



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:00 AM UTC

PDB ID : 1YJ8 / pdb_00001yj8
Title : Initial structural analysis of Plasmodium falciparum Glycerol-3-phosphate dehydrogenase
Authors : Robien, M.A.; Hol, W.G.J.; Structural Genomics of Pathogenic Protozoa Consortium (SGPP)
Deposited on : 2005-01-13
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

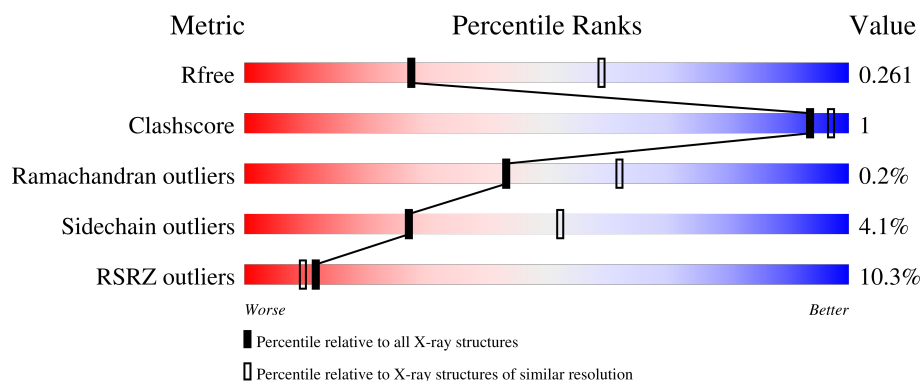
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 $\leq 5\%$. 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	375	6% 90% 5% 5%
1	B	375	11% 87% 7% 5%
1	C	375	12% 87% 8% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8425 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 glycerol-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2812	1806	466	522	18			
1	B	357	Total	C	N	O	S	0	0	0
			2806	1802	464	522	18			
1	C	357	Total	C	N	O	S	0	0	0
			2797	1796	462	521	18			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP Q8I5P5
A	2	ALA	-	cloning artifact	UNP Q8I5P5
A	3	HIS	-	cloning artifact	UNP Q8I5P5
A	4	HIS	-	cloning artifact	UNP Q8I5P5
A	5	HIS	-	cloning artifact	UNP Q8I5P5
A	6	HIS	-	cloning artifact	UNP Q8I5P5
A	7	HIS	-	cloning artifact	UNP Q8I5P5
A	8	HIS	-	cloning artifact	UNP Q8I5P5
B	1	MET	-	cloning artifact	UNP Q8I5P5
B	2	ALA	-	cloning artifact	UNP Q8I5P5
B	3	HIS	-	cloning artifact	UNP Q8I5P5
B	4	HIS	-	cloning artifact	UNP Q8I5P5
B	5	HIS	-	cloning artifact	UNP Q8I5P5
B	6	HIS	-	cloning artifact	UNP Q8I5P5
B	7	HIS	-	cloning artifact	UNP Q8I5P5
B	8	HIS	-	cloning artifact	UNP Q8I5P5
C	1	MET	-	cloning artifact	UNP Q8I5P5
C	2	ALA	-	cloning artifact	UNP Q8I5P5
C	3	HIS	-	cloning artifact	UNP Q8I5P5
C	4	HIS	-	cloning artifact	UNP Q8I5P5
C	5	HIS	-	cloning artifact	UNP Q8I5P5
C	6	HIS	-	cloning artifact	UNP Q8I5P5
C	7	HIS	-	cloning artifact	UNP Q8I5P5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	8	HIS	-	cloning artifact	UNP Q8I5P5

