



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2018 – 05:34 AM EST

PDB ID : 4INO
Title : The crystal structure of Helicobacter pylori Ceue (HP1561)
Authors : Shaik, M.M.; Cendron, L.; Zanotti, G.
Deposited on : 2013-01-05
Resolution : 1.65 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

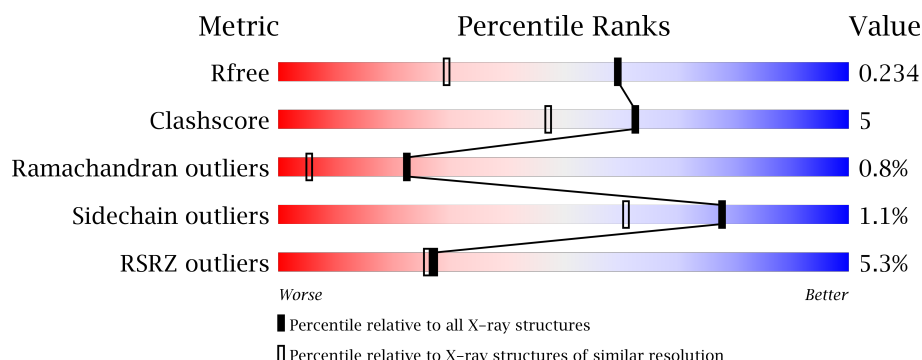
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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}	100719	1368 (1.66-1.66)
Clashscore	112137	1468 (1.66-1.66)
Ramachandran outliers	110173	1438 (1.66-1.66)
Sidechain outliers	110143	1438 (1.66-1.66)
RSRZ outliers	101464	1371 (1.66-1.66)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	334	
1	B	334	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5289 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 Nickel (II) ABC transporter, periplasmic nickel-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2398	1567	391	435	5			
1	B	302	Total	C	N	O	S	0	0	0
			2398	1567	391	435	5			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	ALA	VAL	ENGINEERED MUTATION	UNP B5Z9J2
A	336	LYS	-	EXPRESSION TAG	UNP B5Z9J2
A	337	GLY	-	EXPRESSION TAG	UNP B5Z9J2
A	338	GLU	-	EXPRESSION TAG	UNP B5Z9J2
A	339	LEU	-	EXPRESSION TAG	UNP B5Z9J2
A	340	ASN	-	EXPRESSION TAG	UNP B5Z9J2
A	341	SER	-	EXPRESSION TAG	UNP B5Z9J2
A	342	LYS	-	EXPRESSION TAG	UNP B5Z9J2
A	343	LEU	-	EXPRESSION TAG	UNP B5Z9J2
A	344	GLU	-	EXPRESSION TAG	UNP B5Z9J2
A	345	GLY	-	EXPRESSION TAG	UNP B5Z9J2
A	346	LYS	-	EXPRESSION TAG	UNP B5Z9J2
A	347	PRO	-	EXPRESSION TAG	UNP B5Z9J2
A	348	ILE	-	EXPRESSION TAG	UNP B5Z9J2
A	349	PRO	-	EXPRESSION TAG	UNP B5Z9J2
A	350	ASN	-	EXPRESSION TAG	UNP B5Z9J2
A	351	PRO	-	EXPRESSION TAG	UNP B5Z9J2
A	352	LEU	-	EXPRESSION TAG	UNP B5Z9J2
A	353	LEU	-	EXPRESSION TAG	UNP B5Z9J2
A	354	GLY	-	EXPRESSION TAG	UNP B5Z9J2
A	355	LEU	-	EXPRESSION TAG	UNP B5Z9J2
A	356	ASP	-	EXPRESSION TAG	UNP B5Z9J2
A	357	SER	-	EXPRESSION TAG	UNP B5Z9J2
A	358	THR	-	EXPRESSION TAG	UNP B5Z9J2
A	359	ARG	-	EXPRESSION TAG	UNP B5Z9J2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	360	THR	-	EXPRESSION TAG	UNP B5Z9J2
A	361	GLY	-	EXPRESSION TAG	UNP B5Z9J2
A	362	HIS	-	EXPRESSION TAG	UNP B5Z9J2
A	363	HIS	-	EXPRESSION TAG	UNP B5Z9J2
A	364	HIS	-	EXPRESSION TAG	UNP B5Z9J2
A	365	HIS	-	EXPRESSION TAG	UNP B5Z9J2
A	366	HIS	-	EXPRESSION TAG	UNP B5Z9J2
A	367	HIS	-	EXPRESSION TAG	UNP B5Z9J2
B	104	ALA	VAL	ENGINEERED MUTATION	UNP B5Z9J2
B	336	LYS	-	EXPRESSION TAG	UNP B5Z9J2
B	337	GLY	-	EXPRESSION TAG	UNP B5Z9J2
B	338	GLU	-	EXPRESSION TAG	UNP B5Z9J2
B	339	LEU	-	EXPRESSION TAG	UNP B5Z9J2
B	340	ASN	-	EXPRESSION TAG	UNP B5Z9J2
B	341	SER	-	EXPRESSION TAG	UNP B5Z9J2
B	342	LYS	-	EXPRESSION TAG	UNP B5Z9J2
B	343	LEU	-	EXPRESSION TAG	UNP B5Z9J2
B	344	GLU	-	EXPRESSION TAG	UNP B5Z9J2
B	345	GLY	-	EXPRESSION TAG	UNP B5Z9J2
B	346	LYS	-	EXPRESSION TAG	UNP B5Z9J2
B	347	PRO	-	EXPRESSION TAG	UNP B5Z9J2
B	348	ILE	-	EXPRESSION TAG	UNP B5Z9J2
B	349	PRO	-	EXPRESSION TAG	UNP B5Z9J2
B	350	ASN	-	EXPRESSION TAG	UNP B5Z9J2
B	351	PRO	-	EXPRESSION TAG	UNP B5Z9J2
B	352	LEU	-	EXPRESSION TAG	UNP B5Z9J2
B	353	LEU	-	EXPRESSION TAG	UNP B5Z9J2
B	354	GLY	-	EXPRESSION TAG	UNP B5Z9J2
B	355	LEU	-	EXPRESSION TAG	UNP B5Z9J2
B	356	ASP	-	EXPRESSION TAG	UNP B5Z9J2
B	357	SER	-	EXPRESSION TAG	UNP B5Z9J2
B	358	THR	-	EXPRESSION TAG	UNP B5Z9J2
B	359	ARG	-	EXPRESSION TAG	UNP B5Z9J2
B	360	THR	-	EXPRESSION TAG	UNP B5Z9J2
B	361	GLY	-	EXPRESSION TAG	UNP B5Z9J2
B	362	HIS	-	EXPRESSION TAG	UNP B5Z9J2
B	363	HIS	-	EXPRESSION TAG	UNP B5Z9J2
B	364	HIS	-	EXPRESSION TAG	UNP B5Z9J2
B	365	HIS	-	EXPRESSION TAG	UNP B5Z9J2
B	366	HIS	-	EXPRESSION TAG	UNP B5Z9J2
B	367	HIS	-	EXPRESSION TAG	UNP B5Z9J2

