



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:37 PM GMT

PDB ID : 2PME  
Title : The Apo crystal Structure of the glycyl-tRNA synthetase  
Authors : Xie, W.  
Deposited on : 2007-04-21  
Resolution : 2.90 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

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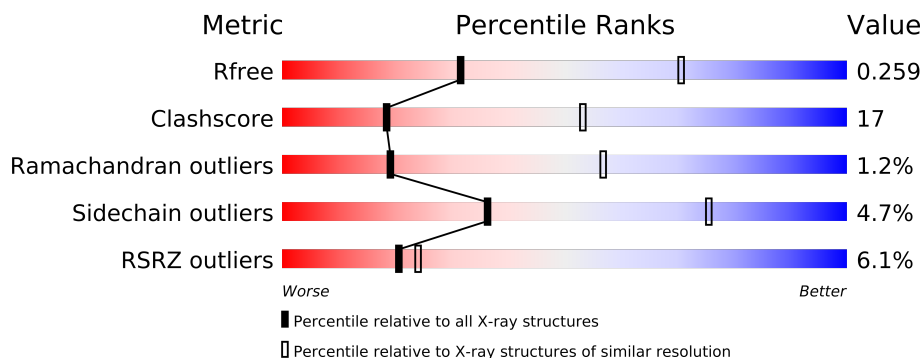
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	693	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4258 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Glycyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	0	0
			4136	2632	715	766	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	686	LEU	-	CLONING ARTIFACT	UNP P41250
A	687	GLU	-	CLONING ARTIFACT	UNP P41250
A	688	HIS	-	CLONING ARTIFACT	UNP P41250
A	689	HIS	-	CLONING ARTIFACT	UNP P41250
A	690	HIS	-	CLONING ARTIFACT	UNP P41250
A	691	HIS	-	CLONING ARTIFACT	UNP P41250
A	692	HIS	-	CLONING ARTIFACT	UNP P41250
A	693	HIS	-	CLONING ARTIFACT	UNP P41250

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	122	Total	O	0	0
			122	122		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.74Å 91.74Å 247.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.83 – 2.90 36.83 – 2.90	Depositor EDS
% Data completeness (in resolution range)	77.3 (36.83-2.90) 77.4 (36.83-2.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.28 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.230 , 0.271 0.223 , 0.259	Depositor DCC
$R_{free}$ test set	978 reflections (5.50%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.1	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 33.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 18744 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4258	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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	0.24	0/4229	0.43	0/5711

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	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	GLY	Peptide
1	A	625	LYS	Peptide

