



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:38 am BST

PDB ID : 3PHL
Title : The apo-form UDP-glucose 6-dehydrogenase
Authors : Chen, Y.Y.; Ko, T.P.; Lin, C.H.; Chen, W.H.; Wang, A.H.J.
Deposited on : 2010-11-04
Resolution : 1.90 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

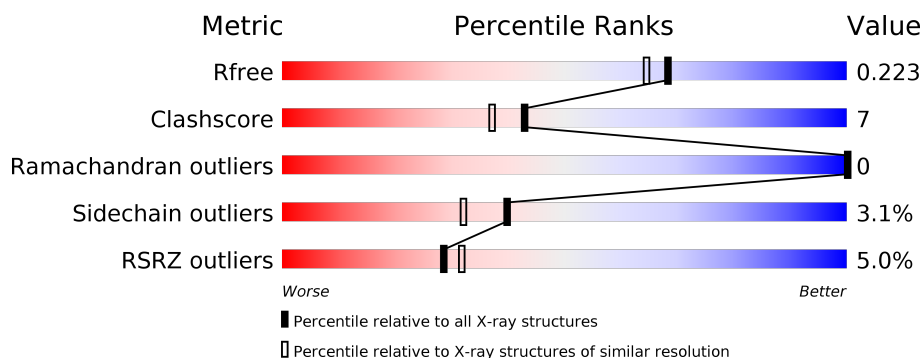
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 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 $\leq 5\%$. 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	424	<div> <div>4%</div> <div>78%</div> <div>11%</div> <div>11%</div> </div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3466 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 UDP-glucose 6-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			2994	1901	511	574	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	964	MET	-	expression tag	UNP C4XAX5
A	965	GLY	-	expression tag	UNP C4XAX5
A	966	SER	-	expression tag	UNP C4XAX5
A	967	SER	-	expression tag	UNP C4XAX5
A	968	HIS	-	expression tag	UNP C4XAX5
A	969	HIS	-	expression tag	UNP C4XAX5
A	970	HIS	-	expression tag	UNP C4XAX5
A	971	HIS	-	expression tag	UNP C4XAX5
A	972	HIS	-	expression tag	UNP C4XAX5
A	973	HIS	-	expression tag	UNP C4XAX5
A	974	SER	-	expression tag	UNP C4XAX5
A	975	SER	-	expression tag	UNP C4XAX5
A	976	GLY	-	expression tag	UNP C4XAX5
A	977	LEU	-	expression tag	UNP C4XAX5
A	978	VAL	-	expression tag	UNP C4XAX5
A	979	PRO	-	expression tag	UNP C4XAX5
A	980	ARG	-	expression tag	UNP C4XAX5
A	981	GLY	-	expression tag	UNP C4XAX5
A	982	SER	-	expression tag	UNP C4XAX5
A	983	HIS	-	expression tag	UNP C4XAX5
A	984	MET	-	expression tag	UNP C4XAX5
A	985	ALA	-	expression tag	UNP C4XAX5
A	986	SER	-	expression tag	UNP C4XAX5
A	987	MET	-	expression tag	UNP C4XAX5
A	988	THR	-	expression tag	UNP C4XAX5
A	989	GLY	-	expression tag	UNP C4XAX5
A	990	GLY	-	expression tag	UNP C4XAX5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	991	GLN	-	expression tag	UNP C4XAX5
A	992	GLN	-	expression tag	UNP C4XAX5
A	993	MET	-	expression tag	UNP C4XAX5
A	994	GLY	-	expression tag	UNP C4XAX5
A	995	ARG	-	expression tag	UNP C4XAX5
A	996	GLY	-	expression tag	UNP C4XAX5
A	997	SER	-	expression tag	UNP C4XAX5
A	998	GLU	-	expression tag	UNP C4XAX5
A	999	PHE	-	expression tag	UNP C4XAX5

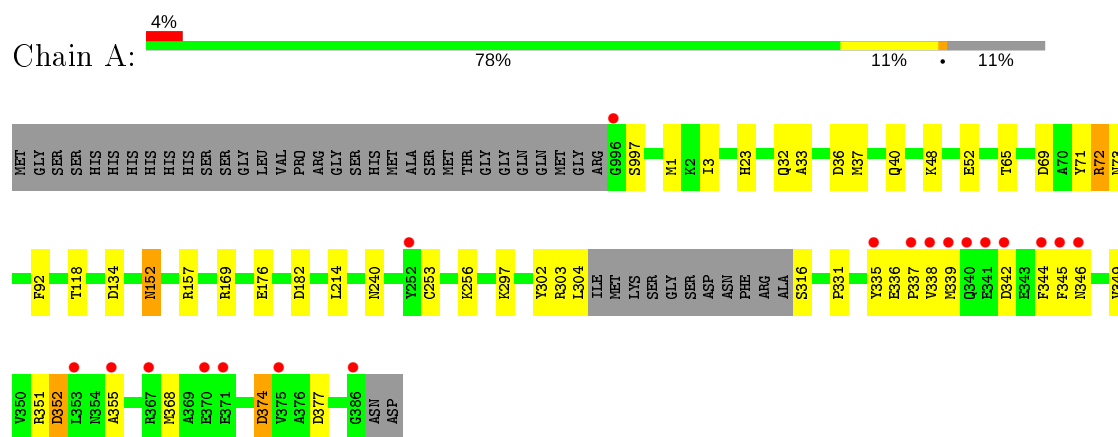
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	472	Total O 472 472	0	0

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.

