



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2G15 / pdb_00002g15
Title : Structural Characterization of autoinhibited c-Met kinase
Authors : Wang, W.; Marimuthu, A.; Tsai, J.; Kumar, A.; Krupka, H.I.; Zhang, C.;
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Deposited on : 2006-02-13
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

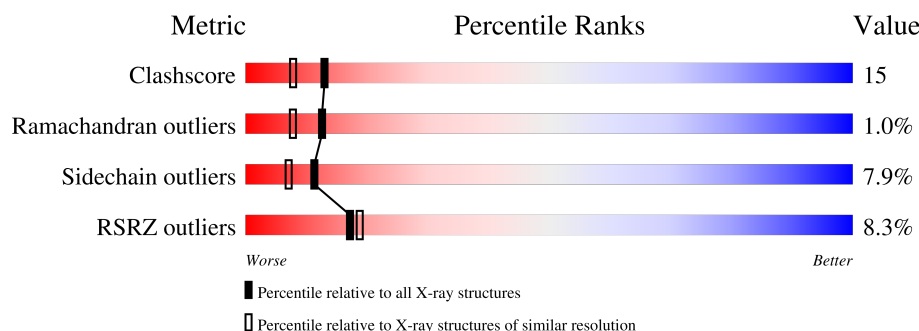
1 Overall quality at a glance

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))
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	318	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2546 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 activated met oncogene.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	301	2396	1545	409	427	15	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1029	MET	-	expression tag	GB 487742
A	1030	GLY	-	expression tag	GB 487742
A	1031	HIS	-	expression tag	GB 487742
A	1032	HIS	-	expression tag	GB 487742
A	1033	HIS	-	expression tag	GB 487742
A	1034	HIS	-	expression tag	GB 487742
A	1035	HIS	-	expression tag	GB 487742
A	1036	HIS	-	expression tag	GB 487742
A	1037	MET	-	expression tag	GB 487742

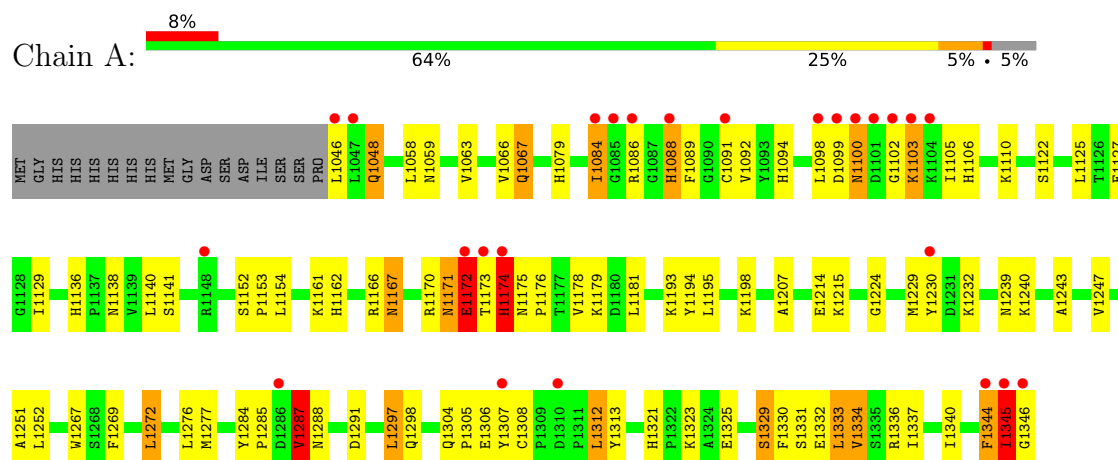
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	150	Total	O	0	0
			150	150		