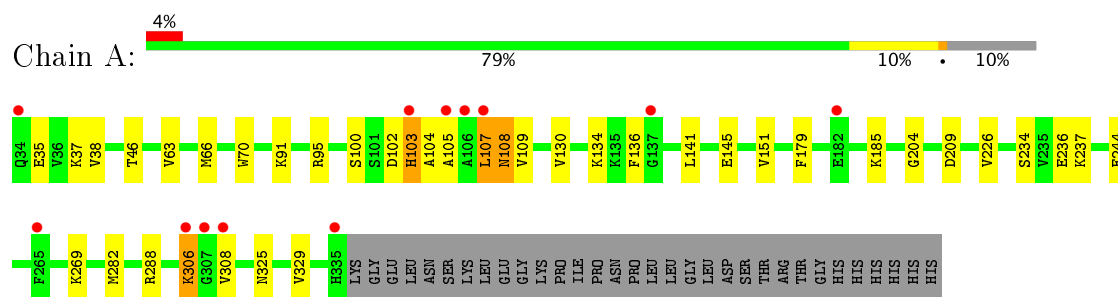
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	216	Total 216	O 216	0	0
2	B	277	Total 277	O 277	0	0

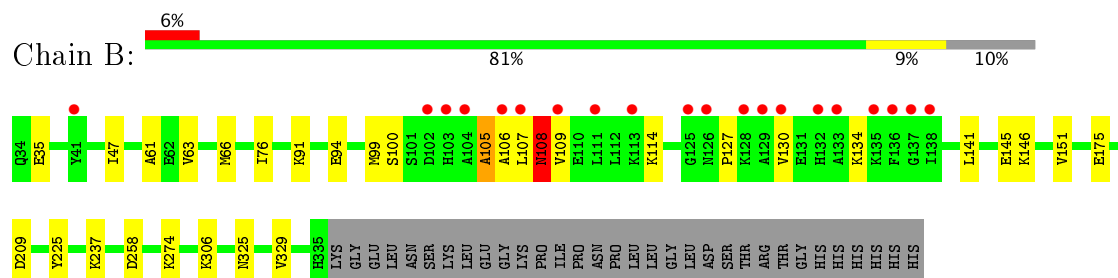
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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: Nickel (II) ABC transporter, periplasmic nickel-binding protein



- Molecule 1: Nickel (II) ABC transporter, periplasmic nickel-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.37Å 87.02Å 105.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.23 – 1.65 45.23 – 1.65	Depositor EDS
% Data completeness (in resolution range)	96.7 (45.23-1.65) 96.7 (45.23-1.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.5.0109, PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.193 , 0.225 0.199 , 0.234	Depositor DCC
R_{free} test set	3661 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5289	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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	0.34	0/2452	0.52	0/3310
1	B	0.38	0/2452	0.57	0/3310
All	All	0.36	0/4904	0.54	0/6620

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2398	0	2474	26	0
1	B	2398	0	2474	23	0
2	A	216	0	0	6	1
2	B	277	0	0	10	1
All	All	5289	0	4948	49	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 5.

All (49) 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:94:GLU:OE1	2:B:520:HOH:O	1.97	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:SER:O	2:A:559:HOH:O	1.98	0.80
1:A:244:GLU:OE2	2:A:424:HOH:O	2.08	0.71
1:B:209:ASP:OD2	2:B:598:HOH:O	2.08	0.71
1:A:209:ASP:OD1	2:A:541:HOH:O	2.08	0.70
1:B:99:MET:HA	1:B:107:LEU:HD12	1.75	0.69
1:B:274:LYS:NZ	2:B:653:HOH:O	2.25	0.67
1:B:146:LYS:NZ	2:B:670:HOH:O	2.27	0.67
1:B:61:ALA:HA	1:B:76:ILE:HD11	1.81	0.61