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4136	0	4039	137	0
2	A	122	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4258	0	4039	137	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (137) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:542:ARG:HG2	1:A:542:ARG:HH11	1.12	1.06
1:A:622:THR:HA	2:A:808:HOH:O	1.57	1.03
1:A:507:PHE:CE2	1:A:517:VAL:HG22	2.02	0.93
1:A:617:THR:HG23	1:A:631:THR:HG23	1.50	0.91
1:A:225:ASN:OD1	2:A:799:HOH:O	1.91	0.89
1:A:542:ARG:CG	1:A:542:ARG:HH11	1.90	0.84
1:A:140:HIS:HB3	1:A:227:MET:CE	2.10	0.81
1:A:212:PRO:HD2	1:A:213:ILE:H	1.45	0.81
1:A:314:VAL:HG11	1:A:357:GLY:HA3	1.62	0.80
1:A:210:LYS:O	1:A:211:SER:O	2.00	0.80
1:A:629:THR:N	2:A:808:HOH:O	2.17	0.77
1:A:633:ARG:HG3	1:A:640:GLN:HG2	1.65	0.76
1:A:553:PHE:O	1:A:635:ARG:NH2	2.18	0.76
1:A:140:HIS:CB	1:A:227:MET:HE1	2.16	0.75
1:A:140:HIS:HB3	1:A:227:MET:HE1	1.69	0.75
1:A:227:MET:SD	2:A:790:HOH:O	2.45	0.74
1:A:265:LEU:HB2	1:A:266:PRO:HD3	1.70	0.73
1:A:534:VAL:O	1:A:538:THR:HB	1.91	0.70
1:A:538:THR:HG23	1:A:552:SER:N	2.06	0.70
1:A:172:MET:HE1	2:A:780:HOH:O	1.90	0.69
1:A:571:GLN:O	1:A:573:PHE:N	2.26	0.69
1:A:664:ASP:O	1:A:668:ARG:HD2	1.93	0.67
1:A:538:THR:HG23	1:A:552:SER:H	1.59	0.67
1:A:140:HIS:O	2:A:799:HOH:O	2.12	0.66
1:A:248:GLN:NE2	2:A:700:HOH:O	2.28	0.66
1:A:144:PHE:CD2	1:A:144:PHE:O	2.49	0.65
1:A:542:ARG:NH1	1:A:542:ARG:HG2	1.94	0.65
1:A:227:MET:CE	1:A:244:PRO:HG3	2.26	0.65
1:A:69:LYS:NZ	2:A:804:HOH:O	2.29	0.64
1:A:113:GLN:HA	1:A:117:GLN:HG3	1.78	0.64
1:A:507:PHE:CD2	1:A:517:VAL:HG22	2.33	0.64
1:A:227:MET:HE2	1:A:244:PRO:HG3	1.79	0.63
1:A:648:LEU:HD23	1:A:651:ILE:HD11	1.81	0.63
1:A:213:ILE:O	1:A:214:THR:C	2.37	0.63
1:A:565:LEU:CD2	1:A:594:ASP:HB3	2.29	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:131:PRO:HB2	1:A:133:PRO:HD2	1.80	0.62
1:A:212:PRO:CD	1:A:213:ILE:H	2.12	0.62
1:A:210:LYS:C	1:A:211:SER:O	2.38	0.61
1:A:229:LYS:HG2	1:A:241:TYR:HE2	1.67	0.60
1:A:608:ASP:OD2	1:A:633:ARG:NH2	2.34	0.58
1:A:510:THR:CG2	1:A:514:GLU:HB3	2.34	0.57
1:A:571:GLN:C	1:A:573:PHE:H	2.07	0.57
1:A:213:ILE:O	1:A:214:THR:O	2.23	0.57
1:A:571:GLN:O	1:A:574:MET:N	2.34	0.57
1:A:574:MET:O	1:A:578:LYS:HB2	2.04	0.57
1:A:530:ILE:O	1:A:534:VAL:HG23	2.05	0.57
1:A:146:ASP:OD1	1:A:159:ARG:NH2	2.37	0.56
1:A:608:ASP:CG	1:A:633:ARG:HH22	2.09	0.56
1:A:229:LYS:HG2	1:A:241:TYR:CE2	2.41	0.56
1:A:210:LYS:O	1:A:211:SER:C	2.45	0.55
1:A:246:THR:HB	1:A:296:GLU:HG3	1.88	0.55
1:A:168:LEU:O	1:A:172:MET:HB2	2.06	0.54
1:A:571:GLN:C	1:A:573:PHE:N	2.61	0.54
1:A:622:THR:O	1:A:628:HIS:HD2	1.92	0.53
1:A:314:VAL:CG1	1:A:357:GLY:HA3	2.33	0.53
1:A:664:ASP:O	1:A:668:ARG:CD	2.57	0.53
1:A:378:HIS:HB3	2:A:695:HOH:O	2.08	0.53
1:A:77:ARG:HH22	1:A:606:ARG:HB3	1.74	0.53
1:A:378:HIS:H	1:A:378:HIS:CD2	2.25	0.52
1:A:510:THR:HG22	1:A:514:GLU:HB3	1.90	0.52
1:A:323:SER:O	1:A:327:GLN:HG3	2.09	0.52
1:A:324:ALA:HB1	1:A:379:MET:HB3	1.92	0.52
1:A:249:GLY:O	1:A:253:ASN:ND2	2.33	0.52
1:A:132:GLU:N	1:A:133:PRO:CD	2.73	0.51
1:A:322:TYR:CE2	1:A:327:GLN:HG2	2.45	0.51
1:A:543:GLU:O	1:A:544:GLY:C	2.49	0.51
1:A:608:ASP:OD1	1:A:633:ARG:NH2	2.44	0.50
1:A:172:MET:CE	2:A:780:HOH:O	2.55	0.50
