



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 02:38 AM UTC

PDB ID : 9Z0Y / pdb_00009z0y
Title : Crystal structure of Neisseria gonorrhoeae penicillin-binding protein 2 from strain FA19 containing seven resistance mutations and three epistatic mutations
Authors : Singh, A.; Bala, S.; Davies, C.
Deposited on : 2025-11-03
Resolution : 1.46 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

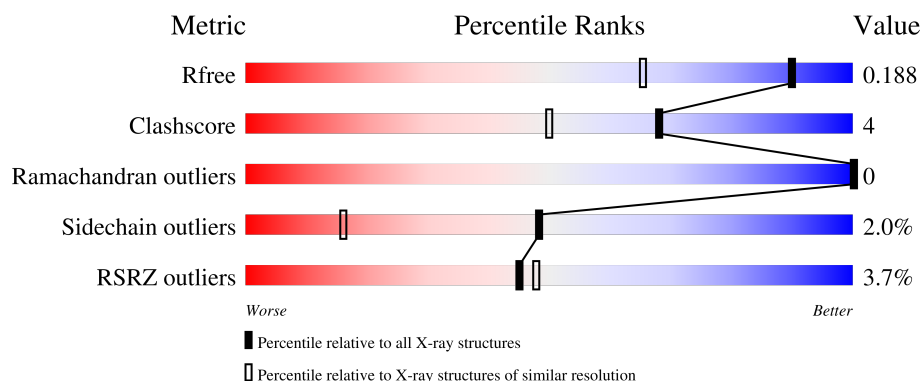
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

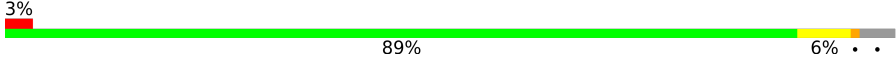
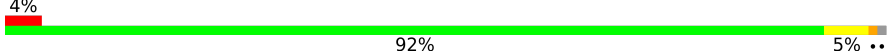
The reported resolution of this entry is 1.46 Å.

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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	329	
1	B	329	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5391 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 Penicillin-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	8	0
			2445	1555	431	449	10			
1	B	325	Total	C	N	O	S	0	11	0
			2545	1615	451	471	8			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	GLY	-	expression tag	UNP A0AB74EE38
A	233	SER	-	expression tag	UNP A0AB74EE38
A	234	GLY	-	expression tag	UNP A0AB74EE38
A	235	GLY	-	expression tag	UNP A0AB74EE38
A	236	ALA	-	expression tag	UNP A0AB74EE38
A	297	GLY	ALA	conflict	UNP A0AB74EE38
A	?	-	TYR	deletion	UNP A0AB74EE38
A	?	-	ASP	deletion	UNP A0AB74EE38
A	?	-	PRO	deletion	UNP A0AB74EE38
A	?	-	ASN	deletion	UNP A0AB74EE38
A	?	-	ARG	deletion	UNP A0AB74EE38
A	?	-	PRO	deletion	UNP A0AB74EE38
A	?	-	GLY	deletion	UNP A0AB74EE38
A	?	-	ARG	deletion	UNP A0AB74EE38
A	?	-	ALA	deletion	UNP A0AB74EE38
A	?	-	ASP	deletion	UNP A0AB74EE38
A	?	-	SER	deletion	UNP A0AB74EE38
A	?	-	GLU	deletion	UNP A0AB74EE38
A	?	-	GLN	deletion	UNP A0AB74EE38
A	?	-	ARG	deletion	UNP A0AB74EE38
A	311	VAL	ALA	engineered mutation	UNP A0AB74EE38
A	312	MET	ILE	engineered mutation	UNP A0AB74EE38
A	316	PRO	VAL	engineered mutation	UNP A0AB74EE38
A	437	VAL	ALA	engineered mutation	UNP A0AB74EE38
A	447	VAL	LEU	engineered mutation	UNP A0AB74EE38

