



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:39 PM UTC

PDB ID : 7XS2 / pdb_00007xs2
Title : Monomer structure of HtrA from Helicobacter pylori
Authors : Cui, L.; Liu, W.
Deposited on : 2022-05-12
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
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

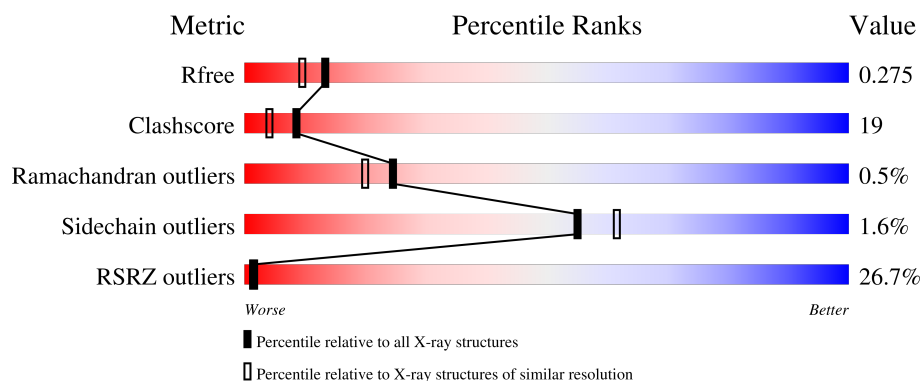
1 Overall quality at a glance

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	441	23% 60% 24% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2923 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 Periplasmic serine endoprotease DegP-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2851	1782	495	571	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MET	-	initiating methionine	UNP O25663
A	36	GLY	-	expression tag	UNP O25663
A	37	HIS	-	expression tag	UNP O25663
A	38	HIS	-	expression tag	UNP O25663
A	39	HIS	-	expression tag	UNP O25663
A	40	HIS	-	expression tag	UNP O25663
A	41	HIS	-	expression tag	UNP O25663
A	42	HIS	-	expression tag	UNP O25663

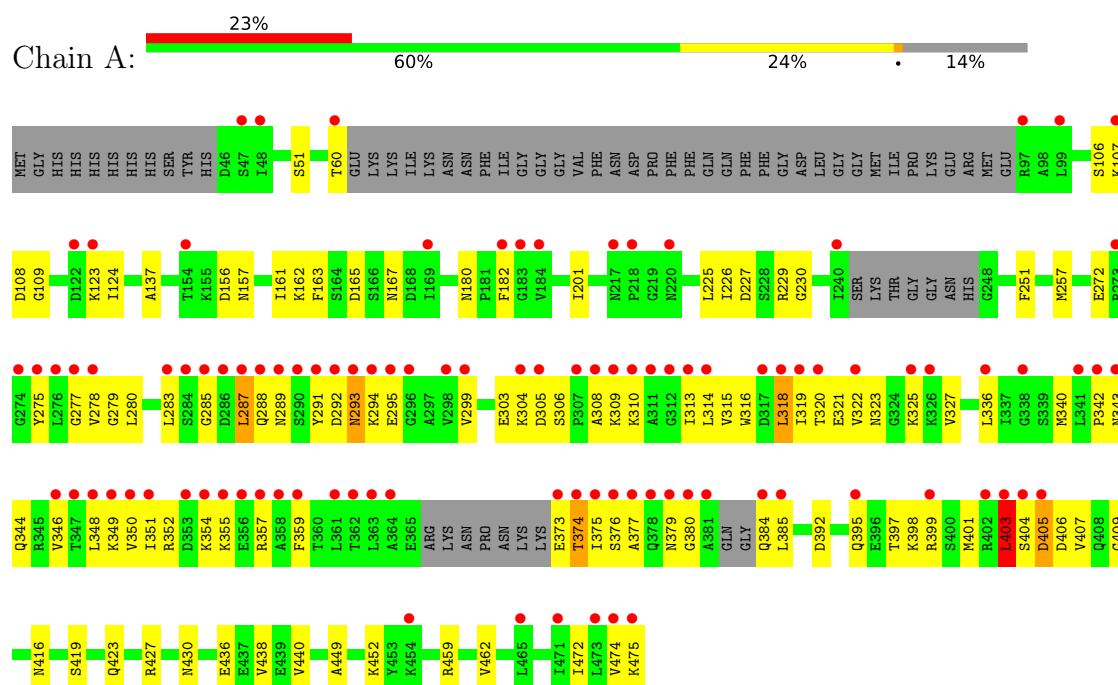
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	72	Total	O	0	0
			72	72		

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: Periplasmic serine endoprotease DegP-like



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	146.20Å 146.20Å 94.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	63.31 – 2.15 63.31 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (63.31-2.15) 100.0 (63.31-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.243 , 0.270 0.251 , 0.275	Depositor DCC
R_{free} test set	1662 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 80.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2923	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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	0.37	0/2875	0.67	2/3877 (0.1%)

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	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	403	LEU	CA-C-N	6.64	133.66	121.70
1	A	403	LEU	C-N-CA	6.64	133.66	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	293	ASN	Peptide
1	A	374	THR	Peptide
1	A	403	LEU	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	2851	0	2924	109	0
2	A	72	0	0	11	0
All	All	2923	0	2924	109	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 19.