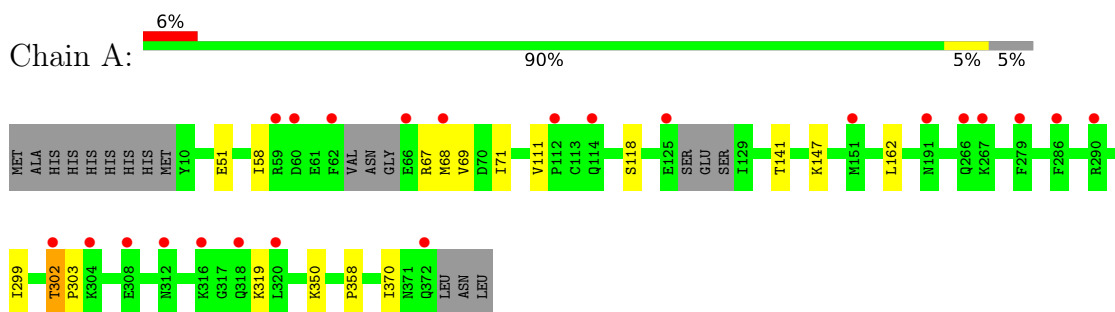
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total 4	O 4	0	0
2	B	3	Total 3	O 3	0	0
2	C	3	Total 3	O 3	0	0

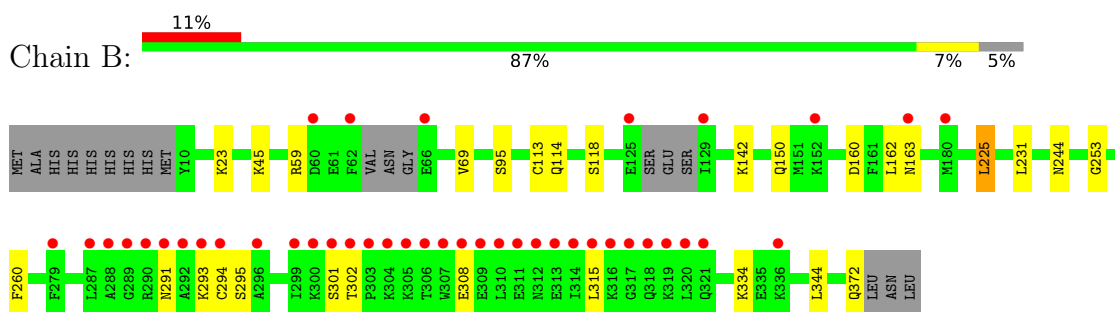
3 Residue-property plots [i](#)

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.

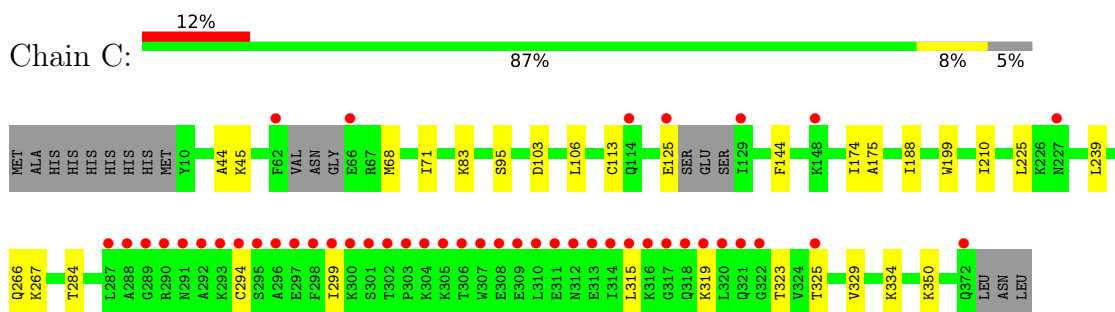
- Molecule 1: glycerol-3-phosphate dehydrogenase



- Molecule 1: glycerol-3-phosphate dehydrogenase



- Molecule 1: glycerol-3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	177.46Å 177.46Å 232.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.54 – 2.85 44.54 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.0 (44.54-2.85) 99.0 (44.54-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.236 , 0.256 0.240 , 0.261	Depositor DCC
R_{free} test set	2557 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	58.7	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8425	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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	0.47	0/2862	0.76	1/3861 (0.0%)
1	B	0.50	0/2856	0.74	1/3855 (0.0%)
1	C	0.48	0/2847	0.74	0/3844
All	All	0.48	0/8565	0.75	2/11560 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	LEU	N-CA-C	-5.07	103.35	110.35
1	A	162	LEU	N-CA-C	-5.03	103.41	110.35

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	2812	0	2844	8	0
1	B	2806	0	2826	5	0
1	C	2797	0	2808	10	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	1	0
All	All	8425	0	8478	23	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 1.

