



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:33 PM UTC

PDB ID : 7PCR / pdb_00007pcr
Title : Helicobacter pylori RNase J
Authors : Luisi, B.F.; Pei, X.Y.
Deposited on : 2021-08-03
Resolution : 2.75 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

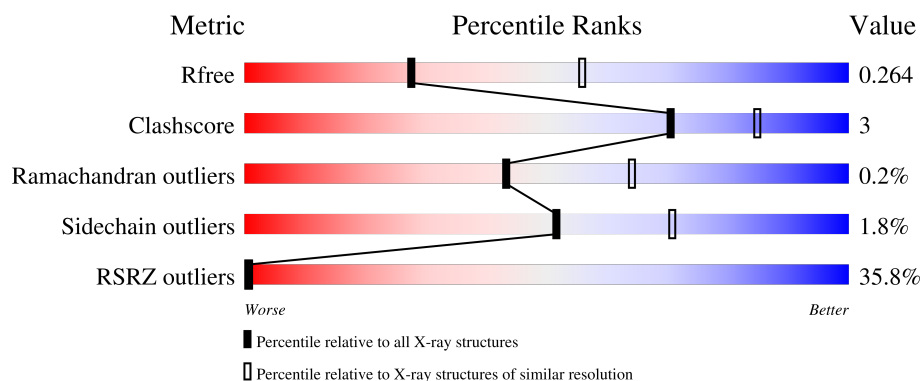
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	553	36% 90% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7943 atoms, of which 3869 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 Ribonuclease J.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	553	Total	C	H	N	O	S	0	1	0
			7933	2584	3869	701	767	12			

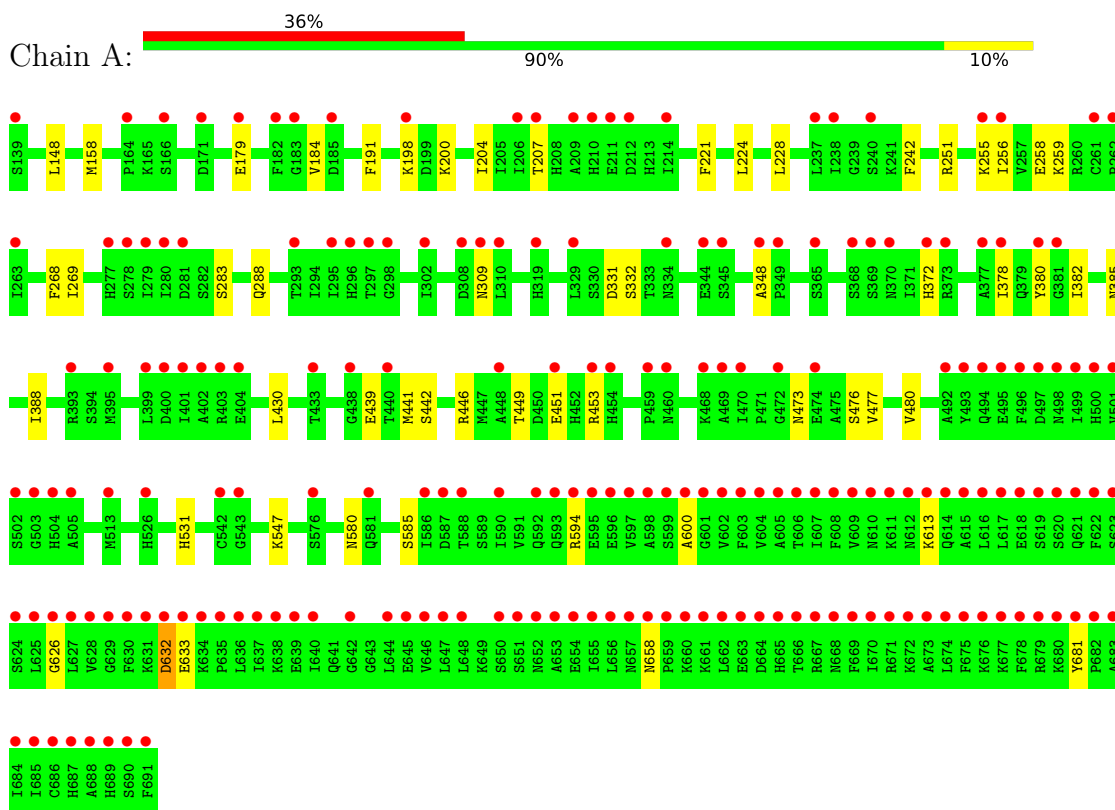
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	10	Total	O	0	0
			10	10		

