



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:54 AM UTC

PDB ID : 8S3G / pdb_00008s3g
Title : Atomic structure of truncated worm GdH
Authors : Mourao, A.; Sattler, M.; Geerlof, A.
Deposited on : 2024-02-20
Resolution : 2.29 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

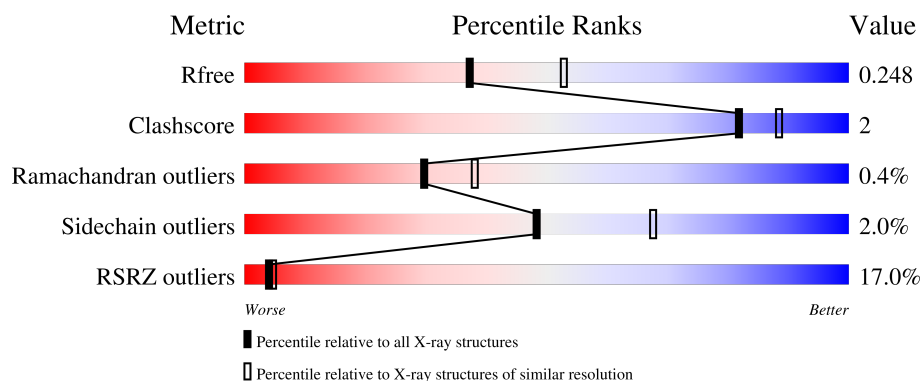
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	537	5% 88% 5% 6%
1	B	537	27% 86% 7% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7920 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 Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	2	0
			3882	2470	667	722	23			
1	B	504	Total	C	N	O	S	0	0	0
			3864	2458	662	722	22			

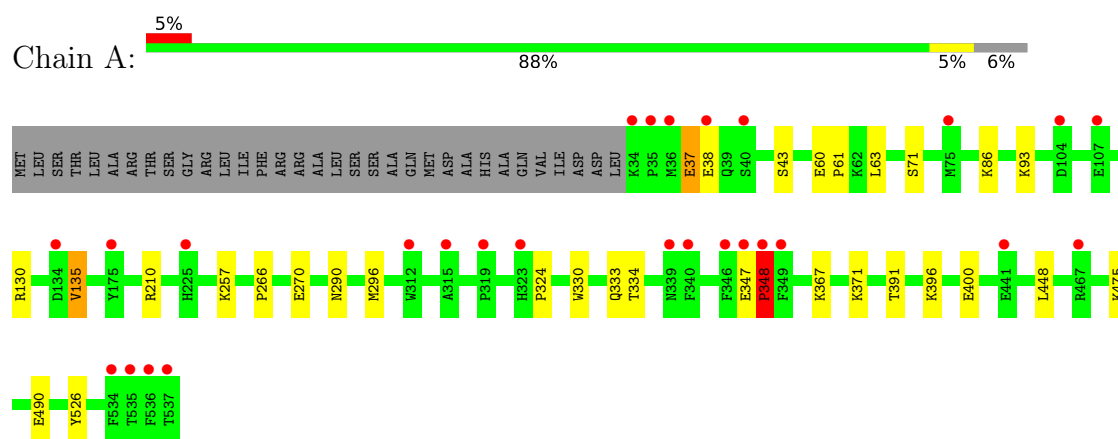
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	95	Total	O	0	0
			95	95		
2	B	79	Total	O	0	0
			79	79		

