



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 03:57 AM UTC

PDB ID : 9Z0W / pdb_00009z0w
Title : Crystal structure of Neisseria gonorrhoeae penicillin-binding protein 2 from strain FA19 containing six resistance mutations
Authors : Singh, A.; Bala, S.; Davies, C.
Deposited on : 2025-11-03
Resolution : 2.15 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

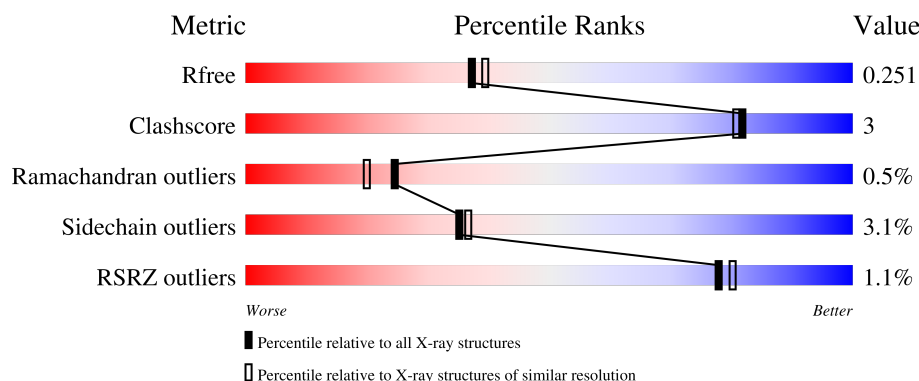
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

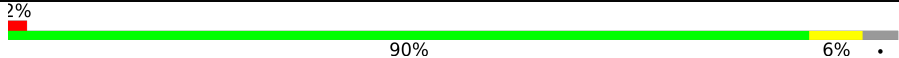

The reported resolution of this entry is 2.15 Å.

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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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 3 unique types of molecules in this entry. The entry contains 4957 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	0	0
			2404	1525	426	445	8			
1	B	325	Total	C	N	O	S	0	0	0
			2472	1567	439	458	8			

There are 52 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	504	LEU	PHE	engineered mutation	UNP A0AB74EE38
A	512	TYR	ASN	engineered mutation	UNP A0AB74EE38

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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	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 PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		

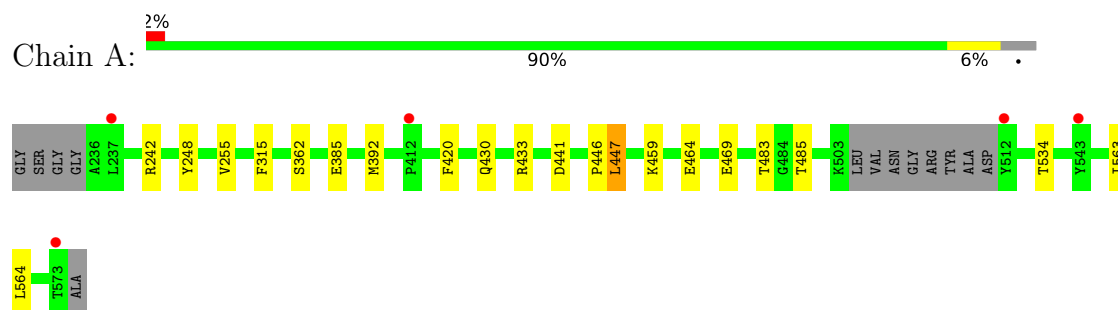
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total	O	0	0
			22	22		
3	B	54	Total	O	0	0
			54	54		

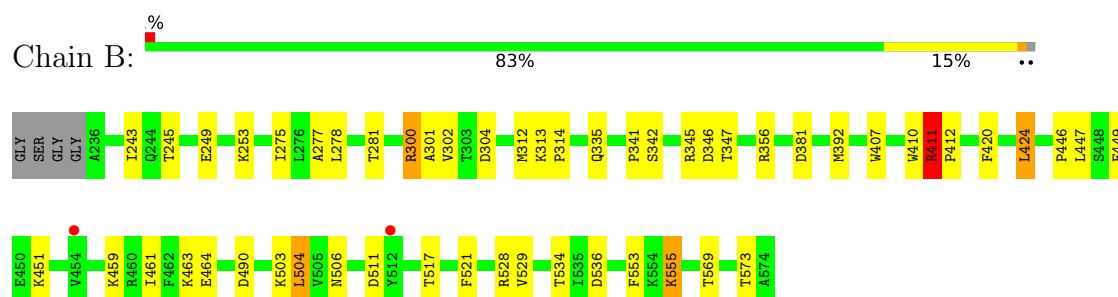
3 Residue-property plots [i](#)

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: 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	44.88Å 77.05Å 87.78Å 90.00° 91.95° 90.00°	Depositor
Resolution (Å)	35.85 – 2.15 35.85 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.7 (35.85-2.15) 94.7 (35.85-2.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.187 , 0.246 0.193 , 0.251	Depositor DCC
R_{free} test set	1760 reflections (5.37%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4957	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% 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

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.59	0/2454	1.11	5/3326 (0.2%)
1	B	0.65	0/2524	1.20	15/3423 (0.4%)
All	All	0.62	0/4978	1.16	20/6749 (0.3%)