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Chain	Residue	Modelled	Actual	Comment	Reference
A	462	ILE	PHE	engineered mutation	UNP A0AB74EE38
A	483	SER	THR	engineered mutation	UNP A0AB74EE38
A	504	LEU	PHE	engineered mutation	UNP A0AB74EE38
A	512	TYR	ASN	engineered mutation	UNP A0AB74EE38
A	545	SER	GLY	engineered mutation	UNP A0AB74EE38
B	232	GLY	-	expression tag	UNP A0AB74EE38
B	233	SER	-	expression tag	UNP A0AB74EE38
B	234	GLY	-	expression tag	UNP A0AB74EE38
B	235	GLY	-	expression tag	UNP A0AB74EE38
B	236	ALA	-	expression tag	UNP A0AB74EE38
B	297	GLY	ALA	conflict	UNP A0AB74EE38
B	?	-	TYR	deletion	UNP A0AB74EE38
B	?	-	ASP	deletion	UNP A0AB74EE38
B	?	-	PRO	deletion	UNP A0AB74EE38
B	?	-	ASN	deletion	UNP A0AB74EE38
B	?	-	ARG	deletion	UNP A0AB74EE38
B	?	-	PRO	deletion	UNP A0AB74EE38
B	?	-	GLY	deletion	UNP A0AB74EE38
B	?	-	ARG	deletion	UNP A0AB74EE38
B	?	-	ALA	deletion	UNP A0AB74EE38
B	?	-	ASP	deletion	UNP A0AB74EE38
B	?	-	SER	deletion	UNP A0AB74EE38
B	?	-	GLU	deletion	UNP A0AB74EE38
B	?	-	GLN	deletion	UNP A0AB74EE38
B	?	-	ARG	deletion	UNP A0AB74EE38
B	311	VAL	ALA	engineered mutation	UNP A0AB74EE38
B	312	MET	ILE	engineered mutation	UNP A0AB74EE38
B	316	PRO	VAL	engineered mutation	UNP A0AB74EE38
B	437	VAL	ALA	engineered mutation	UNP A0AB74EE38
B	447	VAL	LEU	engineered mutation	UNP A0AB74EE38
B	462	ILE	PHE	engineered mutation	UNP A0AB74EE38
B	483	SER	THR	engineered mutation	UNP A0AB74EE38
B	504	LEU	PHE	engineered mutation	UNP A0AB74EE38
B	512	TYR	ASN	engineered mutation	UNP A0AB74EE38
B	545	SER	GLY	engineered mutation	UNP A0AB74EE38

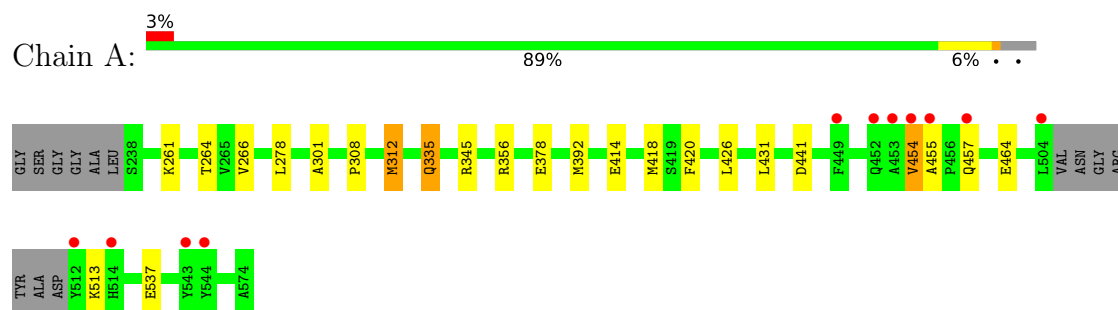
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	203	Total O 203 203	0	0
2	B	198	Total O 198 198	0	0