1:A:574:MET:N	1:A:575:PRO:CD	2.74	0.49
1:A:556:VAL:HG13	1:A:557:VAL:HG23	1.95	0.49
1:A:140:HIS:HB3	1:A:227:MET:HE3	1.94	0.49
1:A:378:HIS:N	1:A:378:HIS:CD2	2.81	0.49
1:A:568:SER:HB3	1:A:570:ASN:HB3	1.95	0.49
1:A:355:PHE:O	1:A:359:ILE:HG13	2.13	0.48
1:A:261:ASN:O	1:A:264:LYS:HG2	2.14	0.48
1:A:507:PHE:CE2	1:A:517:VAL:CG2	2.89	0.48
1:A:107:ILE:HD13	1:A:366:VAL:HG13	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:510:THR:HG23	1:A:512:TYR:H	1.80	0.47
1:A:542:ARG:CG	1:A:542:ARG:NH1	2.58	0.47
1:A:366:VAL:HG12	1:A:534:VAL:HG21	1.97	0.47
1:A:174:ASP:OD1	1:A:176:LYS:HG2	2.16	0.46
1:A:234:PRO:O	1:A:236:GLY:N	2.49	0.46
1:A:369:SER:HA	1:A:370:PRO:HD3	1.77	0.46
1:A:538:THR:HG22	1:A:551:PHE:HD2	1.80	0.46
1:A:388:CYS:HB3	1:A:410:ARG:HG3	1.98	0.46
1:A:308:HIS:HA	1:A:309:PRO:HD3	1.80	0.46
1:A:261:ASN:O	1:A:264:LYS:CG	2.65	0.45
1:A:628:HIS:HA	2:A:808:HOH:O	2.16	0.45
1:A:327:GLN:NE2	1:A:377:GLN:O	2.50	0.44
1:A:177:CYS:SG	1:A:181:LYS:HB3	2.56	0.44
1:A:644:GLU:HG3	1:A:646:SER:H	1.81	0.44
1:A:614:PHE:CZ	1:A:655:LEU:HB3	2.53	0.44
1:A:212:PRO:CD	1:A:213:ILE:N	2.76	0.44
1:A:140:HIS:CB	1:A:227:MET:CE	2.82	0.44
1:A:339:GLY:O	1:A:343:GLU:HG3	2.18	0.44
1:A:608:ASP:CG	1:A:633:ARG:NH2	2.71	0.44
1:A:320:TYR:HA	1:A:335:LYS:HA	1.99	0.44
1:A:532:TYR:HA	1:A:535:PHE:CD1	2.52	0.44
1:A:295:ALA:HB3	1:A:525:PHE:HB2	2.00	0.44
1:A:507:PHE:HE2	1:A:517:VAL:HG13	1.82	0.44
1:A:193:ASP:N	1:A:193:ASP:OD2	2.51	0.44
1:A:144:PHE:CE2	1:A:226:LEU:HB2	2.53	0.43
1:A:358:ARG:HD3	2:A:705:HOH:O	2.18	0.43
1:A:565:LEU:HD23	1:A:594:ASP:HB3	1.99	0.43
1:A:378:HIS:CE1	1:A:390:CYS:HB2	2.53	0.43
1:A:648:LEU:N	1:A:649:PRO:CD	2.82	0.43
1:A:211:SER:HB3	1:A:215:GLY:HA2	2.00	0.43
1:A:580:LEU:HD12	1:A:618:ILE:HD11	2.00	0.42
1:A:564:VAL:HG22	1:A:593:VAL:HA	2.00	0.42
1:A:210:LYS:HB3	1:A:210:LYS:HE3	1.86	0.42
1:A:543:GLU:HB2	2:A:805:HOH:O	2.19	0.42
1:A:211:SER:OG	1:A:212:PRO:CD	2.67	0.42
1:A:144:PHE:O	1:A:144:PHE:CG	2.71	0.42
1:A:340:ASP:HA	1:A:343:GLU:CD	2.40	0.42
1:A:227:MET:HE3	1:A:244:PRO:HG3	2.02	0.42
1:A:565:LEU:HD22	1:A:594:ASP:HB3	2.02	0.42
1:A:510:THR:HG21	1:A:514:GLU:HB3	2.01	0.42
1:A:340:ASP:O	1:A:343:GLU:HB2	2.20	0.42
1:A:288:ARG:NH1	2:A:764:HOH:O	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:507:PHE:CE2	1:A:517:VAL:HG13	2.55	0.42
1:A:77:ARG:HD3	1:A:77:ARG:HA	1.79	0.42
1:A:542:ARG:NH2	1:A:635:ARG:O	2.53	0.41
1:A:140:HIS:HB2	1:A:227:MET:HE1	1.99	0.41
1:A:604:TYR:OH	1:A:617:THR:HG22	2.20	0.41
1:A:641:ILE:HD13	1:A:665:VAL:CG1	2.50	0.41
1:A:622:THR:O	1:A:628:HIS:CD2	2.72	0.41
1:A:258:LEU:HD22	1:A:508:GLN:HG2	2.03	0.41
1:A:363:LEU:HB3	1:A:368:ILE:HD12	2.02	0.41
1:A:172:MET:HE2	1:A:172:MET:HB2	1.91	0.41
1:A:580:LEU:HD11	1:A:616:VAL:HG11	2.03	0.41
1:A:393:ALA:HB3	1:A:405:VAL:HB	2.03	0.41
1:A:594:ASP:OD1	1:A:594:ASP:C	2.59	0.41
1:A:135:LEU:HD13	1:A:227:MET:SD	2.61	0.40
1:A:297:ILE:HB	1:A:523:PRO:HD2	2.03	0.40
1:A:254:PHE:CD1	1:A:415:LEU:HD11	2.56	0.40
1:A:572:GLU:H	1:A:572:GLU:HG3	1.60	0.40
1:A:76:ARG:NH2	1:A:609:GLU:OE2	2.29	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	513/693 (74%)	476 (93%)	31 (6%)	6 (1%)	19 57