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: activated met oncogene



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	103.80Å 103.80Å 103.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.15 20.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.15) 99.6 (20.00-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.1.25	Depositor
R, R_{free}	0.223 , 0.259 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.046 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2546	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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	0.72	14/2455 (0.6%)	1.19	27/3325 (0.8%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1136	HIS	ND1-CE1	5.52	1.38	1.32
1	A	1167	ASN	CG-OD1	5.52	1.34	1.23
1	A	1298	GLN	CD-OE1	5.38	1.33	1.23
1	A	1100	ASN	CG-OD1	5.36	1.33	1.23
1	A	1088	HIS	ND1-CE1	5.35	1.38	1.32
1	A	1162	HIS	ND1-CE1	5.34	1.37	1.32
1	A	1321	HIS	ND1-CE1	5.28	1.37	1.32
1	A	1106	HIS	ND1-CE1	5.26	1.37	1.32
1	A	1079	HIS	ND1-CE1	5.26	1.37	1.32
1	A	1138	ASN	CG-OD1	5.20	1.33	1.23
1	A	1059	ASN	CG-OD1	5.17	1.33	1.23
1	A	1239	ASN	CG-OD1	5.12	1.33	1.23
1	A	1067	GLN	CD-OE1	5.06	1.33	1.23
1	A	1288	ASN	CG-OD1	5.05	1.33	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1173	THR	N-CA-C	-18.66	86.70	111.71
1	A	1285	PRO	N-CA-C	-7.95	103.51	113.84
1	A	1287	VAL	N-CA-C	7.18	119.41	108.71
1	A	1048	GLN	N-CA-C	6.77	119.50	111.71
1	A	1172	GLU	N-CA-C	6.72	119.70	109.62
1	A	1321	HIS	CB-CG-CD2	-6.68	122.51	131.20
1	A	1247	VAL	N-CA-C	6.66	117.35	110.36
1	A	1088	HIS	CB-CG-CD2	-6.62	122.59	131.20
1	A	1136	HIS	CB-CG-CD2	-6.49	122.77	131.20
1	A	1162	HIS	CB-CG-CD2	-6.42	122.85	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1079	HIS	CB-CG-CD2	-6.35	122.94	131.20
1	A	1106	HIS	CB-CG-CD2	-6.20	123.14	131.20
1	A	1084	ILE	N-CA-C	6.08	117.58	109.37
1	A	1102	GLY	N-CA-C	-5.90	105.65	112.50
1	A	1088	HIS	CB-CG-ND1	5.76	131.34	122.70
1	A	1321	HIS	CB-CG-ND1	5.76	131.34	122.70
1	A	1345	ILE	N-CA-C	-5.68	97.53	109.34
1	A	1136	HIS	CB-CG-ND1	5.66	131.19	122.70
1	A	1161	LYS	N-CA-C	5.60	118.10	111.33
1	A	1162	HIS	CB-CG-ND1	5.52	130.98	122.70
1	A	1079	HIS	CB-CG-ND1	5.49	130.94	122.70
1	A	1136	HIS	CA-C-N	5.47	125.82	119.47
1	A	1136	HIS	C-N-CA	5.47	125.82	119.47
1	A	1106	HIS	CB-CG-ND1	5.39	130.78	122.70
1	A	1329	SER	N-CA-C	-5.15	103.89	110.53
1	A	1344	PHE	CA-C-N	5.08	131.10	121.97
1	A	1344	PHE	C-N-CA	5.08	131.10	121.97

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	2396	0	2421	72	0
2	A	150	0	0	4	0
All	All	2546	0	2421	72	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 15.

All (72) 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:1099:ASP:HB3	1:A:1103:LYS:HD3	1.49	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1179:LYS:HD2	1:A:1345:ILE:HD12	1.51	0.89
1:A:1323:LYS:HB3	1:A:1325:GLU:OE2	1.77	0.84
1:A:1175:ASN:N	1:A:1176:PRO:HD2	1.97	0.79
1:A:1110:LYS:HD2	1:A:1229:MET:HE3	1.65	0.79
1:A:1089:PHE:HA	1:A:1230:TYR:HD1	1.47	0.78
1:A:1171:ASN:OD1	1:A:1172:GLU:N	2.19	0.76
1:A:1174:HIS:C	1:A:1176:PRO:HD2	2.10	0.75
1:A:1332:GLU:O	1:A:1336:ARG:HG3	1.89	0.72
1:A:1141:SER:HB3	2:A:636:HOH:O	1.88	0.71
1:A:1099:ASP:OD1	1:A:1100:ASN:N	2.20	0.69
1:A:1089:PHE:HA	1:A:1230:TYR:CD1	2.26	0.69
1:A:1179:LYS:CD	1:A:1345:ILE:HD12	2.24	0.67
1:A:1252:LEU:HD21	1:A:1297:LEU:HD13	1.80	0.63
1:A:1179:LYS:HE2	1:A:1344:PHE:O	1.98	0.63
1:A:1345:ILE:O	1:A:1345:ILE:HG23	1.97	0.63
1:A:1175:ASN:N	1:A:1176:PRO:CD	2.62	0.62
1:A:1066:VAL:CG1	1:A:1129:ILE:HD11	2.29	0.61
1:A:1066:VAL:HG12	1:A:1129:ILE:HD11	1.83	0.61
1:A:1284:TYR:HB3	1:A:1287:VAL:HG13	1.84	0.60
1:A:1329:SER:OG	1:A:1332:GLU:HG3	2.03	0.59
1:A:1099:ASP:HB3	1:A:1103:LYS:CD	2.29	0.59
1:A:1066:VAL:HG11	1:A:1125:LEU:HB3	1.84	0.58
1:A:1194:TYR:O	1:A:1198:LYS:HG2	2.04	0.58
1:A:1172:GLU:HA	1:A:1174:HIS:HB2	1.86	0.58
1:A:1171:ASN:OD1	1:A:1171:ASN:C	2.46	0.58
1:A:1333:LEU:O	1:A:1337:ILE:HG12	2.04	0.57
1:A:1305:PRO:HG2	1:A:1308:CYS:HB2	1.88	0.56
1:A:1331:SER:O	1:A:1334:VAL:HG13	2.05	0.55
1:A:1330:PHE:O	1:A:1334:VAL:HG12	2.07	0.55
1:A:1058:LEU:HD22	1:A:1122:SER:HB3	1.89	0.55
1:A:1178:VAL:HG13	1:A:1277:MET:HE1	1.88	0.55
1:A:1063:VAL:O	1:A:1066:VAL:HG22	2.07	0.54
1:A:1166:ARG:O	1:A:1170:