

wwPDB X-ray Structure Validation Summary Report (i)

Nov 7, 2023 – 12:09 AM JST

PDB ID	:	8HGF
Title	:	Human PKM2 mutant - $C326S$
Authors	:	Chen, YC.; Lin, KT.; Cheng, HC.
Deposited on	:	2022-11-14
Resolution	:	3.10 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
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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 3.10 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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% 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	А	551	% 63%	27%	• 8%
1	В	551	2% 61%	29%	• 8%
1	С	551	% 56% 17%	·	25%
1	D	551	^{2%} 62%	27%	• 8%



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 30019 atoms, of which 15162 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		Atoms				ZeroOcc	AltConf	Trace	
1	Δ	508	Total	С	Η	Ν	0	\mathbf{S}	0	0	0
1	Л	508	7865	2447	3975	689	731	23	0	0	0
1	В	508	Total	С	Η	Ν	0	S	0	0	0
1	D	508	7861	2447	3971	689	731	23	0	0	0
1	П	508	Total	С	Η	Ν	0	S	0	0	0
1		508	7860	2447	3970	689	731	23	0	0	0
1	C	414	Total	С	Η	Ν	0	S	0	0	0
		414	6433	2002	3246	575	590	20		0	U

• Molecule 1 is a protein called Pyruvate kinase PKM.

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-19	MET	-	initiating methionine	UNP P14618
А	-18	GLY	-	expression tag	UNP P14618
А	-17	SER	-	expression tag	UNP P14618
А	-16	SER	-	expression tag	UNP P14618
А	-15	HIS	-	expression tag	UNP P14618
А	-14	HIS	-	expression tag	UNP P14618
А	-13	HIS	-	expression tag	UNP P14618
А	-12	ARG	-	expression tag	UNP P14618
А	-11	HIS	-	expression tag	UNP P14618
А	-10	HIS	-	expression tag	UNP P14618
А	-9	SER	-	expression tag	UNP P14618
А	-8	SER	-	expression tag	UNP P14618
А	-7	GLY	-	expression tag	UNP P14618
А	-6	LEU	-	expression tag	UNP P14618
А	-5	VAL	-	expression tag	UNP P14618
А	-4	PRO	-	expression tag	UNP P14618
А	-3	ARG	-	expression tag	UNP P14618
A	-2	GLY	-	expression tag	UNP P14618
A	-1	SER	-	expression tag	UNP P14618
А	0	HIS	-	expression tag	UNP P14618
А	326	SER	CYS	engineered mutation	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
В	-19	MET	_	initiating methionine	UNP P14618
В	-18	GLY	_	expression tag	UNP P14618
В	-17	SER	-	expression tag	UNP P14618
В	-16	SER	-	expression tag	UNP P14618
В	-15	HIS	-	expression tag	UNP P14618
В	-14	HIS	-	expression tag	UNP P14618
В	-13	HIS	-	expression tag	UNP P14618
В	-12	ARG	_	expression tag	UNP P14618
В	-11	HIS	_	expression tag	UNP P14618
В	-10	HIS	-	expression tag	UNP P14618
В	-9	SER	-	expression tag	UNP P14618
В	-8	SER	-	expression tag	UNP P14618
В	-7	GLY	-	expression tag	UNP P14618
В	-6	LEU	-	expression tag	UNP P14618
В	-5	VAL	-	expression tag	UNP P14618
В	-4	PRO	-	expression tag	UNP P14618
В	-3	ARG	-	expression tag	UNP P14618
В	-2	GLY	-	expression tag	UNP P14618
В	-1	SER	-	expression tag	UNP P14618
В	0	HIS	-	expression tag	UNP P14618
В	326	SER	CYS	engineered mutation	UNP P14618
D	-19	MET	-	initiating methionine	UNP P14618
D	-18	GLY	-	expression tag	UNP P14618
D	-17	SER	-	expression tag	UNP P14618
D	-16	SER	-	expression tag	UNP P14618
D	-15	HIS	-	expression tag	UNP P14618
D	-14	HIS	-	expression tag	UNP P14618
D	-13	HIS	-	expression tag	UNP P14618
D	-12	ARG	-	expression tag	UNP P14618
D	-11	HIS	-	expression tag	UNP P14618
D	-10	HIS	-	expression tag	UNP P14618
D	-9	SER	-	expression tag	UNP P14618
D	-8	SER	-	expression tag	UNP P14618
D	-7	GLY	-	expression tag	UNP P14618
D	-6	LEU	-	expression tag	UNP P14618
D	-5	VAL	-	expression tag	UNP P14618
D	-4	PRO	-	expression tag	UNP P14618
D	-3	ARG	-	expression tag	UNP P14618
D	-2	GLY	-	expression tag	UNP P14618
D	-1	SER	-	expression tag	UNP P14618
D	0	HIS	-	expression tag	UNP P14618
D	326	SER	CYS	engineered mutation	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
С	-19	MET	-	initiating methionine	UNP P14618
С	-18	GLY	-	expression tag	UNP P14618
С	-17	SER	-	expression tag	UNP P14618
С	-16	SER	-	expression tag	UNP P14618
С	-15	HIS	-	expression tag	UNP P14618
С	-14	HIS	-	expression tag	UNP P14618
С	-13	HIS	-	expression tag	UNP P14618
С	-12	ARG	-	expression tag	UNP P14618
С	-11	HIS	-	expression tag	UNP P14618
С	-10	HIS	-	expression tag	UNP P14618
С	-9	SER	-	expression tag	UNP P14618
С	-8	SER	-	expression tag	UNP P14618
С	-7	GLY	-	expression tag	UNP P14618
С	-6	LEU	-	expression tag	UNP P14618
С	-5	VAL	-	expression tag	UNP P14618
С	-4	PRO	-	expression tag	UNP P14618
С	-3	ARG	-	expression tag	UNP P14618
С	-2	GLY	-	expression tag	UNP P14618
C	-1	SER	-	expression tag	UNP P14618
С	0	HIS	-	expression tag	UNP P14618
C	326	SER	CYS	engineered mutation	UNP P14618