All (23) 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:A:111:VAL:O	1:A:141:THR:HG21	2.02	0.59
1:A:302:THR:HB	1:A:303:PRO:HD3	1.85	0.59
1:A:58:ILE:HD11	1:A:69:VAL:HA	1.87	0.56
1:C:144:PHE:HE1	1:C:325:THR:HG22	1.73	0.53
1:C:294:CYS:SG	1:C:315:LEU:HG	2.49	0.52
1:A:302:THR:CB	1:A:303:PRO:HD3	2.41	0.51
1:B:69:VAL:HG21	1:B:95:SER:HB3	1.95	0.48
1:C:68:MET:HE3	1:C:71:ILE:HB	1.94	0.48
1:C:44:ALA:O	2:C:501:HOH:O	2.20	0.47
1:A:111:VAL:C	1:A:141:THR:HG21	2.40	0.47
1:C:239:LEU:HG	1:C:299:ILE:HG21	1.97	0.45
1:A:302:THR:CB	1:A:303:PRO:CD	2.95	0.45
1:B:294:CYS:SG	1:B:315:LEU:HD21	2.57	0.45
1:B:253:GLY:HA2	1:B:344:LEU:HD23	1.99	0.44
1:C:188:ILE:HD12	1:C:210:ILE:HG21	2.00	0.43
1:B:225:LEU:HD11	1:B:260:PHE:CD2	2.53	0.43
1:C:225:LEU:HD22	1:C:329:VAL:HG21	2.02	0.41
1:B:231:LEU:HD12	1:B:295:SER:HB3	2.02	0.41
1:A:68:MET:HE3	1:A:71:ILE:HB	2.01	0.41
1:C:144:PHE:CE1	1:C:325:THR:HG22	2.53	0.40
1:C:174:ILE:O	1:C:175:ALA:C	2.64	0.40
1:A:299:ILE:HD11	1:A:358:PRO:HB3	2.03	0.40
1:C:106:LEU:HB3	1:C:199:TRP:CH2	2.56	0.40

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	351/375 (94%)	342 (97%)	8 (2%)	1 (0%)	36	54
1	B	351/375 (94%)	338 (96%)	12 (3%)	1 (0%)	36	54
1	C	351/375 (94%)	341 (97%)	10 (3%)	0	100	100
All	All	1053/1125 (94%)	1021 (97%)	30 (3%)	2 (0%)	43	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	THR
1	B	291	ASN

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	314/333 (94%)	307 (98%)	7 (2%)	45	69
1	B	312/333 (94%)	294 (94%)	18 (6%)	18	38
1	C	310/333 (93%)	297 (96%)	13 (4%)	26	51
All	All	936/999 (94%)	898 (96%)	38 (4%)	27	52

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	GLU
1	A	67	ARG
1	A	118	SER
1	A	147	LYS
1	A	319	LYS
1	A	350	LYS
1	A	370	ILE
1	B	23	LYS
1	B	45	LYS
1	B	59	ARG
1	B	113	CYS

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Mol	Chain	Res	Type
1	B	114	GLN
1	B	118	SER
1	B	142	LYS
1	B	150	GLN
1	B	160	ASP
1	B	163	ASN
1	B	225	LEU
1	B	244	ASN
1	B	293	LYS
1	B	301	SER
1	B	302	THR
1	B	308	GLU
1	B	334	LYS
1	B	372	GLN
1	C	45	LYS
1	C	83	LYS
1	C	95	SER
1	C	103	ASP
1	C	113	CYS
1	C	125	GLU
1	C	266	GLN
1	C	267	LYS
1	C	284	THR
1	C	319	LYS
1	C	323	THR
1	C	334	LYS
1	C	350	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	191	ASN
1	B	114	GLN
1	B	150	GLN
1	B	156	ASN
1	B	163	ASN
1	B	191	ASN
1	B	200	GLN
1	B	355	ASN
1	C	74	ASN
1	C	114	GLN

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Mol	Chain	Res	Type
1	C	150	GLN
1	C	173	ASN
1	C	182	ASN
1	C	191	ASN

