



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:57 AM GMT

PDB ID : 3GPD
Title : TWINNING IN CRYSTALS OF HUMAN SKELETAL MUSCLE D-GLYCE
RALDEHYDE-3-PHOSPHATE DEHYDROGENASE
Authors : Watson, H.C.; Campbell, J.C.
Deposited on : 1983-06-20
Resolution : 3.50 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
<http://wwpdb.org/validation/2016/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
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

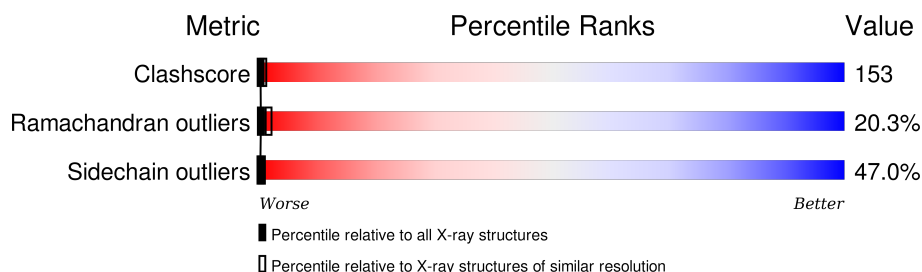
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)

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. 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	SO4	G	338	-	-	X	-
2	SO4	G	340	-	-	X	-
2	SO4	R	338	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAD	G	336	X	-	-	-

2 Entry composition [i](#)

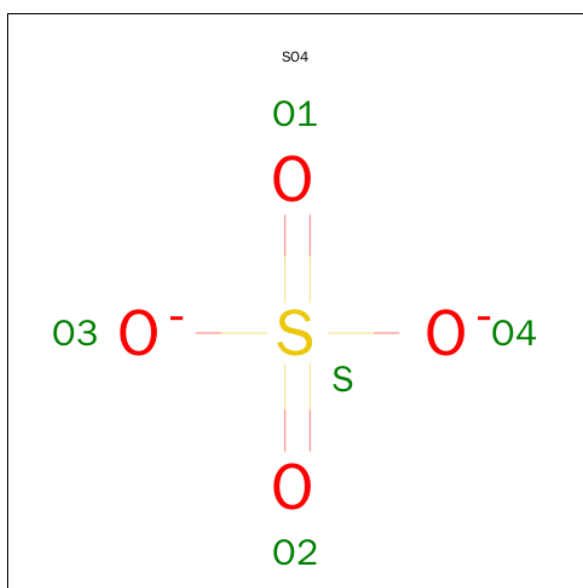
There are 3 unique types of molecules in this entry. The entry contains 5154 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

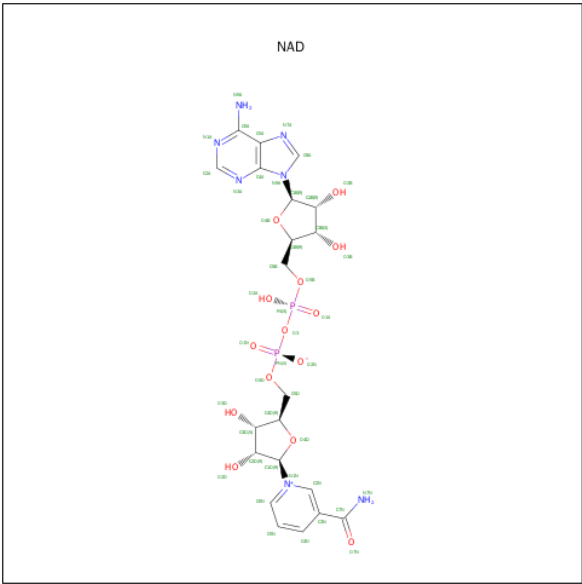
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	334	Total	C	N	O	S	0	0	0
			2523	1601	431	479	12			
1	G	334	Total	C	N	O	S	0	0	0
			2523	1601	431	479	12			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	R	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



