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	66.7	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 66.9	EDS
L-test for twinning ²	$< L > = 0.39, < L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.105 for h,-k,-l	Xtriage
Reported twinning fraction	0.200 for h,-k,-l	Depositor
Outliers	0 of 86165 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	28376	wwPDB-VP
Average B, all atoms $(Å^2)$	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: NMN

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
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.56	0/3790	0.79	0/5146
1	В	0.55	0/3696	0.82	0/5028
1	С	0.53	0/3079	0.78	0/4224
1	D	0.55	0/3620	0.81	0/4945
1	Ε	0.56	0/3660	0.80	0/4983
1	F	0.58	0/3444	0.81	0/4692
1	G	0.52	0/3810	0.78	0/5173
1	H	0.54	0/3754	0.79	0/5104
All	All	0.55	0/28853	0.80	0/39295

There are no bond length outliers.

There are no bond angle outliers.

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	3712	0	3640	246	0
1	В	3625	0	3513	271	0
1	С	3027	0	2453	157	0
1	D	3545	0	3326	204	0
1	Е	3587	0	3445	257	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3378	0	3145	213	0
1	G	3735	0	3668	223	0
1	Н	3679	0	3590	268	0
2	А	22	0	14	16	0
2	В	22	0	14	7	0
2	Е	22	0	14	4	0
2	G	22	0	14	5	0
All	All	28376	0	26836	1754	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 32.

The worst 5 of 1754 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:E:54:PHE:CD2	1:E:84:PHE:HA	1.76	1.21
1:E:54:PHE:CE2	1:E:84:PHE:HA	1.84	1.13
1:A:144:LYS:HE3	2:A:501:NMN:C6	1.78	1.12
1:E:54:PHE:HE2	1:E:84:PHE:CB	1.63	1.11
1:E:54:PHE:HE2	1:E:84:PHE:HB3	1.10	1.10

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	Perce	entiles
1	А	480/487~(99%)	446 (93%)	34 (7%)	0	100	100
1	В	473/487~(97%)	438 (93%)	35 (7%)	0	100	100
1	С	457/487~(94%)	408 (89%)	49 (11%)	0	100	100
1	D	475/487 (98%)	430 (90%)	45 (10%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	Ε	470/487~(96%)	423 (90%)	45 (10%)	2~(0%)	34	67
1	F	452/487~(93%)	413 (91%)	39~(9%)	0	100	100
1	G	483/487~(99%)	453~(94%)	30~(6%)	0	100	100
1	Н	477/487~(98%)	431 (90%)	46 (10%)	0	100	100
All	All	3767/3896~(97%)	3442 (91%)	323 (9%)	2~(0%)	51	82

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All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Е	57	PHE
1	Е	117	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	386/409~(94%)	304 (79%)	82 (21%)	1	4
1	В	372/409~(91%)	301 (81%)	71 (19%)	1	6
1	С	214/409~(52%)	182 (85%)	32 (15%)	3	12
1	D	352/409~(86%)	295~(84%)	57 (16%)	2	10
1	Е	364/409~(89%)	294 (81%)	70 (19%)	1	6
1	F	321/409~(78%)	263~(82%)	58 (18%)	1	7
1	G	392/409~(96%)	320~(82%)	72 (18%)	1	7
1	Н	383/409~(94%)	317 (83%)	66 (17%)	2	9
All	All	2784/3272 (85%)	2276 (82%)	508 (18%)	1	7

 $5~{\rm of}~508$ residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	D	380	SER
1	Н	16	ASP



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Mol	Chain	Res	Type
1	Е	335	ARG
1	G	473	ILE
1	Н	186	THR

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such side chains are listed below:

Mol	Chain	Res	Type
1	Н	19	GLN
1	Н	346	GLN
1	D	378	GLN
1	D	205	HIS
1	Н	394	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	Type	Chain	Ros	Link	Bond lengths			Bond angles		
	Ullalli	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
2	NMN	В	501	-	22,23,23	0.91	2 (9%)	30,34,34	1.07	3 (10%)



Mol Type		Chain	Dec	Bood lengths				Bond angles		
MOI	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NMN	G	501	-	22,23,23	0.88	1 (4%)	30,34,34	1.14	3 (10%)
2	NMN	Е	501	-	22,23,23	0.81	2 (9%)	30,34,34	1.09	3 (10%)
2	NMN	А	501	-	22,23,23	0.86	1 (4%)	30,34,34	1.18	4 (13%)

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	NMN	В	501	-	-	2/14/30/30	0/2/2/2
2	NMN	G	501	-	-	1/14/30/30	0/2/2/2
2	NMN	Е	501	-	-	6/14/30/30	0/2/2/2
2	NMN	А	501	-	-	2/14/30/30	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
2	В	501	NMN	O4R-C1R	2.87	1.45	1.41
2	В	501	NMN	C2-N1	2.51	1.38	1.35
2	G	501	NMN	C2-N1	2.40	1.37	1.35
2	Е	501	NMN	C2-N1	2.36	1.37	1.35
2	А	501	NMN	O4R-C1R	2.35	1.44	1.41

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	G	501	NMN	O3R-C3R-C2R	-3.81	99.49	111.82
2	В	501	NMN	C6-N1-C2	-3.02	119.22	121.97
2	Е	501	NMN	C3-C2-N1	-2.87	117.63	120.43
2	Е	501	NMN	C2-C3-C4	2.60	121.21	118.26
2	А	501	NMN	C6-N1-C2	-2.43	119.76	121.97

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	501	NMN	O4R-C1R-N1-C2
2	Е	501	NMN	O4R-C1R-N1-C2
2	Е	501	NMN	O4R-C1R-N1-C6



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Mol	Chain	Res	Type	Atoms
2	Е	501	NMN	C2R-C1R-N1-C2
2	Е	501	NMN	C2R-C1R-N1-C6

There are no ring outliers.

4 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	501	NMN	7	0
2	G	501	NMN	5	0
2	Е	501	NMN	4	0
2	А	501	NMN	16	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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^{th} 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	$OWAB(Å^2)$	Q<0.9
1	А	482/487~(98%)	0.13	7 (1%) 73 71	31, 65, 96, 135	0
1	В	479/487~(98%)	0.20	18 (3%) 40 37	26, 63, 129, 151	0
1	С	463/487~(95%)	0.12	14 (3%) 50 48	49, 95, 152, 209	0
1	D	479/487~(98%)	0.15	12 (2%) 57 53	48, 83, 113, 166	0
1	E	476/487~(97%)	0.19	12 (2%) 57 53	40, 81, 116, 139	0
1	F	462/487~(94%)	0.40	36 (7%) 13 12	42, 82, 173, 204	0
1	G	485/487~(99%)	0.10	4 (0%) 86 86	27, 64, 103, 142	0
1	Н	481/487~(98%)	0.10	3 (0%) 89 89	33, 68, 106, 137	0
All	All	3807/3896~(97%)	0.17	106 (2%) 53 50	26, 76, 130, 209	0

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	133	LEU	6.7
1	С	14	THR	6.3
1	В	75	ALA	5.1
1	А	109	GLY	5.1
1	С	25	ALA	4.7

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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	$B-factors(A^2)$	Q<0.9
2	NMN	В	501	22/22	0.75	0.43	87,100,104,172	0
2	NMN	Е	501	22/22	0.85	0.23	76,88,102,162	0
2	NMN	А	501	22/22	0.89	0.24	66,73,78,87	0
2	NMN	G	501	22/22	0.91	0.23	59,71,81,92	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.















6.5 Other polymers (i)

There are no such residues in this entry.