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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: Pyruvate kinase PKM



A411 15.15 A412 55.17 54.20 55.19 6.419 15.22 5.420 15.23 74.12 15.23 74.13 15.23 74.13 15.27 74.23 15.27 74.26 15.21 74.23 15.21 74.26 16.27 74.46 74.45 74.46

• Molecule 1: Pyruvate kinase PKM



В





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	181.51Å 156.37Å 121.59Å	Depositor
a, b, c, α , β , γ	90.00° 114.20° 90.00°	Depositor
Bosolution (Å)	29.79 - 3.10	Depositor
Resolution (A)	29.79 - 3.10	EDS
% Data completeness	63.9 (29.79-3.10)	Depositor
(in resolution range)	86.3 (29.79-3.10)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.86 (at 3.11 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
P. P.	0.182 , 0.237	Depositor
Π, Π_{free}	0.182 , 0.236	DCC
R_{free} test set	2000 reflections $(4.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	53.6	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.38, 38.1	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	30019	wwPDB-VP
Average B, all atoms $(Å^2)$	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.02% 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)

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		Bo	ond lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	1.07	19/3953~(0.5%)	1.04	10/5338~(0.2%)	
1	В	0.98	9/3953~(0.2%)	1.00	6/5338~(0.1%)	
1	С	0.93	9/3242~(0.3%)	0.94	1/4379~(0.0%)	
1	D	1.14	24/3953~(0.6%)	1.07	11/5338~(0.2%)	
All	All	1.04	61/15101~(0.4%)	1.02	28/20393~(0.1%)	

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	А	0	3
1	В	0	1
1	С	0	2
1	D	0	2
All	All	0	8

