



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 4, 2025 – 04:10 PM JST

PDB ID : 9V4C / pdb\_00009v4c  
Title : Selective Production of Versatile L-Glyceraldehyde from C1 and/or C2 aldehydes  
Authors : Duysak, T.; Seo, P.W.; Kim, J.S.  
Deposited on : 2025-05-23  
Resolution : 2.00 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

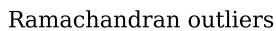
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

i

## X-RAY DIFFRACTION

A.

Metric	Percentile Banks	Value
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 $R_{free}$ 

that have poor fit to the electron density. The numeric value is given above the bar.

1

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Mol	Chain	Length	Quality of chain
1	G	222	 92% 7%
1	H	222	 91% 7% .
1	I	222	 91% 6% ..
1	J	222	 90% 9% .

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18062 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 Fructose-6-phosphate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	1	0
			1662	1070	272	313	7			
1	B	222	Total	C	N	O	S	0	1	0
			1666	1072	273	314	7			
1	C	222	Total	C	N	O	S	0	0	0
			1663	1070	273	314	6			
1	D	221	Total	C	N	O	S	0	1	0
			1662	1070	272	313	7			
1	E	221	Total	C	N	O	S	0	2	0
			1670	1075	275	313	7			
1	F	221	Total	C	N	O	S	0	1	0
			1662	1070	272	313	7			
1	G	221	Total	C	N	O	S	0	0	0
			1659	1068	272	313	6			
1	H	221	Total	C	N	O	S	0	2	0
			1670	1075	275	313	7			
1	I	220	Total	C	N	O	S	0	0	0
			1655	1066	271	312	6			
1	J	221	Total	C	N	O	S	0	0	0
			1659	1068	272	313	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A1B9MNE3
A	0	GLY	-	expression tag	UNP A0A1B9MNE3
B	-1	GLY	-	expression tag	UNP A0A1B9MNE3
B	0	GLY	-	expression tag	UNP A0A1B9MNE3
C	-1	GLY	-	expression tag	UNP A0A1B9MNE3
C	0	GLY	-	expression tag	UNP A0A1B9MNE3
D	-1	GLY	-	expression tag	UNP A0A1B9MNE3
D	0	GLY	-	expression tag	UNP A0A1B9MNE3
E	-1	GLY	-	expression tag	UNP A0A1B9MNE3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	GLY	-	expression tag	UNP A0A1B9MNE3
F	-1	GLY	-	expression tag	UNP A0A1B9MNE3
F	0	GLY	-	expression tag	UNP A0A1B9MNE3
G	-1	GLY	-	expression tag	UNP A0A1B9MNE3
G	0	GLY	-	expression tag	UNP A0A1B9MNE3
H	-1	GLY	-	expression tag	UNP A0A1B9MNE3
H	0	GLY	-	expression tag	UNP A0A1B9MNE3
I	-1	GLY	-	expression tag	UNP A0A1B9MNE3
I	0	GLY	-	expression tag	UNP A0A1B9MNE3
J	-1	GLY	-	expression tag	UNP A0A1B9MNE3
J	0	GLY	-	expression tag	UNP A0A1B9MNE3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	155	Total O 155 155	0	0
2	B	147	Total O 147 147	0	0
2	C	163	Total O 163 163	0	0
2	D	183	Total O 183 183	0	0
2	E	140	Total O 140 140	0	0
2	F	142	Total O 142 142	0	0
2	G	134	Total O 134 134	0	0
2	H	135	Total O 135 135	0	0
2	I	129	Total O 129 129	0	0
2	J	106	Total O 106 106	0	0

### 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: Fructose-6-phosphate aldolase

Chain A:  96%



- Molecule 1: Fructose-6-phosphate aldolase

Chain B:  96%



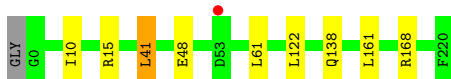
- Molecule 1: Fructose-6-phosphate aldolase

Chain C:  94% 6%



- Molecule 1: Fructose-6-phosphate aldolase

Chain D:  95%

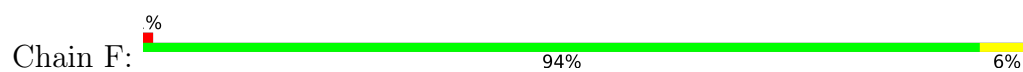


- Molecule 1: Fructose-6-phosphate aldolase

Chain E:  91% 8%



- Molecule 1: Fructose-6-phosphate aldolase



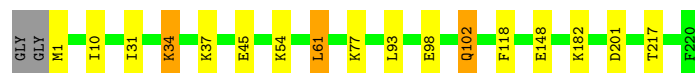
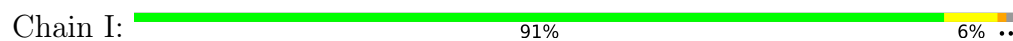
- Molecule 1: Fructose-6-phosphate aldolase



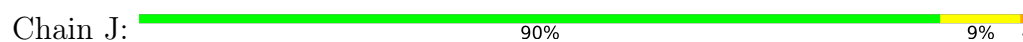
- Molecule 1: Fructose-6-phosphate aldolase



- Molecule 1: Fructose-6-phosphate aldolase



- Molecule 1: Fructose-6-phosphate aldolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.82Å 117.35Å 204.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.41 – 2.00 49.41 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.6 (49.41-2.00) 95.7 (49.41-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158)	Depositor
R, $R_{free}$	0.172 , 0.218 0.176 , 0.219	Depositor DCC
$R_{free}$ test set	6144 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.4	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 38.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18062	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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](#)