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	4

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	347	THR	CA-CB-OG1	-6.82	99.37	109.60
1	B	503	LYS	N-CA-CB	-6.78	100.07	110.65
1	B	503	LYS	CB-CA-C	6.71	121.29	110.16
1	B	446	PRO	CB-CA-C	-6.55	102.54	112.11
1	B	490	ASP	CA-CB-CG	6.40	119.00	112.60
1	A	248	TYR	N-CA-CB	6.08	118.89	110.07
1	A	483	THR	CA-CB-OG1	-5.98	100.63	109.60
1	B	253	LYS	N-CA-CB	-5.84	101.52	110.16
1	B	281	THR	CA-CB-OG1	-5.80	100.90	109.60
1	A	385	GLU	N-CA-CB	-5.80	100.77	110.39
1	B	312	MET	CG-SD-CE	-5.70	88.36	100.90
1	B	573	THR	CA-CB-OG1	-5.69	101.07	109.60
1	B	511	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	420	PHE	CA-CB-CG	5.60	119.40	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	ASP	CA-CB-CG	5.52	118.12	112.60
1	B	420	PHE	CA-CB-CG	5.46	119.26	113.80
1	B	341	PRO	CB-CA-C	-5.40	104.45	112.55
1	A	315	PHE	CA-CB-CG	-5.36	108.44	113.80
1	B	536	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	569	THR	CA-CB-OG1	-5.15	101.87	109.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	300	ARG	Sidechain
1	B	356	ARG	Sidechain
1	B	411	ARG	Sidechain
1	B	528	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	2404	0	2439	7	0
1	B	2472	0	2505	19	0
2	B	5	0	0	0	0
3	A	22	0	0	0	0
3	B	54	0	0	1	0
All	All	4957	0	4944	25	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 3.

All (25) 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:275:ILE:HD13	1:B:449:PHE:CE2	2.29	0.66
1:A:433:ARG:HG3	1:A:447:LEU:HD13	1.78	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:LEU:HD23	1:B:504:LEU:C	2.24	0.62
1:B:517:THR:HG22	1:B:534:THR:HG22	1.83	0.60
1:A:446:PRO:O	1:A:447:LEU:HB2	2.01	0.59
1:B:300:ARG:HG2	1:B:304:ASP:OD2	2.08	0.54
1:B:459:LYS:HE3	1:B:461:ILE:HD11	1.94	0.48
1:B:313:LYS:N	1:B:314:PRO:CD	2.78	0.46
1:B:243:ILE:HG22	1:B:277:ALA:HB2	1.96	0.46
1:B:521:PHE:HA	1:B:529:VAL:O	2.14	0.46
1:A:441:ASP:HB3	1:A:464:GLU:HG3	1.99	0.45
1:B:411:ARG:HH11	1:B:412:PRO:HD2	1.82	0.44
1:B:555:LYS:N	1:B:555:LYS:HD3	2.33	0.44
1:A:392:MET:HE2	1:A:430:GLN:CG	2.49	0.43
1:B:245:THR:O	1:B:249:GLU:HG3	2.19	0.43
1:B:463:LYS:NZ	3:B:710:HOH:O	2.51	0.43
1:B:278:LEU:HD11	1:B:301:ALA:HB3	1.99	0.42
1:A:392:MET:HE2	1:A:430:GLN:HG3	2.01	0.42
1:B:424:LEU:HD23	1:B:424:LEU:O	2.19	0.42
1:B:553:PHE:CD2	1:B:553:PHE:C	2.98	0.42
1:B:392:MET:HE3	1:B:392:MET:HB3	1.84	0.42
1:A:242:ARG:HB3	1:A:563:ILE:HD13	2.02	0.41
1:A:459:LYS:NZ	1:B:381:ASP:OD2	2.48	0.41
1:B:407:TRP:HA	1:B:410:TRP:CD1	2.54	0.41
1:B:275:ILE:HD13	1:B:449:PHE:CD2	2.55	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	312/329 (95%)	309 (99%)	2 (1%)	1 (0%)	36	34
1	B	323/329 (98%)	317 (98%)	4 (1%)	2 (1%)	21	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	635/658 (96%)	626 (99%)	6 (1%)	3 (0%)	24	20

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	506	ASN
1	A	447	LEU
1	B	447	LEU

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	252/259 (97%)	246 (98%)	6 (2%)	43	47
1	B	258/259 (100%)	248 (96%)	10 (4%)	28	28
All	All	510/518 (98%)	494 (97%)	16 (3%)	35	37

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

Mol	Chain	Res	Type
1	A	255	VAL
1	A	362	SER
1	A	469	GLU
1	A	485	THR
1	A	534	THR
1	A	564	LEU
1	B	302	VAL
1	B	335	GLN
1	B	342	SER
1	B	345	ARG
1	B	411	ARG
1	B	424	LEU
1	B	451	LYS
1	B	464	GLU
1	B	504	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	555	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	335	GLN
1	A	425	GLN
1	A	472	ASN
1	B	425	GLN

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](#)

1 ligand is 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	$\# Z > 2$
2	PO4	B	601	-	4,4,4	1.00	0	6,6,6	0.35	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

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%)	0.19	5 (1%) 70 74	34, 53, 72, 97	0
1	B	325/329 (98%)	0.01	2 (0%) 85 87	30, 41, 61, 79	0
All	All	641/658 (97%)	0.10	7 (1%) 78 80	30, 47, 70, 97	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	412	PRO	3.6
1	A	512	TYR	3.2
1	A	543	TYR	2.5
1	B	512	TYR	2.2
1	A	573	THR	2.1
1	A	237	LEU	2.1
1	B	454	VAL	2.1

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PO4	B	601	5/5	0.91	0.17	54,60,67,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.