All (109) 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:405:ASP:H	1:A:406:ASP:HA	1.11	1.10
1:A:405:ASP:N	1:A:406:ASP:HA	1.74	1.01
1:A:295:GLU:O	2:A:501:HOH:O	1.93	0.86
1:A:308:ALA:HB1	1:A:313:ILE:HD11	1.58	0.86
1:A:226:ILE:HD12	1:A:227:ASP:O	1.75	0.85
1:A:283:LEU:HD11	1:A:318:LEU:HD21	1.57	0.85
1:A:403:LEU:HD13	1:A:404:SER:O	1.78	0.83
1:A:283:LEU:HD12	1:A:295:GLU:HA	1.60	0.82
1:A:226:ILE:HD13	1:A:230:GLY:HA2	1.62	0.81
1:A:60:THR:HG22	1:A:123:LYS:HG2	1.64	0.78
1:A:395:GLN:OE1	2:A:502:HOH:O	2.02	0.76
1:A:373:GLU:OE2	2:A:503:HOH:O	2.04	0.75
1:A:452:LYS:NZ	2:A:506:HOH:O	2.22	0.73
1:A:438:VAL:HG11	1:A:449:ALA:HB2	1.72	0.71
1:A:283:LEU:HD11	1:A:318:LEU:CD2	2.22	0.69
1:A:294:LYS:N	2:A:508:HOH:O	2.27	0.67
1:A:288:GLN:O	1:A:291:TYR:N	2.26	0.67
1:A:403:LEU:HD12	1:A:403:LEU:O	1.96	0.66
1:A:403:LEU:HD12	1:A:403:LEU:C	2.21	0.66
1:A:398:LYS:HG2	1:A:403:LEU:HD11	1.76	0.66
1:A:322:VAL:HA	1:A:348:LEU:HD12	1.79	0.64
1:A:403:LEU:HA	1:A:404:SER:HB2	1.80	0.63
1:A:322:VAL:HA	1:A:348:LEU:CD1	2.30	0.62
1:A:318:LEU:C	1:A:318:LEU:HD12	2.25	0.62
1:A:405:ASP:H	1:A:406:ASP:CA	2.00	0.61
1:A:397:THR:HG22	1:A:401:MET:HE2	1.83	0.60
1:A:351:ILE:HG23	1:A:354:LYS:HA	1.85	0.59
1:A:288:GLN:NE2	2:A:511:HOH:O	2.33	0.59
1:A:318:LEU:HD12	1:A:319:ILE:N	2.17	0.59
1:A:419:SER:O	1:A:423:GLN:HG2	2.03	0.58
1:A:384:GLN:HA	1:A:475:LYS:HD3	1.86	0.57
1:A:180:ASN:ND2	1:A:182:PHE:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LYS:H	1:A:107:LYS:HD2	1.71	0.55
1:A:285:GLY:O	1:A:287:LEU:HD22	2.06	0.55
1:A:304:LYS:HD2	1:A:305:ASP:CG	2.32	0.54
1:A:374:THR:HG22	1:A:392:ASP:HB2	1.89	0.54
1:A:395:GLN:O	1:A:399:ARG:HG2	2.06	0.54
1:A:352:ARG:O	1:A:355:LYS:N	2.40	0.53
1:A:289:ASN:O	1:A:293:ASN:HB3	2.08	0.53
1:A:474:VAL:HG22	1:A:475:LYS:HG3	1.89	0.53
1:A:60:THR:O	1:A:123:LYS:HE2	2.09	0.53
1:A:303:GLU:O	1:A:304:LYS:HB3	2.08	0.52
1:A:124:ILE:HG22	1:A:137:ALA:HB3	1.91	0.52
1:A:322:VAL:HG22	1:A:348:LEU:CD1	2.40	0.51
1:A:156:ASP:CG	1:A:157:ASN:H	2.18	0.51
1:A:403:LEU:CD1	1:A:404:SER:O	2.56	0.51
1:A:106:SER:OG	1:A:108:ASP:HB3	2.11	0.50
1:A:322:VAL:HG22	1:A:348:LEU:HD12	1.93	0.50
1:A:404:SER:OG	1:A:405:ASP:HB3	2.12	0.50
1:A:375:ILE:HG13	1:A:376:SER:H	1.77	0.49
1:A:291:TYR:CZ	2:A:509:HOH:O	2.62	0.49
1:A:226:ILE:CD1	1:A:230:GLY:HA2	2.39	0.49
1:A:322:VAL:HG23	1:A:327:VAL:HG11	1.93	0.49
1:A:162:LYS:HE3	1:A:163:PHE:H	1.77	0.49
1:A:409:GLY:HA2	1:A:440:VAL:O	2.13	0.49
1:A:314:LEU:HD23	1:A:352:ARG:CZ	2.44	0.48