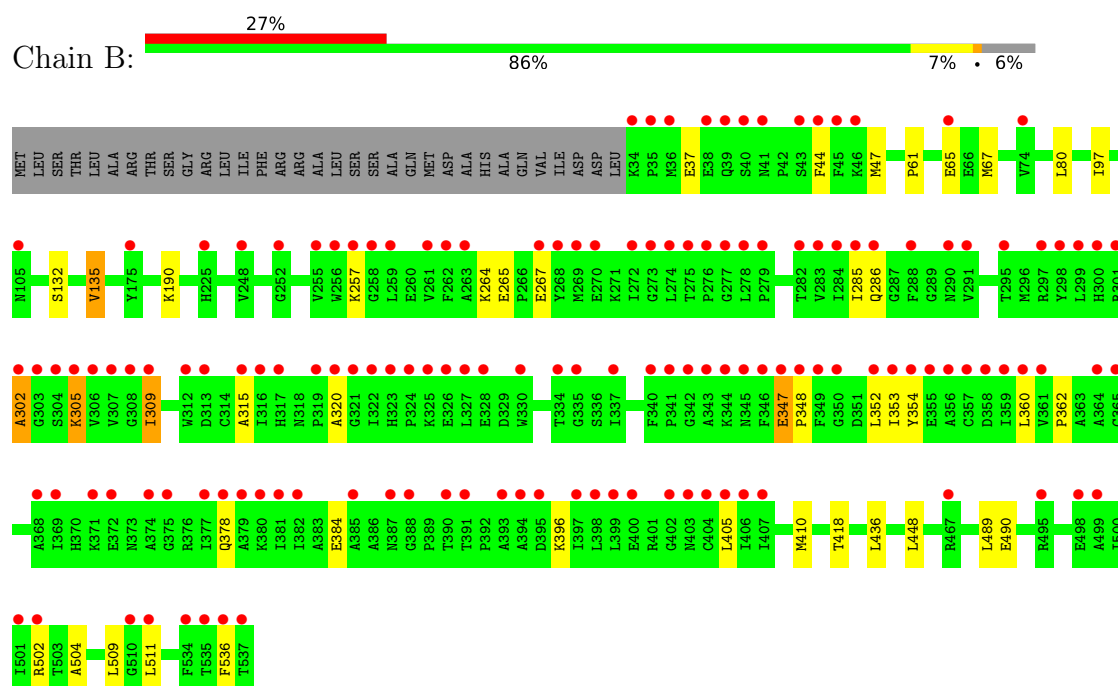
3 Residue-property plots [i](#)

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: Glutamate dehydrogenase



- Molecule 1: Glutamate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.25Å 151.25Å 146.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.51 – 2.29 97.51 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.3 (97.51-2.29) 99.4 (97.51-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.224 , 0.248 0.224 , 0.248	Depositor DCC
R_{free} test set	4222 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7920	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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	0.38	0/3974	0.52	0/5376
1	B	0.38	0/3949	0.50	0/5343
All	All	0.38	0/7923	0.51	0/10719

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	302	ALA	Peptide

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	3882	0	3853	14	0
1	B	3864	0	3826	25	0
2	A	95	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	79	0	0	3	0
All	All	7920	0	7679	38	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.

All (38) 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:B:315:ALA:HB1	1:B:352:LEU:HD12	1.48	0.96
1:B:257:LYS:HE3	1:B:490:GLU:HG2	1.62	0.81
1:B:44:PHE:HA	1:B:47:MET:HE3	1.68	0.75
1:B:37:GLU:OE2	1:B:37:GLU:N	2.25	0.66
1:B:37:GLU:HB2	1:B:396:LYS:HD2	1.82	0.60
1:A:38:GLU:O	1:A:371:LYS:NZ	2.34	0.57
1:A:347:GLU:O	1:A:348:PRO:C	2.46	0.56
1:B:285:ILE:HB	1:B:309:ILE:HD13	1.87	0.55
1:B:353:ILE:HG22	1:B:360:LEU:HD11	1.89	0.54
1:A:93:LYS:HG2	1:B:97:ILE:HG22	1.88	0.54
1:B:286:GLN:HB3	1:B:362:PRO:HA	1.89	0.53
1:B:302:ALA:HB1	2:B:660:HOH:O	2.11	0.50
1:A:266:PRO:O	1:A:270:GLU:HG2	2.12	0.50
1:B:61:PRO:O	1:B:65:GLU:HG2	2.12	0.48
1:B:418:THR:HG21	1:B:489:LEU:HA	1.95	0.48
1:B:347:GLU:CB	1:B:348:PRO:HD3	2.44	0.48
1:A:37:GLU:HB2	1:A:396:LYS:HD3	1.96	0.47
1:B:265:GLU:HG3	1:B:267:GLU:OE2	2.14	0.47
1:A:396:LYS:HE3	1:A:400:GLU:OE2	2.15	0.47
1:B:502:ARG:HB3	2:B:625:HOH:O	2.13	0.46
1:B:410:MET:HE2	1:B:410:MET:HB2	1.80	0.46
1:A:296:MET:HE3	1:A:324:PRO:HB3	1.97	0.46
1:B:354:TYR:O	1:B:378:GLN:NE2	2.50	0.45
1:B:504:ALA:HA	1:B:509:LEU:HD12	1.99	0.45
1:A:290:ASN:ND2	2:A:602:HOH:O	2.50	0.45
1:A:330:TRP:CE2	1:A:334:THR:HG21	2.52	0.44
1:B:37:GLU:H	1:B:37:GLU:CD	2.20	0.44
1:A:63:LEU:HD22	1:A:526:TYR:CD2	2.53	0.43
1:B:405:LEU:HD13	1:B:511:LEU:HD22	2.00	0.43
1:A:130:ARG:HD2	1:A:135:VAL:HG12	2.01	0.43
1:A:60:GLU:HB3	1:A:61:PRO:HD3	2.01	0.42
1:A:257:LYS:HE2	1:A:490:GLU:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:SER:O	1:B:135:VAL:HG13	2.20	0.42
1:B:405:LEU:HB2	1:B:511:LEU:HD22	2.02	0.42
1:A:367:LYS:HG2	1:A:391:THR:HG22	2.02	0.41
1:B:67:MET:SD	1:B:80:LEU:HD23	2.61	0.41
1:B:305:LYS:HE3	1:B:320:ALA:O	2.21	0.40
1:B:264:LYS:HD2	2:B:636:HOH:O	2.21	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	504/537 (94%)	489 (97%)	14 (3%)	1 (0%)	43	55
1	B	502/537 (94%)	474 (94%)	25 (5%)	3 (1%)	21	27
All	All	1006/1074 (94%)	963 (96%)	39 (4%)	4 (0%)	30	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	348	PRO
1	B	536	PHE
1	B	384	GLU
1	B	347	GLU