1:A:70:TRP:O	1:A:95:ARG:NH2	2.37	0.57
1:B:258:ASP:OD1	2:B:619:HOH:O	2.17	0.57
1:B:306:LYS:O	2:B:572:HOH:O	2.18	0.57
1:A:37:LYS:HG2	1:A:46:THR:HG22	1.87	0.56
1:A:134:LYS:NZ	2:A:572:HOH:O	2.16	0.55
1:A:325:ASN:O	1:A:329:VAL:HG23	2.07	0.55
1:B:325:ASN:O	1:B:329:VAL:HG23	2.10	0.51
1:B:105:ALA:HB1	1:B:108:ASN:ND2	2.25	0.51
1:B:225:TYR:CE1	1:B:237:LYS:HD3	2.45	0.51
1:A:179:PHE:HZ	1:A:308:VAL:HG11	1.74	0.51
1:A:109:VAL:HG11	1:A:136:PHE:CD1	2.47	0.50
1:A:234:SER:OG	1:A:237:LYS:HG3	2.12	0.49
1:B:130:VAL:O	1:B:134:LYS:HG3	2.12	0.49
1:A:236:GLU:HG2	2:A:547:HOH:O	2.14	0.47
1:B:108:ASN:HB3	1:B:109:VAL:H	1.56	0.47
1:A:244:GLU:HG2	1:A:269:LYS:HE2	1.97	0.46
1:B:100:SER:OG	1:B:106:ALA:HB3	2.14	0.46
1:A:130:VAL:O	1:A:134:LYS:HG3	2.16	0.46
1:B:105:ALA:HA	2:B:625:HOH:O	2.15	0.46
1:A:102:ASP:O	1:A:104:ALA:HA	2.16	0.45
1:A:145:GLU:HG3	1:A:151:VAL:HG22	1.99	0.45
1:A:185:LYS:HE3	2:A:563:HOH:O	2.15	0.45
1:A:63:VAL:O	1:A:66:MET:HG2	2.17	0.45
1:B:145:GLU:HG3	1:B:151:VAL:HG22	1.97	0.45
1:B:175:GLU:OE1	2:B:634:HOH:O	2.20	0.45
1:A:107:LEU:HA	1:A:107:LEU:HD23	1.69	0.44
1:A:141:LEU:HA	1:A:141:LEU:HD23	1.89	0.43
1:B:47:ILE:HD11	1:B:141:LEU:HD21	2.01	0.43
1:B:91:LYS:HA	1:B:91:LYS:HD3	1.83	0.43
1:A:282:MET:HG2	1:A:288:ARG:CZ	2.48	0.43
1:B:127:PRO:C	2:B:671:HOH:O	2.56	0.43
1:A:306:LYS:HD3	1:A:306:LYS:HA	1.95	0.43
1:B:114:LYS:HB2	2:B:623:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LYS:HD3	1:A:91:LYS:HA	1.84	0.42
1:A:204:GLY:HA3	1:A:226:VAL:HB	2.02	0.41
1:A:38:VAL:HG21	1:A:141:LEU:HD21	2.03	0.41
1:A:103:HIS:HA	1:A:104:ALA:HA	1.82	0.40
1:B:63:VAL:O	1:B:66:MET:HG2	2.21	0.40
1:B:141:LEU:HA	1:B:141:LEU:HD23	1.95	0.40
1:A:179:PHE:CZ	1:A:308:VAL:HG11	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)
2:A:590:HOH:O	2:B:631:HOH:O[3_755]	1.68	0.52