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	0.29	0/1691	0.44	0/2301
1	B	0.29	0/1695	0.44	0/2306
1	C	0.31	0/1689	0.46	0/2297
1	D	0.31	0/1691	0.47	0/2301
1	E	0.29	0/1702	0.44	0/2315
1	F	0.29	0/1691	0.43	0/2301
1	G	0.25	0/1685	0.40	0/2292
1	H	0.27	0/1702	0.42	0/2315
1	I	0.29	0/1681	0.44	0/2287
1	J	0.27	0/1685	0.41	0/2292
All	All	0.29	0/16912	0.44	0/23007

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	1662	0	1737	4	0
1	B	1666	0	1740	3	0
1	C	1663	0	1735	8	0
1	D	1662	0	1737	3	0
1	E	1670	0	1750	12	0
1	F	1662	0	1737	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1659	0	1732	10	0
1	H	1670	0	1750	11	0
1	I	1655	0	1729	10	0
1	J	1659	0	1732	11	0
2	A	155	0	0	1	0
2	B	147	0	0	0	0
2	C	163	0	0	0	0
2	D	183	0	0	1	0
2	E	140	0	0	4	0
2	F	142	0	0	0	0
2	G	134	0	0	3	0
2	H	135	0	0	2	0
2	I	129	0	0	2	0
2	J	106	0	0	0	0
All	All	18062	0	17379	69	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 2.

The worst 5 of 69 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:J:98:GLU:OE2	1:J:102:GLN:NE2	2.17	0.76
1:E:10:ILE:HG13	1:E:49:VAL:HG21	1.68	0.75
1:D:15:ARG:NH1	2:D:301:HOH:O	2.13	0.71
1:G:11:VAL:HA	1:G:14:LYS:HE2	1.73	0.69
1:I:201:ASP:OD1	2:I:301:HOH:O	2.13	0.66

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	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
1	B	221/222 (100%)	217 (98%)	4 (2%)	0	100	100
1	C	220/222 (99%)	216 (98%)	3 (1%)	1 (0%)	25	21
1	D	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
1	E	221/222 (100%)	216 (98%)	5 (2%)	0	100	100
1	F	220/222 (99%)	218 (99%)	2 (1%)	0	100	100
1	G	219/222 (99%)	216 (99%)	3 (1%)	0	100	100
1	H	221/222 (100%)	215 (97%)	6 (3%)	0	100	100
1	I	218/222 (98%)	216 (99%)	2 (1%)	0	100	100
1	J	219/222 (99%)	214 (98%)	5 (2%)	0	100	100
All	All	2199/2220 (99%)	2161 (98%)	37 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	0	GLY

### 5.3.2 Protein sidechains ⓘ

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	182/181 (101%)	178 (98%)	4 (2%)	47	51
1	B	182/181 (101%)	177 (97%)	5 (3%)	40	42
1	C	181/181 (100%)	177 (98%)	4 (2%)	47	51
1	D	182/181 (101%)	175 (96%)	7 (4%)	28	28
1	E	183/181 (101%)	178 (97%)	5 (3%)	40	42
1	F	182/181 (101%)	179 (98%)	3 (2%)	58	64
1	G	181/181 (100%)	178 (98%)	3 (2%)	56	61
1	H	183/181 (101%)	177 (97%)	6 (3%)	33	33
1	I	181/181 (100%)	174 (96%)	7 (4%)	27	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	181/181 (100%)	173 (96%)	8 (4%)	24	22
All	All	1818/1810 (100%)	1766 (97%)	52 (3%)	37	39

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	10	ILE
1	H	138	GLN
1	J	138	GLN
1	G	61	LEU
1	H	48	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	138	GLN
1	J	74	GLN
1	F	150	GLN
1	I	138	GLN
1	F	74	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 oligosaccharides 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 ⓘ

### 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, 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	221/222 (99%)	-0.60	1 (0%) 87 86	18, 28, 48, 66	1 (0%)
1	B	222/222 (100%)	-0.65	1 (0%) 87 86	19, 29, 45, 62	1 (0%)
1	C	222/222 (100%)	-0.64	3 (1%) 73 72	20, 29, 45, 82	0
1	D	221/222 (99%)	-0.70	1 (0%) 87 86	18, 27, 40, 66	1 (0%)
1	E	221/222 (99%)	-0.54	1 (0%) 87 86	20, 30, 48, 76	2 (0%)
1	F	221/222 (99%)	-0.55	2 (0%) 81 80	19, 30, 51, 68	1 (0%)
1	G	221/222 (99%)	-0.33	1 (0%) 87 86	23, 36, 56, 90	0
1	H	221/222 (99%)	-0.53	1 (0%) 87 86	22, 33, 51, 82	2 (0%)
1	I	220/222 (99%)	-0.49	0 100 100	21, 31, 47, 60	0
1	J	221/222 (99%)	-0.44	1 (0%) 87 86	24, 36, 54, 85	0
All	All	2211/2220 (99%)	-0.55	12 (0%) 87 86	18, 31, 51, 90	8 (0%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	0	GLY	3.9
1	G	0	GLY	3.1
1	F	217	THR	2.9
1	C	-1	GLY	2.9
1	D	53	ASP	2.8

### 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 oligosaccharides 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.