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	A	402/435 (92%)	392 (98%)	10 (2%)	42	60
1	B	399/435 (92%)	393 (98%)	6 (2%)	57	75
All	All	801/870 (92%)	785 (98%)	16 (2%)	48	67

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	43	SER
1	A	71	SER
1	A	86	LYS
1	A	135	VAL
1	A	210	ARG
1	A	333	GLN
1	A	348	PRO
1	A	448	LEU
1	A	475	LYS
1	B	135	VAL
1	B	190	LYS
1	B	305	LYS
1	B	309	ILE
1	B	436	LEU
1	B	448	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	HIS
1	A	290	ASN
1	A	413	ASN
1	A	450	GLN
1	B	290	ASN
1	B	294	HIS
1	B	387	ASN
1	B	445	ASN

5.3.3 RNA ⓘ

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	504/537 (93%)	0.50	27 (5%) 31 33	25, 40, 64, 85	2 (0%)
1	B	504/537 (93%)	1.27	144 (28%) 1 1	25, 46, 87, 105	0
All	All	1008/1074 (93%)	0.88	171 (16%) 4 5	25, 42, 80, 105	2 (0%)

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	536	PHE	8.3
1	B	536	PHE	8.1
1	B	320	ALA	6.5
1	B	321	GLY	6.5
1	B	306	VAL	6.4
1	B	35	PRO	6.2
1	B	348	PRO	6.0
1	A	34	LYS	5.9
1	B	353	ILE	5.6
1	A	323[A]	HIS	5.5
1	B	40	SER	5.3
1	B	38	GLU	5.2
1	B	34	LYS	5.1
1	B	537	THR	5.0
1	B	356	ALA	5.0
1	B	382	ILE	4.9
1	B	352	LEU	4.9
1	B	263	ALA	4.9
1	B	175	TYR	4.9
1	B	302	ALA	4.9
1	A	537	THR	4.9
1	B	256	TRP	4.6
1	B	36	MET	4.6
1	B	534	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	404	CYS	4.5
1	B	535	THR	4.4
1	A	348	PRO	4.4
1	B	304	SER	4.4
1	B	369	ILE	4.4
1	B	349	PHE	4.4
1	B	379	ALA	4.4
1	B	343	ALA	4.3
1	B	340	PHE	4.3
1	B	262	PHE	4.3
1	B	347	GLU	4.2
1	B	277	GLY	4.2
1	B	377	ILE	4.2
1	A	35	PRO	4.2
1	B	357	CYS	4.2
1	A	40	SER	4.1
1	A	535	THR	4.1
1	B	39	GLN	4.1
1	B	309	ILE	4.0
1	B	312	TRP	4.0
1	B	399	LEU	3.9
1	B	298	TYR	3.9
1	A	347	GLU	3.9
1	B	381	ILE	3.8
1	B	360	LEU	3.8
1	B	346	PHE	3.8
1	B	270	GLU	3.7
1	B	313	ASP	3.7
1	B	380	LYS	3.7
1	B	368	ALA	3.7
1	B	322	ILE	3.6
1	B	278	LEU	3.5
1	B	325	LYS	3.5
1	B	288	PHE	3.5
1	B	395	ASP	3.5
1	B	74	VAL	3.4
1	B	365	CYS	3.4
1	A	175	TYR	3.4
1	B	308	GLY	3.4