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: Ribonuclease J



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	158.49Å 158.49Å 214.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.03 – 2.75 56.03 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.2 (56.03-2.75) 99.1 (56.03-2.75)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.245 , 0.267 0.241 , 0.264	Depositor DCC
R_{free} test set	1805 reflections (0.84%)	wwPDB-VP
Wilson B-factor (Å ²)	75.8	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 86.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.020 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.027 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7943	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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	0.60	2/4147 (0.0%)	0.89	9/5627 (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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	633	GLU	C-O	6.08	1.31	1.24
1	A	633	GLU	N-CA	5.15	1.52	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	ARG	N-CA-C	-7.94	103.48	113.01
1	A	613	LYS	N-CA-C	-6.60	105.80	114.31
1	A	632	ASP	O-C-N	-6.12	114.41	122.42
1	A	681	TYR	CA-C-N	6.09	126.06	120.03
1	A	681	TYR	C-N-CA	6.09	126.06	120.03
1	A	658	ASN	CA-C-N	5.87	126.28	119.47
1	A	658	ASN	C-N-CA	5.87	126.28	119.47
1	A	331	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	242	PHE	CA-CB-CG	5.08	118.88	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	632	ASP	Mainchain

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	4064	3869	3869	27	1
2	A	10	0	0	0	0
All	All	4074	3869	3869	27	1

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 (27) 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:388:ILE:HD12	1:A:430:LEU:HD23	1.81	0.63
1:A:473:ASN:O	1:A:477:VAL:HG23	2.00	0.61
1:A:547:LYS:H	1:A:547:LYS:HE2	1.69	0.57
1:A:378:ILE:HG12	1:A:388:ILE:HG21	1.90	0.53
1:A:158:MET:HE1	1:A:191:PHE:HD1	1.74	0.52
1:A:269:ILE:HB	1:A:288:GLN:HB2	1.91	0.52
1:A:332:SER:O	1:A:531:HIS:HB3	2.11	0.51
1:A:476:SER:O	1:A:480:VAL:HG23	2.10	0.51
1:A:441:MET:HB3	1:A:480:VAL:HG21	1.95	0.49
1:A:148:LEU:HD13	1:A:158:MET:HE3	1.93	0.49
1:A:221:PHE:HA	1:A:224:LEU:O	2.13	0.48
1:A:378:ILE:O	1:A:382:ILE:HG23	2.14	0.47
1:A:441:MET:HE1	1:A:476:SER:CB	2.44	0.47
1:A:439:GLU:OE2	1:A:580:ASN:ND2	2.43	0.47
1:A:453:ARG:CZ	1:A:453:ARG:HA	2.45	0.47
1:A:179:GLU:HB2	1:A:184:VAL:HG12	1.96	0.46
1:A:204:ILE:HB	1:A:228:LEU:HD23	1.98	0.45
1:A:441:MET:HE1	1:A:476:SER:HB2	2.00	0.43
1:A:268:PHE:O	1:A:269:ILE:HD13	2.18	0.43
1:A:442:SER:O	1:A:446:ARG:HG3	2.19	0.43
1:A:348:ALA:HB1	1:A:380:TYR:OH	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:THR:HG22	1:A:451:GLU:HG3	2.01	0.42
1:A:256:ILE:HD12	1:A:256:ILE:C	2.46	0.41
1:A:259:LYS:HE2	1:A:283:SER:OG	2.20	0.41
1:A:441:MET:HE1	1:A:476:SER:HB3	2.03	0.40
1:A:200:LYS:HE3	1:A:200:LYS:HB3	1.92	0.40
1:A:385:ASN:O	1:A:385:ASN:ND2	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:ARG:NE	1:A:626:GLY:O[16_445]	1.72	0.48