1:A:321:GLU:HG3	1:A:325:LYS:C	2.39	0.48
1:A:323:ASN:ND2	2:A:516:HOH:O	2.47	0.48
1:A:60:THR:C	1:A:123:LYS:HG3	2.39	0.47
1:A:162:LYS:HD2	1:A:162:LYS:HA	1.75	0.47
1:A:283:LEU:CD1	1:A:295:GLU:HA	2.39	0.47
1:A:310:LYS:HD3	1:A:310:LYS:HA	1.64	0.47
1:A:320:THR:C	1:A:327:VAL:HG22	2.39	0.47
1:A:323:ASN:OD1	1:A:346:VAL:HG23	2.14	0.47
1:A:277:GLY:HA3	1:A:306:SER:HB2	1.97	0.46
1:A:436:GLU:OE2	1:A:459:ARG:HG3	2.16	0.46
1:A:108:ASP:OD1	1:A:108:ASP:C	2.58	0.46
1:A:321:GLU:HG3	1:A:325:LYS:O	2.15	0.46
1:A:403:LEU:HA	1:A:404:SER:CB	2.45	0.46
1:A:272:GLU:OE1	1:A:377:ALA:HA	2.16	0.45
1:A:278:VAL:HG13	1:A:299:VAL:HG23	1.98	0.45
1:A:283:LEU:HD22	1:A:288:GLN:OE1	2.16	0.45
1:A:229:ARG:H	1:A:229:ARG:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:GLN:O	1:A:291:TYR:HB3	2.16	0.45
1:A:315:VAL:HG12	1:A:316:TRP:CD1	2.51	0.45
1:A:321:GLU:OE2	1:A:349:LYS:HD2	2.17	0.45
1:A:201:ILE:HD12	1:A:251:PHE:CE2	2.52	0.44
1:A:398:LYS:NZ	1:A:407:VAL:O	2.50	0.44
1:A:342:PRO:O	1:A:343:ASN:OD1	2.35	0.44
1:A:107:LYS:H	1:A:107:LYS:CD	2.30	0.44
1:A:375:ILE:O	2:A:505:HOH:O	2.21	0.43
1:A:379:ASN:HA	1:A:380:GLY:HA3	1.77	0.43
1:A:309:LYS:HD3	1:A:309:LYS:HA	1.67	0.43
1:A:180:ASN:HD22	1:A:180:ASN:C	2.25	0.43
1:A:403:LEU:C	1:A:403:LEU:CD1	2.92	0.43
1:A:416:ASN:O	1:A:419:SER:OG	2.34	0.43
1:A:293:ASN:O	1:A:293:ASN:OD1	2.38	0.42
1:A:291:TYR:CE1	2:A:509:HOH:O	2.57	0.42
1:A:340:MET:HE3	1:A:340:MET:HB2	1.78	0.42
1:A:51:SER:HA	1:A:161:ILE:HG12	2.02	0.42
1:A:201:ILE:H	1:A:201:ILE:HG12	1.75	0.42
1:A:308:ALA:HB1	1:A:313:ILE:CD1	2.41	0.42
1:A:165:ASP:OD1	1:A:167:ASN:HB2	2.20	0.42
1:A:323:ASN:HB2	2:A:516:HOH:O	2.19	0.41
1:A:352:ARG:HH22	1:A:359:PHE:HZ	1.68	0.41
1:A:357:ARG:HH11	1:A:357:ARG:HB2	1.84	0.41
1:A:318:LEU:O	1:A:350:VAL:HA	2.20	0.41
1:A:257:MET:HE3	1:A:257:MET:HB3	1.88	0.41
1:A:279:GLY:O	1:A:299:VAL:HA	2.21	0.41
1:A:285:GLY:C	1:A:287:LEU:H	2.29	0.41
1:A:384:GLN:HB2	1:A:385:LEU:H	1.64	0.41
1:A:278:VAL:HG12	1:A:280:LEU:HG	2.02	0.41
1:A:427:ARG:H	1:A:430:ASN:ND2	2.19	0.41
1:A:462:VAL:HG21	1:A:472:ILE:HD12	2.03	0.41
1:A:275:TYR:OH	1:A:303:GLU:HG2	2.21	0.40
1:A:340:MET:HG3	1:A:344:GLN:OE1	2.21	0.40
1:A:283:LEU:O	1:A:285:GLY:N	2.54	0.40
1:A:292:ASP:O	1:A:293:ASN:OD1	2.39	0.40
1:A:354:LYS:O	1:A:354:LYS:HG3	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	368/441 (83%)	341 (93%)	25 (7%)	2 (0%)	24	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	405	ASP
1	A	109	GLY

