



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 12:51 pm BST

PDB ID : 6C4K  
Title : Full length hUGDH with A104L substitution in the absence of ligand  
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Deposited on : 2018-01-12  
Resolution : 2.65 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
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

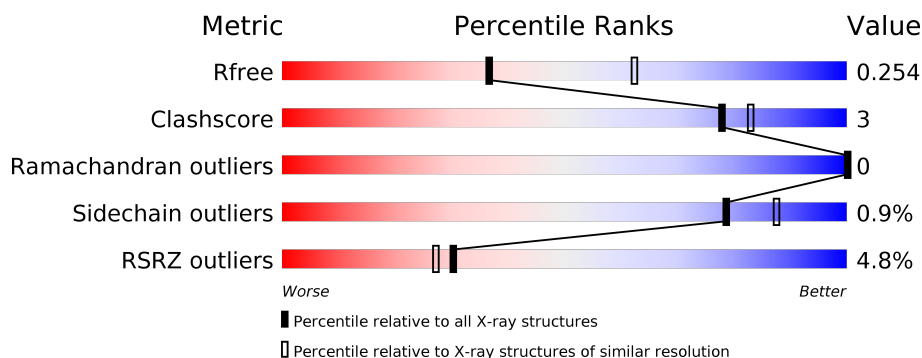
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 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	494	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>5%</div> <div>7%</div> </div> </div>
1	B	494	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>6%</div> </div> </div>
1	C	494	<div> <div>8%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>8%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10895 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.

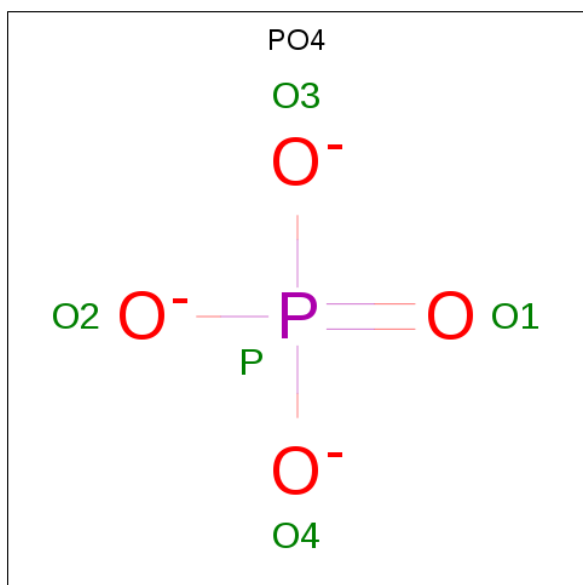
- Molecule 1 is a protein called UDP-glucose 6-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	1	0
			3603	2282	622	679	20			
1	B	462	Total	C	N	O	S	0	1	0
			3626	2294	625	687	20			
1	C	456	Total	C	N	O	S	0	1	0
			3581	2266	619	675	21			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	LEU	ALA	engineered mutation	UNP O60701
B	104	LEU	ALA	engineered mutation	UNP O60701
C	104	LEU	ALA	engineered mutation	UNP O60701

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	B	39	Total	O	0	0
			39	39		
4	C	10	Total	O	0	0
			10	10		

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.

- Chain A:
- 
- | Residue Type | Count | Percentage |
|--------------|-------|------------|
| Red          | 3     | 3%         |
| Yellow       | 87    | 87%        |
| Grey         | 7     | 7%         |

- Chain B:
- 
- | Position | Most Conserved AA | Information Content (bits) |
|----------|-------------------|----------------------------|
| 1        | M                 | 0.15                       |
| 2        | I                 | 0.10                       |
| 3        | I                 | 0.10                       |
| 4        | I                 | 0.10                       |
| 5        | I                 | 0.10                       |
| 6        | I                 | 0.10                       |
| 7        | I                 | 0.10                       |
| 8        | I                 | 0.10                       |
| 9        | I                 | 0.10                       |
| 10       | I                 | 0.10                       |
| 11       | I                 | 0.10                       |
| 12       | I                 | 0.10                       |
| 13       | I                 | 0.10                       |
| 14       | I                 | 0.10                       |
| 15       | I                 | 0.10                       |
| 16       | I                 | 0.10                       |
| 17       | I                 | 0.10                       |
| 18       | I                 | 0.10                       |
| 19       | I                 | 0.10                       |
| 20       | I                 | 0.10                       |
| 21       | I                 | 0.10                       |
| 22       | I                 | 0.10                       |
| 23       | I                 | 0.10                       |
| 24       | I                 | 0.10                       |