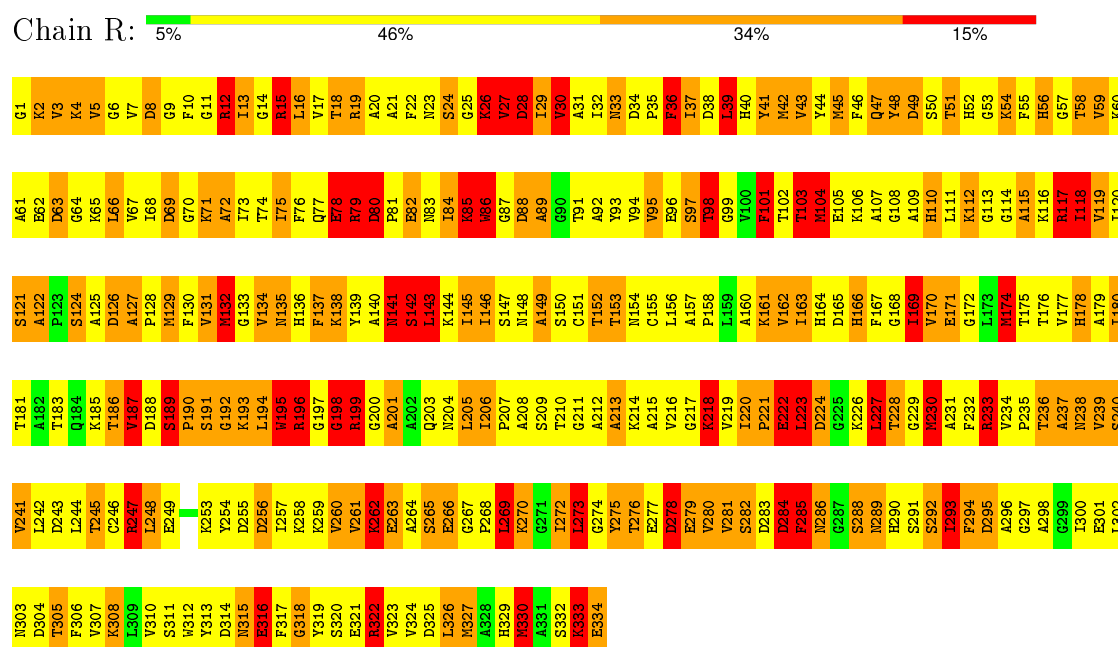
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	R	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

3 Residue-property plots

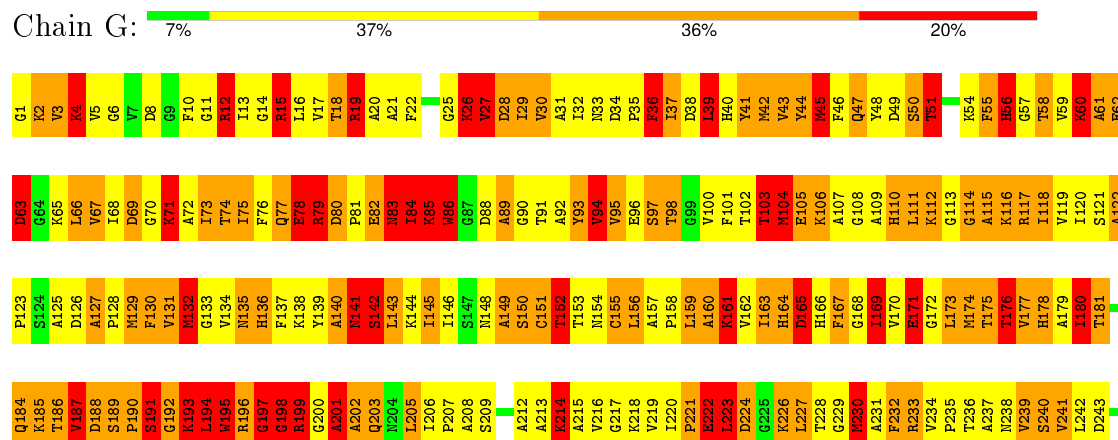
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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



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



C246	F306
R247	V307
I248	K308
E249	I309
K250	V310
P251	S311
A252	K312
K253	Y313
Y254	D314
D255	R315
D256	E316
I257	F317
K258	G318
K259	Y319
V260	S320
Y261	E321
K262	R322
E263	V323
A264	V324
S265	D325
E266	L326
G267	M327
P268	A328
L269	H329
K270	R330
G271	A331
I272	S332
L273	K333
G274	E334
Y275	
T276	
E277	
D278	
E279	
Y280	
V281	
S282	
D283	
D284	
F285	
I286	
G287	
S288	
I288	
H290	
S291	
S292	
L293	
F294	
D295	
A296	
G297	
A298	
G299	
I300	
F301	
L302	
R303	
D304	
T305	

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	132.40Å 97.90Å 81.60Å 90.00° 114.30° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	0.330 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5154	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

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: SO4, NAD

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	1.40	11/2573 (0.4%)	2.06	121/3479 (3.5%)
1	R	1.12	3/2573 (0.1%)	1.67	54/3479 (1.6%)
All	All	1.27	14/5146 (0.3%)	1.87	175/6958 (2.5%)

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	198	GLY	N-CA	8.67	1.59	1.46
1	G	195	TRP	CB-CG	7.61	1.64	1.50
1	G	329	HIS	CB-CG	6.51	1.61	1.50
1	G	70	GLY	N-CA	6.48	1.55	1.46
1	G	279	GLU	N-CA	6.37	1.59	1.46