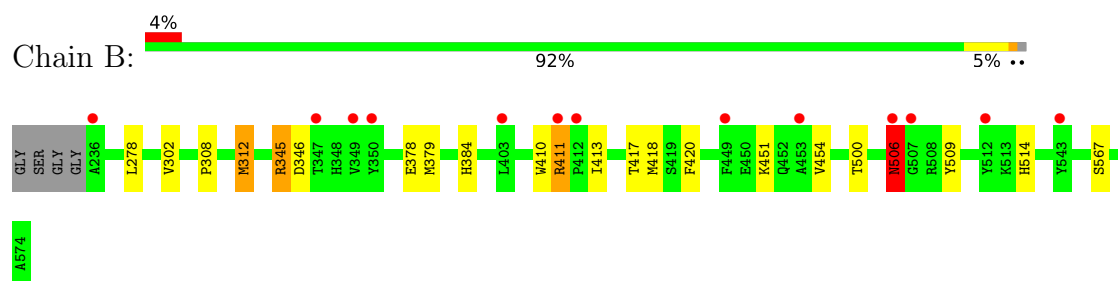
3 Residue-property plots

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: Penicillin-binding protein 2



- Molecule 1: Penicillin-binding protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.34Å 79.59Å 81.37Å 90.00° 90.45° 90.00°	Depositor
Resolution (Å)	36.25 – 1.46 36.25 – 1.46	Depositor EDS
% Data completeness (in resolution range)	99.4 (36.25-1.46) 99.5 (36.25-1.46)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 1.46Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.162 , 0.188 0.162 , 0.188	Depositor DCC
R_{free} test set	5009 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.739	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.012 for -h,-l,-k 0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5391	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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

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	0.70	0/2512	1.08	2/3402 (0.1%)
1	B	0.77	2/2619 (0.1%)	1.20	9/3550 (0.3%)
All	All	0.74	2/5131 (0.0%)	1.15	11/6952 (0.2%)

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	346	ASP	CG-OD2	5.19	1.35	1.25
1	B	384	HIS	ND1-CE1	5.08	1.37	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	ASP	CA-CB-CG	12.39	124.99	112.60
1	B	312	MET	CG-SD-CE	-10.05	78.80	100.90
1	B	506	ASN	CA-CB-CG	-7.67	104.93	112.60
1	B	420	PHE	CB-CA-C	7.54	123.17	111.02
1	B	346	ASP	CB-CA-C	7.34	121.82	109.48
1	A	420	PHE	CA-CB-CG	6.72	120.52	113.80
1	B	345	ARG	CG-CD-NE	-6.03	98.74	112.00
1	B	346	ASP	N-CA-C	-5.66	100.47	109.76
1	A	312	MET	CG-SD-CE	-5.48	88.85	100.90
1	B	379	MET	CG-SD-CE	-5.37	89.09	100.90
1	B	420	PHE	CA-CB-CG	5.12	118.92	113.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	345	ARG	Sidechain
1	B	411	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	A	2445	0	2511	17	0
1	B	2545	0	2594	19	0
2	A	203	0	0	4	0
2	B	198	0	0	2	0
All	All	5391	0	5105	36	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 4.