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	552/553 (100%)	531 (96%)	20 (4%)	1 (0%)	43 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	600	ALA

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	398/475 (84%)	390 (98%)	8 (2%)	48 69

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	LYS
1	A	207	THR
1	A	255[A]	LYS
1	A	255[B]	LYS
1	A	258	GLU
1	A	309	ASN
1	A	372	HIS
1	A	585	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	376	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides 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, 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	553/553 (100%)	1.96	198 (35%) ⓘ ⓘ	58, 106, 273, 394	2 (0%)

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	627	LEU	13.0
1	A	687	HIS	9.8
1	A	655	ILE	8.6
1	A	674	LEU	8.5
1	A	499	ILE	8.1
1	A	686	CYS	8.1
1	A	681	TYR	8.0
1	A	603	PHE	7.9
1	A	680	LYS	7.9
1	A	630	PHE	7.7
1	A	604	VAL	7.6
1	A	600	ALA	7.5
1	A	673	ALA	7.5
1	A	601	GLY	7.4
1	A	678	PHE	7.4
1	A	608	PHE	7.0
1	A	606	THR	7.0
1	A	626	GLY	7.0
1	A	679	ARG	7.0
1	A	682	PRO	7.0
1	A	685	ILE	6.8
1	A	622	PHE	6.7
1	A	618	GLU	6.6
1	A	624	SER	6.5
1	A	621	GLN	6.3
1	A	652	ASN	6.3
1	A	684	ILE	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	664	ASP	6.3
1	A	501	VAL	6.2
1	A	628	VAL	6.2
1	A	656	LEU	6.2
1	A	500	HIS	6.2
1	A	670	ILE	6.2
1	A	454	HIS	5.9
1	A	255[A]	LYS	5.9
1	A	675	PHE	5.9
1	A	689	HIS	5.8
1	A	658	ASN	5.8
1	A	631	LYS	5.8
1	A	261	CYS	5.8
1	A	602	VAL	5.7
1	A	542	CYS	5.7
1	A	625	LEU	5.7
1	A	691	PHE	5.7
1	A	629	GLY	5.6
1	A	610	ASN	5.5
1	A	657	ASN	5.4
1	A	644	LEU	5.4
1	A	587	ASP	5.3
1	A	497	ASP	5.3
1	A	615	ALA	5.2
1	A	668	ASN	5.1
1	A	619	SER	5.0
1	A	526	HIS	5.0
1	A	660	LYS	4.9
1	A	667	ARG	4.9
1	A	502	SER	4.8
1	A	654	GLU	4.8
1	A	594	ARG	4.8
1	A	616	LEU	4.7
1	A	623	SER	4.7
1	A	495	GLU	4.5
1	A	372	HIS	4.5
1	A	690	SER	4.5
1	A	677	LYS	4.5
1	A	676	LYS	4.4
1	A	278	SER	4.3
1	A	683	ALA	4.3
1	A	440	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	661	LYS	4.1
1	A	666	THR	4.0
1	A	498	ASN	4.0
1	A	647	LEU	4.0
1	A	672	LYS	4.0
1	A	308	ASP	3.9
1	A	612	ASN	3.9
1	A	613	LYS	3.8
1	A	596	GLU	3.8
1	A	650	SER	3.8