The worst 5 of 175 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	279	GLU	O-C-N	10.67	139.77	122.70
1	G	278	ASP	O-C-N	-10.53	105.85	122.70
1	G	196	ARG	O-C-N	10.25	140.63	123.20
1	G	196	ARG	CB-CA-C	9.98	130.36	110.40
1	R	27	VAL	O-C-N	9.88	138.50	122.70

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	G	2523	0	2515	794	25
1	R	2523	0	2518	780	20
2	G	10	0	0	6	0
2	R	10	0	0	3	0
3	G	44	0	24	14	0
3	R	44	0	26	8	0
All	All	5154	0	5083	1561	25

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 153.

The worst 5 of 1561 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:R:1:GLY:CA	1:R:28:ASP:HA	1.14	1.57
1:G:3:VAL:H	1:G:27:VAL:CG1	1.19	1.55
1:R:3:VAL:CB	1:R:27:VAL:HG13	1.32	1.55
1:R:1:GLY:C	1:R:28:ASP:HA	1.30	1.49
1:R:3:VAL:HG23	1:R:27:VAL:CG2	1.41	1.48

The worst 5 of 25 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:R:267:GLY:CA	1:G:166:HIS:ND1[3_545]	1.06	1.14
1:R:263:GLU:OE1	1:G:260:VAL:CA[3_545]	1.27	0.93
1:R:308:LYS:CG	1:G:173:LEU:CD1[2_555]	1.33	0.87
1:R:260:VAL:CA	1:G:263:GLU:OE1[3_545]	1.45	0.75
1:R:263:GLU:OE2	1:G:259:LYS:O[3_545]	1.52	0.68

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%)	198 (60%)	68 (20%)	66 (20%)	0	1
1	R	332/334 (99%)	205 (62%)	58 (18%)	69 (21%)	0	1
All	All	664/668 (99%)	403 (61%)	126 (19%)	135 (20%)	0	1

5 of 135 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	2	LYS
1	R	4	LYS
1	R	12	ARG
1	R	26	LYS
1	R	30	VAL

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	G	267/267 (100%)	140 (52%)	127 (48%)	0	0
1	R	267/267 (100%)	143 (54%)	124 (46%)	0	0
All	All	534/534 (100%)	283 (53%)	251 (47%)	0	0

5 of 251 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	301	GLU
1	G	56	HIS
1	G	284	ASP
1	R	308	LYS
1	G	18	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	R	303	ASN
1	R	329	HIS
1	G	154	ASN
1	R	289	ASN
1	G	166	HIS

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 ⓘ

6 ligands are modelled in this entry.

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	336	-	38,48,48	2.76	10 (26%)	47,73,73	2.68	14 (29%)
2	SO4	G	338	-	4,4,4	0.51	0	6,6,6	0.11	0
2	SO4	G	340	1	4,4,4	0.52	0	6,6,6	0.10	0
3	NAD	R	336	-	38,48,48	1.40	4 (10%)	47,73,73	2.14	8 (17%)
2	SO4	R	338	-	4,4,4	0.51	0	6,6,6	0.11	0
2	SO4	R	340	1	4,4,4	0.52	0	6,6,6	0.10	0

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	336	-	1/1/11/11	0/22/62/62	0/5/5/5
2	SO4	G	338	-	-	0/0/0/0	0/0/0/0
2	SO4	G	340	1	-	0/0/0/0	0/0/0/0
3	NAD	R	336	-	-	0/22/62/62	0/5/5/5
2	SO4	R	338	-	-	0/0/0/0	0/0/0/0
2	SO4	R	340	1	-	0/0/0/0	0/0/0/0

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	336	NAD	C2B-C3B	-7.73	1.32	1.53
3	G	336	NAD	C3B-C4B	-6.08	1.36	1.53
3	G	336	NAD	O2B-C2B	-5.74	1.29	1.43
3	R	336	NAD	C6N-N1N	2.08	1.41	1.35
3	G	336	NAD	O4D-C4D	2.10	1.49	1.45

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	336	NAD	C1B-N9A-C4A	-9.61	112.44	126.94
3	G	336	NAD	C5N-C4N-C3N	-6.28	112.44	120.33
3	R	336	NAD	C5N-C4N-C3N	-5.94	112.86	120.33
3	G	336	NAD	C4A-C5A-N7A	-4.23	105.59	109.48
3	G	336	NAD	C2B-C1B-N9A	-3.91	108.33	114.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	336	NAD	C2B

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	336	NAD	14	0
2	G	338	SO4	4	0
2	G	340	SO4	2	0
3	R	336	NAD	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	338	SO4	2	0
2	R	340	SO4	1	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.