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	319/372 (86%)	314 (98%)	5 (2%)	55	61

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	225	LEU
1	A	287	LEU
1	A	318	LEU
1	A	336	LEU
1	A	403	LEU

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	180	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	378/441 (85%)	1.30	101 (26%) 1 1	38, 75, 126, 162	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	381	ALA	8.5
1	A	291	TYR	6.6
1	A	375	ILE	6.5
1	A	284	SER	6.2
1	A	293	ASN	6.1
1	A	285	GLY	6.0
1	A	294	LYS	5.9
1	A	403	LEU	5.7
1	A	358	ALA	5.7
1	A	289	ASN	5.6
1	A	292	ASP	5.4
1	A	404	SER	5.0
1	A	355	LYS	4.8
1	A	288	GLN	4.6
1	A	356	GLU	4.5
1	A	240	ILE	4.5
1	A	350	VAL	4.5
1	A	362	THR	4.4
1	A	283	LEU	4.2
1	A	402	ARG	4.2
1	A	326	LYS	4.2
1	A	351	ILE	4.2
1	A	313	ILE	4.1
1	A	60	THR	4.0
1	A	384	GLN	4.0
1	A	474	VAL	3.9
1	A	320	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	123	LYS	3.9
1	A	290	SER	3.8
1	A	307	PRO	3.8
1	A	341	LEU	3.8
1	A	377	ALA	3.8
1	A	405	ASP	3.7
1	A	359	PHE	3.7
1	A	319	ILE	3.7
1	A	348	LEU	3.7
1	A	309	LYS	3.6
1	A	353	ASP	3.5
1	A	363	LEU	3.5
1	A	169	ILE	3.5
1	A	311	ALA	3.5
1	A	274	GLY	3.4
1	A	286	ASP	3.4
1	A	475	LYS	3.4
1	A	342	PRO	3.3
1	A	346	VAL	3.3
1	A	349	LYS	3.3
1	A	374	THR	3.2
1	A	275	TYR	3.1
1	A	361	LEU	3.1
1	A	318	LEU	3.1
1	A	296	GLY	3.0
1	A	312	GLY	3.0
1	A	314	LEU	3.0
1	A	308	ALA	2.9
1	A	287	LEU	2.9
1	A	184	VAL	2.9
1	A	380	GLY	2.9
1	A	183	GLY	2.8
1	A	298	VAL	2.8
1	A	278	VAL	2.8
1	A	276	LEU	2.7
1	A	48	ILE	2.7
1	A	364	ALA	2.7
1	A	336	LEU	2.7
1	A	220	ASN	2.7
1	A	322	VAL	2.7
1	A	357	ARG	2.7
1	A	395	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	299	VAL	2.6
1	A	97	ARG	2.6
1	A	182	PHE	2.6
1	A	454	LYS	2.6
1	A	373	GLU	2.5
1	A	347	THR	2.5
1	A	273	ARG	2.4
1	A	385	LEU	2.4
1	A	217	ASN	2.3
1	A	343	ASN	2.3
1	A	354	LYS	2.3
1	A	107	LYS	2.3
1	A	304	LYS	2.3
1	A	277	GLY	2.3
1	A	473	LEU	2.3
1	A	47	SER	2.2
1	A	310	LYS	2.2
1	A	317	ASP	2.2
1	A	218	PRO	2.2
1	A	305	ASP	2.2
1	A	465	LEU	2.2
1	A	379	ASN	2.2
1	A	295	GLU	2.1
1	A	378	GLN	2.1
1	A	471	ILE	2.1
1	A	325	LYS	2.1
1	A	99	LEU	2.1
1	A	376	SER	2.1
1	A	122	ASP	2.1
1	A	154	THR	2.0
1	A	399	ARG	2.0
1	A	338	GLY	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.