- Chain C:
- 
- 8% 83% 9% 8%
- M I K C R S N Y T P L Q L D E L N D T E P L P S G A P T K P A L L A P S L P
- SI20 N121 G122 Y123 T127 P133 V134 R135 I143 L152 N153 LEU Q155 V156 L157 E165 I169 K173 R177 L178 L180 G181 G182 D183 E184 L195 V198 Y199 E202 I208 T213 E242 G273 Q278 I304 R313 F323 V326
- I333 L334 F338 K339 R340 A362 H365 I366 Y367 P372 R373 F374 Q375 H382 PRO GLY VAL SER ASP D389 T396 K399 D400 P401 E416 R421 Y425 R443 V444 I462 V466 SER LYS ARG ILE PRO TYR ALA PRO SER GLY ILE PRO

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.52Å 114.47Å 96.88Å 90.00° 116.50° 90.00°	Depositor
Resolution (Å)	48.16 – 2.65 86.70 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.16-2.65) 100.0 (86.70-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.222 , 0.255 0.221 , 0.254	Depositor DCC
$R_{free}$ test set	2147 reflections (4.23%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.4	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 55.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10895	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: NA, 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	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.24	0/3670	0.40	0/4964
1	B	0.25	0/3694	0.41	0/4997
1	C	0.25	0/3645	0.40	0/4925
All	All	0.25	0/11009	0.40	0/14886

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	A	3603	0	3625	17	0
1	B	3626	0	3647	20	0
1	C	3581	0	3605	27	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	B	1	0	0	0	0
4	A	20	0	0	0	0
4	B	39	0	0	0	0
4	C	10	0	0	0	0
All	All	10895	0	10877	63	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 3.

The worst 5 of 63 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:C:372:PRO:HG2	1:C:375:GLN:HB2	1.74	0.70
1:A:205:ARG:NH1	1:A:208:ILE:O	2.36	0.59
1:A:340:LYS:HB3	1:A:416:GLU:HG2	1.84	0.58
1:A:96:TYR:HD1	1:A:96:TYR:O	1.85	0.58
1:C:45:TRP:O	1:C:65:ARG:NH1	2.37	0.57

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	454/494 (92%)	436 (96%)	18 (4%)	0	100	100
1	B	459/494 (93%)	442 (96%)	17 (4%)	0	100	100
1	C	447/494 (90%)	430 (96%)	17 (4%)	0	100	100
All	All	1360/1482 (92%)	1308 (96%)	52 (4%)	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	395/427 (92%)	393 (100%)	2 (0%)	88	94
1	B	399/427 (93%)	394 (99%)	5 (1%)	69	82
1	C	394/427 (92%)	390 (99%)	4 (1%)	76	86
All	All	1188/1281 (93%)	1177 (99%)	11 (1%)	78	87

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	327	THR
1	B	373	ARG
1	C	177	ARG
1	B	205	ARG
1	C	98	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	ASN
1	C	283	ASN
1	C	375	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 4 ligands modelled in this entry, 1 is 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	PO4	C	501	-	4,4,4	0.93	0	6,6,6	0.43	0
2	PO4	A	501	-	4,4,4	0.96	0	6,6,6	0.44	0
2	PO4	B	502	-	4,4,4	0.84	0	6,6,6	0.47	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.

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](#)

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	459/494 (92%)	0.41	14 (3%) 49 45	54, 108, 154, 177	0
1	B	462/494 (93%)	0.37	14 (3%) 50 47	43, 95, 141, 180	0
1	C	456/494 (92%)	0.61	38 (8%) 11 9	57, 113, 151, 197	0
All	All	1377/1482 (92%)	0.46	66 (4%) 30 27	43, 104, 150, 197	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	14	TYR	5.5
1	A	14	TYR	5.0
1	C	195	LEU	4.3
1	B	30	ILE	4.1
1	C	116	ILE	3.9

### 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	B	502	5/5	0.86	0.27	60,61,66,69	5
3	NA	B	501	1/1	0.88	0.15	82,82,82,82	0
2	PO4	C	501	5/5	0.90	0.40	89,89,96,102	5
2	PO4	A	501	5/5	0.91	0.34	69,71,73,74	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.