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	SER
1	A	214	THR
1	A	235	GLY
1	A	572	GLU
1	A	212	PRO

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Mol	Chain	Res	Type
1	A	234	PRO

### 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	446/600 (74%)	425 (95%)	21 (5%)	36 75

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	GLU
1	A	129	LEU
1	A	138	SER
1	A	154	ASN
1	A	210	LYS
1	A	214	THR
1	A	248	GLN
1	A	278	ASN
1	A	301	VAL
1	A	319	LEU
1	A	352	LEU
1	A	378	HIS
1	A	542	ARG
1	A	549	THR
1	A	570	ASN
1	A	571	GLN
1	A	580	LEU
1	A	584	LEU
1	A	590	SER
1	A	617	THR
1	A	631	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	A	169	GLN
1	A	206	ASN
1	A	261	ASN
1	A	278	ASN
1	A	570	ASN
1	A	571	GLN
1	A	628	HIS
1	A	640	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues

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	521/693 (75%)	0.23	32 (6%) 21 24	20, 51, 96, 118	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	511	LEU	6.5
1	A	513	VAL	5.4
1	A	508	GLN	5.4
1	A	153	LYS	5.4
1	A	515	GLU	5.1
1	A	152	VAL	5.0
1	A	420	ARG	4.8
1	A	507	PHE	4.8
1	A	512	TYR	4.5
1	A	154	ASN	3.9
1	A	510	THR	3.5
1	A	142	ASP	3.5
1	A	626	THR	3.5
1	A	505	LYS	3.4
1	A	509	LYS	3.4
1	A	175	LYS	3.3
1	A	63	ASP	3.3
1	A	380	GLU	3.3
1	A	514	GLU	3.2
1	A	572	GLU	3.1
1	A	214	THR	3.1
1	A	237	ASN	2.8
1	A	213	ILE	2.8
1	A	179	VAL	2.7
1	A	569	GLN	2.7
1	A	265	LEU	2.6
1	A	571	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	544	GLY	2.5
1	A	197	GLN	2.3
1	A	173	SER	2.3
1	A	331	GLN	2.3
1	A	194	ASN	2.1

## 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.