1	A	281	ASP	3.8
1	A	605	ALA	3.8
1	A	633	GLU	3.8
1	A	663	GLU	3.8
1	A	651	SER	3.7
1	A	653	ALA	3.7
1	A	632	ASP	3.7
1	A	469	ALA	3.7
1	A	620	SER	3.7
1	A	642	GLY	3.7
1	A	494	GLN	3.6
1	A	638	LYS	3.6
1	A	400	ASP	3.6
1	A	659	PRO	3.6
1	A	662	LEU	3.6
1	A	590	ILE	3.6
1	A	607	ILE	3.6
1	A	646	VAL	3.6
1	A	665	HIS	3.5
1	A	543	GLY	3.5
1	A	139	SER	3.4
1	A	503	GLY	3.4
1	A	598	ALA	3.4
1	A	319	HIS	3.4
1	A	645	GLU	3.3
1	A	640	ILE	3.3
1	A	459	PRO	3.3
1	A	648	LEU	3.3
1	A	581	GLN	3.2
1	A	164	PRO	3.1
1	A	393	ARG	3.1
1	A	611	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	377	ALA	3.1
1	A	597	VAL	3.1
1	A	296	HIS	3.1
1	A	637	ILE	3.1
1	A	368	SER	3.1
1	A	370	ASN	3.0
1	A	493	TYR	3.0
1	A	609	VAL	3.0
1	A	256	ILE	3.0
1	A	395	MET	3.0
1	A	617	LEU	2.9
1	A	237	LEU	2.9
1	A	504	HIS	2.9
1	A	593	GLN	2.9
1	A	182	PHE	2.9
1	A	297	THR	2.8
1	A	492	ALA	2.8
1	A	671	ARG	2.8
1	A	263	ILE	2.8
1	A	277	HIS	2.7
1	A	639	GLU	2.7
1	A	404	GLU	2.7
1	A	669	PHE	2.7
1	A	280	ILE	2.7
1	A	378	ILE	2.7
1	A	210	HIS	2.7
1	A	279	ILE	2.6
1	A	474	GLU	2.6
1	A	399	LEU	2.6
1	A	381	GLY	2.6
1	A	468	LYS	2.6
1	A	586	ILE	2.6
1	A	344	GLU	2.6
1	A	214	ILE	2.5
1	A	576	SER	2.5
1	A	171	ASP	2.5
1	A	635	PRO	2.5
1	A	293	THR	2.5
1	A	460	ASN	2.5
1	A	349	PRO	2.5
1	A	348	ALA	2.5
1	A	592	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	614	GLN	2.5
1	A	334	ASN	2.5
1	A	240	SER	2.5
1	A	209	ALA	2.5
1	A	634	LYS	2.4
1	A	369	SER	2.4
1	A	298	GLY	2.4
1	A	166	SER	2.4
1	A	588	THR	2.4
1	A	302	ILE	2.3
1	A	373	ARG	2.3
1	A	345	SER	2.3
1	A	599	SER	2.3
1	A	438	GLY	2.3
1	A	448	ALA	2.3
1	A	505	ALA	2.3
1	A	207	THR	2.3
1	A	198	LYS	2.3
1	A	211	GLU	2.3
1	A	310	LEU	2.3
1	A	295	ILE	2.3
1	A	380	TYR	2.3
1	A	403	ARG	2.3
1	A	496	PHE	2.3
1	A	688	ALA	2.2
1	A	185	ASP	2.2
1	A	636	LEU	2.2
1	A	179	GLU	2.1
1	A	453	ARG	2.1
1	A	262	PRO	2.1
1	A	472	GLY	2.1
1	A	238	ILE	2.1
1	A	402	ALA	2.1
1	A	451	GLU	2.1
1	A	513	MET	2.1
1	A	206	ILE	2.1
1	A	212	ASP	2.1
1	A	595	GLU	2.1
1	A	309	ASN	2.1
1	A	470	ILE	2.1
1	A	329	LEU	2.0
1	A	183	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	401	ILE	2.0
1	A	365	SER	2.0
1	A	433	THR	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.