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, 95th 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 ²)	Q < 0.9
1	A	357/375 (95%)	0.55	23 (6%)	25 19	35, 55, 78, 92	2 (0%)
1	B	357/375 (95%)	0.68	42 (11%)	9 7	39, 56, 105, 113	0
1	C	357/375 (95%)	0.81	45 (12%)	8 6	39, 56, 108, 115	0
All	All	1071/1125 (95%)	0.68	110 (10%)	12 10	35, 55, 91, 115	2 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	267	LYS	8.2
1	C	303	PRO	7.8
1	C	314	ILE	7.0
1	B	303	PRO	7.0
1	C	302	THR	7.0
1	C	304	LYS	6.8
1	A	266	GLN	6.8
1	B	291	ASN	6.4
1	C	307	TRP	6.1
1	B	302	THR	6.1
1	C	292	ALA	6.0
1	C	320	LEU	5.9
1	B	304	LYS	5.9
1	C	301	SER	5.6
1	C	315	LEU	5.5
1	C	310	LEU	5.4
1	B	314	ILE	4.9
1	C	306	THR	4.9
1	B	306	THR	4.9
1	B	320	LEU	4.8
1	B	292	ALA	4.5
1	B	310	LEU	4.4
1	B	301	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	291	ASN	4.4
1	C	299	ILE	4.3
1	A	279	PHE	4.3
1	C	293	LYS	4.3
1	C	305	LYS	4.3
1	C	319	LYS	4.3
1	B	289	GLY	4.3
1	C	311	GLU	4.2
1	C	300	LYS	4.1
1	C	316	LYS	3.9
1	C	309	GLU	3.9
1	B	318	GLN	3.9
1	C	296	ALA	3.9
1	B	313	GLU	3.8
1	C	318	GLN	3.8
1	C	313	GLU	3.8
1	A	302	THR	3.8
1	C	289	GLY	3.7
1	B	305	LYS	3.7
1	A	114	GLN	3.6
1	B	316	LYS	3.6
1	B	294	CYS	3.6
1	C	312	ASN	3.6
1	B	299	ILE	3.6
1	B	315	LEU	3.6
1	B	288	ALA	3.6
1	B	290	ARG	3.6
1	A	312	ASN	3.5
1	B	287	LEU	3.5
1	B	307	TRP	3.5
1	B	319	LYS	3.4
1	A	66	GLU	3.4
1	C	294	CYS	3.4
1	C	288	ALA	3.4
1	C	317	GLY	3.4
1	C	66	GLU	3.4
1	A	62	PHE	3.3
1	B	293	LYS	3.2
1	B	309	GLU	3.2
1	B	60	ASP	3.2
1	C	287	LEU	3.2
1	B	317	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	66	GLU	3.0
1	C	321	GLN	3.0
1	C	125	GLU	2.9
1	A	318	GLN	2.9
1	A	304	LYS	2.9
1	A	60	ASP	2.9
1	C	298	PHE	2.8
1	B	312	ASN	2.8
1	C	372	GLN	2.7
1	C	290	ARG	2.7
1	B	125	GLU	2.7
1	A	125	GLU	2.7
1	C	322	GLY	2.7
1	B	300	LYS	2.7
1	A	316	LYS	2.6
1	C	129	ILE	2.6
1	B	62	PHE	2.6
1	B	180	MET	2.6
1	B	296	ALA	2.6
1	C	295	SER	2.6
1	B	311	GLU	2.6
1	B	152	LYS	2.6
1	C	325	THR	2.6
1	B	308	GLU	2.5
1	C	227	ASN	2.5
1	A	191	ASN	2.5
1	A	112	PRO	2.5
1	C	148	LYS	2.4
1	A	308	GLU	2.4
1	C	297	GLU	2.4
1	B	163	ASN	2.3
1	A	320	LEU	2.3
1	A	372	GLN	2.3
1	C	114	GLN	2.2
1	C	62	PHE	2.2
1	A	286	PHE	2.2
1	B	129	ILE	2.1
1	B	321	GLN	2.1
1	A	151	MET	2.1
1	B	336	LYS	2.1
1	A	59	ARG	2.0
1	A	290	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	279	PHE	2.0
1	C	308	GLU	2.0
1	A	68	MET	2.0

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 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.