All (36) 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:500:THR:HG23	1:B:514[B]:HIS:CD2	2.04	0.92
1:B:378[A]:GLU:HG3	2:B:767:HOH:O	1.81	0.80
1:B:500:THR:HG23	1:B:514[B]:HIS:HD2	1.45	0.80
1:A:513:LYS:HG3	1:A:537:GLU:CD	2.14	0.73
1:A:266:VAL:HG22	1:A:278:LEU:CD2	2.23	0.69
1:B:308:PRO:CG	1:B:312:MET:HG3	2.28	0.63
1:B:500:THR:CG2	1:B:514[B]:HIS:CD2	2.80	0.63
1:B:308:PRO:HG3	1:B:312:MET:HG3	1.80	0.62
1:A:266:VAL:HG22	1:A:278:LEU:HD23	1.82	0.61
1:A:414:GLU:O	1:A:418[B]:MET:HG3	2.03	0.58
1:B:506:ASN:HB3	1:B:509[A]:TYR:HB2	1.86	0.57
1:B:308:PRO:CG	1:B:312:MET:CG	2.83	0.56
1:B:410:TRP:CE2	1:B:418:MET:HE1	2.41	0.56
1:B:308:PRO:HG3	1:B:312:MET:CG	2.36	0.56
1:B:506:ASN:HB2	2:B:652:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:GLN:NE2	2:A:605:HOH:O	2.43	0.52
1:A:356[A]:ARG:NH2	2:A:601:HOH:O	2.14	0.51
1:A:378:GLU:HG3	2:A:773:HOH:O	2.10	0.50
1:A:426:LEU:HG	1:A:431[B]:LEU:HG	1.95	0.48
1:A:441:ASP:HB3	1:A:464:GLU:HG3	1.96	0.48
1:B:308:PRO:HG2	1:B:312:MET:HG3	1.96	0.47
1:B:278:LEU:C	1:B:278:LEU:HD23	2.40	0.47
1:A:264:THR:CG2	1:A:301:ALA:HB2	2.46	0.46
1:B:411:ARG:HB3	1:B:411:ARG:NH2	2.31	0.45
1:A:312:MET:HE3	1:A:312:MET:HB3	1.72	0.44
1:A:308:PRO:CG	1:A:312:MET:HG3	2.48	0.44
1:A:454:VAL:HG22	1:A:455:ALA:O	2.18	0.44
1:B:312:MET:HB3	1:B:312:MET:HE3	1.49	0.44
1:B:413:ILE:O	1:B:417:THR:HG23	2.18	0.43
1:A:392[A]:MET:HG3	2:A:710:HOH:O	2.19	0.43
1:B:506:ASN:HB3	1:B:509[B]:TYR:HB2	2.01	0.43
1:B:308:PRO:CG	1:B:312:MET:HG2	2.49	0.43
1:A:392[A]:MET:HE2	1:A:392[A]:MET:HB3	1.63	0.43
1:B:411:ARG:CG	1:B:411:ARG:HH21	2.31	0.42
1:A:308:PRO:HG2	1:A:312:MET:HG3	2.02	0.41
1:A:264:THR:HG21	1:A:301:ALA:HB2	2.03	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	320/329 (97%)	318 (99%)	2 (1%)	0	100	100
1	B	334/329 (102%)	330 (99%)	4 (1%)	0	100	100
All	All	654/658 (99%)	648 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	260/260 (100%)	255 (98%)	5 (2%)	50	17
1	B	270/260 (104%)	265 (98%)	5 (2%)	50	17
All	All	530/520 (102%)	520 (98%)	10 (2%)	48	17

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	261	LYS
1	A	335	GLN
1	A	345	ARG
1	A	454	VAL
1	A	457	GLN
1	B	302	VAL
1	B	451	LYS
1	B	454	VAL
1	B	506	ASN
1	B	567	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	335	GLN
1	A	360	GLN
1	A	425	GLN
1	A	472	ASN
1	B	241	GLN
1	B	506	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	316/329 (96%)	0.06	11 (3%)	47 49	9, 21, 38, 58	8 (2%)
1	B	325/329 (98%)	0.11	13 (4%)	42 45	8, 20, 35, 51	11 (3%)
All	All	641/658 (97%)	0.09	24 (3%)	45 48	8, 21, 36, 58	19 (2%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	507	GLY	5.5
1	A	504	LEU	5.3
1	A	454	VAL	4.5
1	B	543	TYR	4.4
1	B	347	THR	3.9
1	A	543	TYR	3.8
1	B	506	ASN	3.7
1	A	512	TYR	3.5
1	A	544	TYR	3.4
1	A	455	ALA	3.3
1	B	236	ALA	3.2
1	B	449	PHE	2.7
1	B	350	TYR	2.6
1	B	411	ARG	2.6
1	B	512	TYR	2.5
1	A	514	HIS	2.5
1	A	453	ALA	2.4
1	B	412	PRO	2.4
1	B	349	VAL	2.3
1	A	457	GLN	2.3
1	A	452	GLN	2.3
1	B	403	LEU	2.3
1	B	453	ALA	2.1
1	A	449	PHE	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.