



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:40 PM GMT

PDB ID : 1GPD  
Title : STUDIES OF ASYMMETRY IN THE THREE-DIMENSIONAL STRUCTURE OF LOBSTER D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE  
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Deposited on : 1975-07-01  
Resolution : 2.90 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

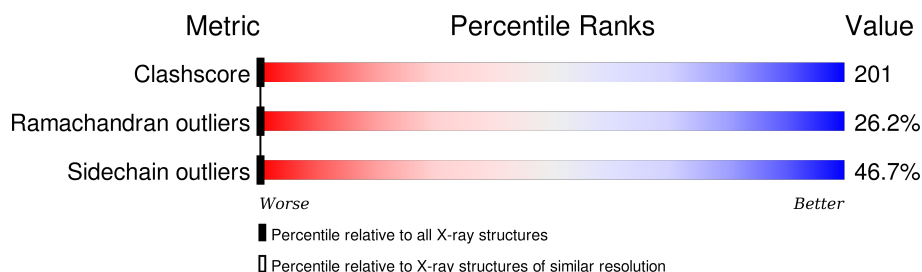
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	G	334	
1	R	334	

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	PO4	R	338	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5112 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 D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE.

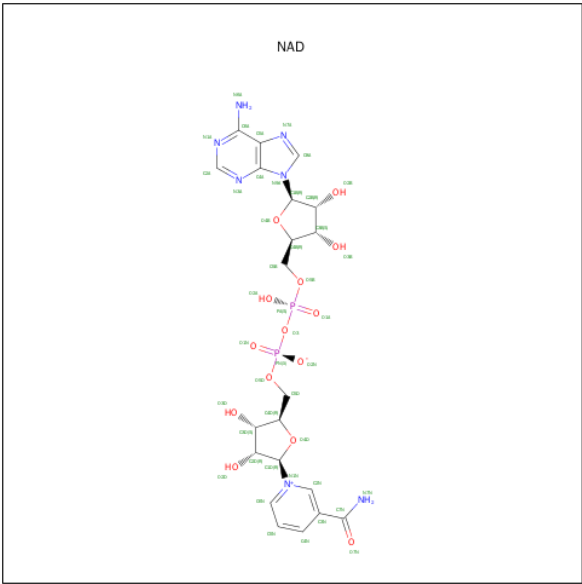
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	334	Total	C	N	O	S	0	0	0
			2510	1593	419	483	15			
1	R	334	Total	C	N	O	S	0	0	0
			2510	1593	419	483	15			

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



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	R	1	Total	P	0	0
			1	1		
2	R	1	Total	P	0	0
			1	1		
2	R	1	Total	P	0	0
			1	1		
2	R	1	Total	P	0	0
			1	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



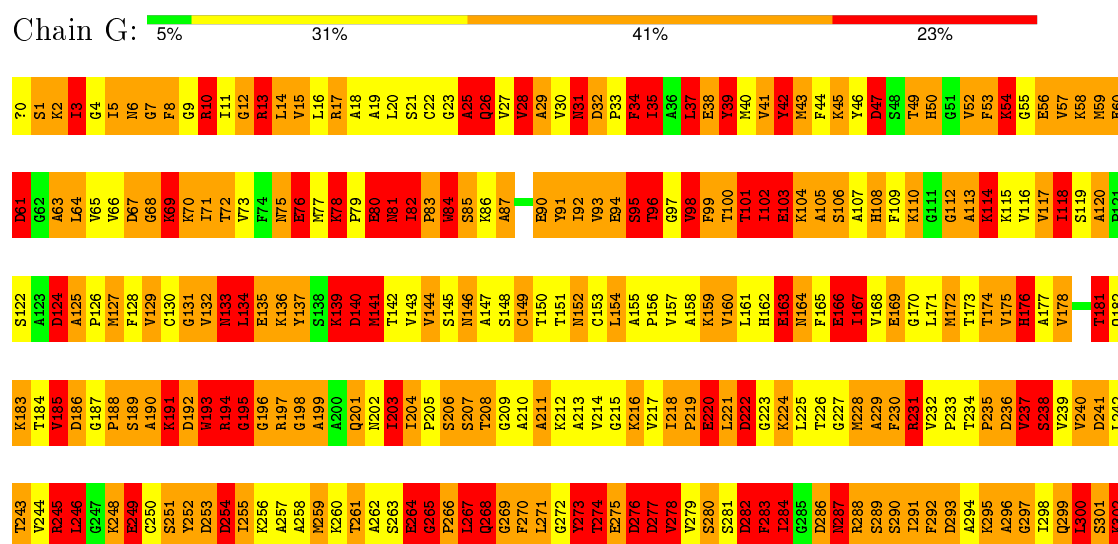
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	R	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