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	434	SER	CB-OG	11.79	1.57	1.42
1	С	423	CYS	CB-SG	-11.21	1.63	1.82
1	D	31	CYS	CB-SG	-8.79	1.67	1.82
1	D	332	GLU	CG-CD	8.64	1.65	1.51
1	А	423	CYS	CB-SG	-8.58	1.67	1.82

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$\operatorname{Ideal}(^{o})$
1	D	386	GLU	OE1-CD-OE2	8.72	133.76	123.30
1	В	401	LEU	C-N-CA	7.84	141.30	121.70
1	А	386	GLU	OE1-CD-OE2	7.82	132.68	123.30

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	447	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	D	500	ARG	O-C-N	-6.61	111.96	123.20

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	423	CYS	Peptide
1	А	518	GLY	Peptide
1	А	526	ARG	Sidechain
1	В	447	ARG	Sidechain
1	D	56	ARG	Sidechain

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	3890	3975	3976	121	1
1	В	3890	3971	3976	149	0
1	С	3187	3246	3249	79	0
1	D	3890	3970	3976	126	1
All	All	14857	15162	15177	448	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 15.

The worst 5 of 448 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:D:118:GLU:OE1	1:D:120:ARG:NH1	1.90	1.04
1:C:71:VAL:HG22	1:C:109:ALA:HB3	1.40	1.03
1:B:400:ARG:HG3	1:C:422:LYS:NZ	1.78	0.98
1:B:395:PHE:CZ	1:B:421:PHE:CE2	2.51	0.98
1:A:41:THR:HG22	1:A:42:ALA:O	1.64	0.98

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)
1:A:35:ILE:O	1:D:305:LYS:NZ[2_556]	1.90	0.30

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	Pe	erce	ntiles
1	А	506/551~(92%)	456 (90%)	48 (10%)	2 (0%)	4° 9	34	69
1	В	506/551~(92%)	452 (89%)	50 (10%)	4 (1%)		19	54
1	С	410/551~(74%)	369~(90%)	37~(9%)	4 (1%)	-	15	49
1	D	506/551~(92%)	456 (90%)	48 (10%)	2(0%)	4. e	34	69
All	All	1928/2204 (88%)	1733 (90%)	183 (10%)	12 (1%)	، 4	25	59

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	125	LYS
1	В	411	ALA
1	В	516	ARG
1	С	406	SER
1	А	156	ILE

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	419/453~(92%)	412 (98%)	7(2%)	60 83		
1	В	419/453~(92%)	410 (98%)	9~(2%)	53 79		
1	С	342/453~(76%)	335~(98%)	7(2%)	55 80		
1	D	419/453~(92%)	413 (99%)	6 (1%)	67 86		
All	All	1599/1812~(88%)	1570 (98%)	29 (2%)	59 82		

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	В	436	ARG
1	С	445	ARG
1	D	188	LYS
1	С	383	ARG
1	D	154	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	378	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 monosaccharides 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)

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>	#RSR2	L>2	$OWAB(Å^2)$	Q<0.9
1	А	508/551~(92%)	-0.14	8 (1%) 72	51	23, 49, 102, 113	0
1	В	508/551~(92%)	-0.10	9 (1%) 68	47	36, 55, 84, 116	0
1	С	414/551~(75%)	-0.03	8 (1%) 66	46	35, 60, 87, 120	0
1	D	508/551~(92%)	-0.11	12 (2%) 59) 37	25, 46, 73, 99	0
All	All	1938/2204 (87%)	-0.10	37 (1%) 66	6 46	23, 53, 90, 120	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	402	ALA	6.9
1	D	402	ALA	4.5
1	D	519	SER	4.5
1	D	517	PRO	4.4
1	D	403	PRO	4.3

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)

There are no ligands in this entry.



6.5 Other polymers (i)

There are no such residues in this entry.