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	300/334 (90%)	291 (97%)	6 (2%)	3 (1%)	18	3
1	B	300/334 (90%)	289 (96%)	9 (3%)	2 (1%)	25	7
All	All	600/668 (90%)	580 (97%)	15 (2%)	5 (1%)	22	5

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	108	ASN
1	A	105	ALA
1	B	105	ALA
1	A	108	ASN
1	A	107	LEU

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	261/289 (90%)	257 (98%)	4 (2%)	70	48
1	B	261/289 (90%)	259 (99%)	2 (1%)	85	73
All	All	522/578 (90%)	516 (99%)	6 (1%)	78	61

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	103	HIS
1	A	108	ASN
1	A	306	LYS
1	B	35	GLU
1	B	108	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	302/334 (90%)	0.19	12 (3%) 39 40	16, 28, 49, 65	0
1	B	302/334 (90%)	0.36	20 (6%) 19 18	14, 25, 57, 68	0
All	All	604/668 (90%)	0.27	32 (5%) 27 26	14, 26, 53, 68	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	107	LEU	15.3
1	A	107	LEU	12.3
1	B	106	ALA	9.4
1	B	103	HIS	6.2
1	A	106	ALA	5.8
1	B	130	VAL	5.3
1	B	109	VAL	5.0
1	B	102	ASP	4.8
1	A	105	ALA	4.2
1	B	125	GLY	4.2
1	B	128	LYS	4.2
1	B	129	ALA	4.0
1	B	126	ASN	3.9
1	A	335	HIS	3.8
1	B	104	ALA	3.7
1	A	307	GLY	3.7
1	B	137	GLY	3.4
1	A	103	HIS	3.3
1	B	113	LYS	3.0
1	A	308	VAL	3.0
1	B	133	ALA	3.0
1	B	132	HIS	2.9
1	A	34	GLN	2.9
1	B	138	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	182	GLU	2.2
1	B	135	LYS	2.1
1	B	136	PHE	2.1
1	B	111	LEU	2.1
1	B	41	TYR	2.1
1	A	306	LYS	2.1
1	A	265	PHE	2.0
1	A	137	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 carbohydrates 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.