#### • Molecule 1: D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE



L242	K302
L243	T303
V244	F304
R245	V305
L246	K306
G247	V307
R248	V308
E249	S309
C250	W310
S251	Y311
Y252	D312
D253	N313
D254	E314
I255	F315
K256	G316
A257	Y317
W259	S318
K260	Q319
T261	R320
A262	V321
S263	I322
E264	D323
G265	L324
P266	L325
L267	K326
Q268	H327
G269	M328
F270	Q329
L271	K330
G272	V331
V273	D332
T274	S333
E275	A334
D276	
D277	
V278	
Y279	
S280	
S281	
D282	
F283	
I284	
G285	
D286	
D287	
R288	
S289	
S290	
I291	
F292	
D293	
A294	
K295	
A296	
G297	
I298	
Q299	
L300	
S301	

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.00Å 139.10Å 80.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	unknown	Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5112	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, NAD, ACE

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	G	1.18	30/2554 (1.2%)	2.05	168/3453 (4.9%)
1	R	1.18	30/2554 (1.2%)	1.88	130/3453 (3.8%)
All	All	1.18	60/5108 (1.2%)	1.97	298/6906 (4.3%)

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	G	0	5
1	R	0	7
All	All	0	12

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	84	TRP	NE1-CE2	-7.38	1.27	1.37
1	R	84	TRP	NE1-CE2	-7.35	1.27	1.37
1	R	310	TRP	NE1-CE2	-7.34	1.28	1.37
1	R	193	TRP	NE1-CE2	-7.33	1.28	1.37
1	G	310	TRP	NE1-CE2	-7.31	1.28	1.37

The worst 5 of 298 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	277	ASP	N-CA-C	13.71	148.02	111.00
1	G	300	LEU	N-CA-C	13.61	147.75	111.00
1	R	198	GLY	N-CA-C	12.19	143.56	113.10
1	R	195	GLY	N-CA-C	12.14	143.44	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	198	GLY	N-CA-C	12.06	143.25	113.10

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	13	ARG	Sidechain
1	G	194	ARG	Sidechain
1	G	231	ARG	Sidechain
1	G	245	ARG	Sidechain
1	G	320	ARG	Sidechain

## 5.2 Too-close contacts

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	G	2510	0	2519	1064	7
1	R	2510	0	2522	1004	7
2	R	4	0	0	8	0
3	G	44	0	26	20	0
3	R	44	0	26	8	0
All	All	5112	0	5093	2047	7

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 201.

The worst 5 of 2047 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:G:117:VAL:HG21	1:G:328:MET:SD	1.23	1.70
1:R:324:LEU:HD11	1:R:328:MET:SD	1.24	1.66
1:G:173:THR:HG22	1:G:228:MET:SD	1.39	1.60
1:R:137:TYR:CD1	1:R:331:VAL:HG11	1.47	1.47
1:R:5:ILE:CG1	1:R:30:VAL:HG13	1.02	1.47

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes

the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:GLU:CB	1:R:220:GLU:OE2[4_555]	1.21	0.99
1:G:135:GLU:CG	1:R:220:GLU:OE2[4_555]	1.26	0.94
1:G:135:GLU:N	1:R:220:GLU:OE1[4_555]	1.32	0.88
1:G:135:GLU:CA	1:R:220:GLU:OE1[4_555]	1.53	0.67
1:G:135:GLU:CB	1:R:220:GLU:CD[4_555]	1.61	0.59

## 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	G	332/334 (99%)	178 (54%)	73 (22%)	81 (24%)	0	0
1	R	332/334 (99%)	167 (50%)	72 (22%)	93 (28%)	0	0
All	All	664/668 (99%)	345 (52%)	145 (22%)	174 (26%)	0	0

5 of 174 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	2	LYS
1	G	10	ARG
1	G	13	ARG
1	G	25	ALA
1	G	28	VAL

### 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	G	271/271 (100%)	149 (55%)	122 (45%)	0	0
1	R	271/271 (100%)	140 (52%)	131 (48%)	0	0
All	All	542/542 (100%)	289 (53%)	253 (47%)	0	0

5 of 253 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	313	ASN
1	R	47	ASP
1	R	291	ILE
1	G	324	LEU
1	R	15	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	327	HIS
1	R	26	GLN
1	R	299	GLN
1	G	313	ASN
1	G	319	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are modelled with single atom - leaving 2 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	$\# Z  > 2$
3	NAD	G	335	-	38,48,48	0.73	1 (2%)	47,73,73	0.76	1 (2%)
3	NAD	R	339	-	38,48,48	0.72	1 (2%)	47,73,73	1.58	2 (4%)

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
3	NAD	G	335	-	-	0/22/62/62	0/5/5/5
3	NAD	R	339	-	-	0/22/62/62	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	339	NAD	C8A-N7A	-2.33	1.30	1.34
3	G	335	NAD	C8A-N7A	-2.31	1.30	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	339	NAD	O2A-PA-O1A	-6.71	76.17	112.53
3	G	335	NAD	O2A-PA-O5B	2.26	119.85	108.46
3	R	339	NAD	O2A-PA-O5B	7.09	144.21	108.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	335	NAD	20	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	339	NAD	8	0

## 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](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.