- Molecule 1: UDP-glucose 6-dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	106.94Å 63.73Å 78.12Å 90.00° 113.08° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 25.90 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.7 (30.00-1.90) 94.6 (25.90-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.175 , 0.222 0.175 , 0.223	Depositor DCC
R_{free} test set	1803 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3466	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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	0.92	1/3045 (0.0%)	0.86	1/4124 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	TYR	CD2-CE2	5.00	1.46	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	ASN	N-CA-C	5.35	125.44	111.00

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	A	2994	0	3008	41	0
2	A	472	0	0	15	1
All	All	3466	0	3008	41	1

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 7.

All (41) 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:72:ARG:HG3	1:A:72:ARG:HH11	1.32	0.92
1:A:72:ARG:HD3	2:A:410:HOH:O	1.68	0.91
1:A:304:LEU:HD21	1:A:344:PHE:CE2	2.11	0.84
1:A:352:ASP:OD2	1:A:355:ALA:N	2.12	0.82
1:A:72:ARG:HG3	1:A:72:ARG:NH1	1.98	0.74
1:A:72:ARG:CD	2:A:410:HOH:O	2.31	0.73
1:A:118:THR:HG22	2:A:1361:HOH:O	1.88	0.72
1:A:69:ASP:HA	1:A:72:ARG:HE	1.58	0.68
1:A:72:ARG:HG2	1:A:73:ASN:ND2	2.09	0.67
1:A:316:SER:N	2:A:394:HOH:O	2.28	0.66
1:A:37:MET:HE1	2:A:408:HOH:O	1.96	0.64
1:A:23:HIS:HE1	1:A:176:GLU:OE1	1.83	0.60
1:A:169:ARG:HD3	2:A:427:HOH:O	2.03	0.58
1:A:374:ASP:OD1	1:A:374:ASP:N	2.30	0.56
1:A:304:LEU:HD21	1:A:344:PHE:CZ	2.44	0.53
1:A:345:PHE:O	1:A:346:ASN:HB3	2.07	0.53
1:A:36:ASP:O	1:A:40:GLN:HG3	2.10	0.52
1:A:997:SER:HA	1:A:1:MET:HG3	1.93	0.51
1:A:336:GLU:OE2	1:A:338:VAL:HB	2.10	0.51
1:A:169:ARG:CD	2:A:427:HOH:O	2.59	0.49
1:A:304:LEU:HD21	1:A:344:PHE:CD2	2.48	0.48
1:A:72:ARG:HG2	1:A:73:ASN:HD22	1.76	0.47
1:A:316:SER:N	2:A:395:HOH:O	2.47	0.47
1:A:368:MET:HB3	2:A:1375:HOH:O	2.13	0.47
1:A:368:MET:CB	2:A:1375:HOH:O	2.62	0.47
1:A:118:THR:CG2	2:A:1361:HOH:O	2.53	0.46
1:A:335:TYR:CZ	1:A:337:PRO:HD3	2.51	0.46
1:A:253:CYS:SG	2:A:399:HOH:O	2.61	0.45
1:A:256:LYS:HG3	2:A:1363:HOH:O	2.15	0.45
1:A:316:SER:HB2	2:A:393:HOH:O	2.17	0.44
1:A:48:LYS:HG2	1:A:52:GLU:OE1	2.17	0.43
1:A:33:ALA:O	1:A:37:MET:HG3	2.18	0.43
1:A:297:LYS:O	1:A:331:PRO:HD2	2.20	0.42
1:A:349:VAL:HG11	1:A:351:ARG:NH2	2.34	0.42
1:A:169:ARG:HD3	2:A:428:HOH:O	2.19	0.42
1:A:339:MET:O	1:A:351:ARG:NH2	2.53	0.42
1:A:214:LEU:HD23	1:A:214:LEU:C	2.40	0.42
1:A:152:ASN:HD22	1:A:152:ASN:HA	1.74	0.41
1:A:302:TYR:CD2	1:A:303:ARG:HG2	2.55	0.41
1:A:32:GLN:OE1	1:A:65:THR:HG21	2.21	0.40
1:A:3:ILE:N	1:A:3:ILE:HD12	2.35	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1261:HOH:O	2:A:1289:HOH:O[4_657]	2.02	0.18

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	375/424 (88%)	364 (97%)	11 (3%)	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	326/362 (90%)	316 (97%)	10 (3%)	40	32

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ARG
1	A	92	PHE
1	A	134	ASP
1	A	152	ASN
1	A	157	ARG
1	A	182	ASP

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Mol	Chain	Res	Type
1	A	342	ASP
1	A	352	ASP
1	A	374	ASP
1	A	377	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	40	GLN
1	A	73	ASN
1	A	152	ASN
1	A	240	ASN
1	A	319	GLN
1	A	346	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 ⓘ

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, 95th 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	A	379/424 (89%)	-0.11	19 (5%)	28 32	11, 21, 55, 73	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	345	PHE	5.8
1	A	252	TYR	5.1
1	A	386	GLY	3.9
1	A	370	GLU	3.8
1	A	339	MET	3.5
1	A	346	ASN	3.4
1	A	338	VAL	3.4
1	A	375	VAL	3.2
1	A	335	TYR	2.9
1	A	342	ASP	2.8
1	A	996	GLY	2.8
1	A	340	GLN	2.8
1	A	344	PHE	2.7
1	A	353	LEU	2.6
1	A	341	GLU	2.3
1	A	337	PRO	2.3
1	A	355	ALA	2.1
1	A	371	GLU	2.1
1	A	367	ARG	2.1

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

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.