1	B	398	LEU	3.4
1	B	388	GLY	3.3
1	B	276	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	364	ALA	3.3
1	B	406	ILE	3.3
1	B	324	PRO	3.3
1	A	38	GLU	3.3
1	B	344	LYS	3.3
1	B	319	PRO	3.2
1	B	337	ILE	3.2
1	B	350	GLY	3.2
1	B	397	ILE	3.2
1	B	269	MET	3.2
1	B	291	VAL	3.2
1	B	359	ILE	3.2
1	B	402	GLY	3.1
1	B	390	THR	3.1
1	B	307	VAL	3.1
1	B	316	ILE	3.0
1	B	511	LEU	3.0
1	B	295	THR	2.9
1	B	248	VAL	2.9
1	B	361	VAL	2.9
1	B	282	THR	2.9
1	B	323	HIS	2.9
1	B	299	LEU	2.9
1	B	341	PRO	2.8
1	B	394	ALA	2.8
1	B	326	GLU	2.8
1	B	301	ARG	2.8
1	B	317	HIS	2.8
1	B	330	TRP	2.8
1	B	391	THR	2.8
1	B	495	ARG	2.8
1	B	510	GLY	2.8
1	A	75[A]	MET	2.8
1	A	534	PHE	2.8
1	B	261	VAL	2.8
1	B	45	PHE	2.7
1	B	375	GLY	2.7
1	A	107	GLU	2.7
1	A	349	PHE	2.7
1	B	284	ILE	2.7
1	B	257	LYS	2.7
1	B	267	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	41	ASN	2.7
1	B	315	ALA	2.6
1	B	342	GLY	2.6
1	B	345	ASN	2.6
1	B	393	ALA	2.6
1	B	283	VAL	2.6
1	B	305	LYS	2.6
1	B	378	GLN	2.6
1	A	315	ALA	2.6
1	B	44	PHE	2.6
1	B	354	TYR	2.6
1	B	403	ASN	2.5
1	B	358	ASP	2.5
1	B	334	THR	2.5
1	A	441	GLU	2.5
1	B	268	TYR	2.5
1	B	335	GLY	2.5
1	B	43	SER	2.5
1	B	286	GLN	2.5
1	B	290	ASN	2.4
1	B	255	VAL	2.4
1	B	272	ILE	2.4
1	A	134	ASP	2.4
1	A	312	TRP	2.4
1	B	300	HIS	2.4
1	A	340	PHE	2.4
1	B	400	GLU	2.4
1	B	371	LYS	2.3
1	B	407	ILE	2.3
1	B	502	ARG	2.3
1	B	498	GLU	2.3
1	B	303	GLY	2.3
1	B	467	ARG	2.3
1	B	501	ILE	2.3
1	B	279	PRO	2.3
1	B	65	GLU	2.3
1	B	328	GLU	2.3
1	A	319	PRO	2.2
1	B	385	ALA	2.2
1	B	285	ILE	2.2
1	B	274	LEU	2.2
1	A	339	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	36	MET	2.2
1	B	275	THR	2.2
1	B	297	ARG	2.2
1	B	387	ASN	2.2
1	B	374	ALA	2.2
1	A	225	HIS	2.2
1	B	252	GLY	2.2
1	B	258	GLY	2.2
1	B	46	LYS	2.1
1	A	104	ASP	2.1
1	A	346	PHE	2.1
1	B	327	LEU	2.1
1	B	355	GLU	2.1
1	B	372	GLU	2.1
1	B	273	GLY	2.1
1	B	405	LEU	2.1
1	B	105	ASN	2.1
1	B	499	ALA	2.0
1	B	259	LEU	2.0
1	B	225	HIS	2.0
1	A	467	ARG	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.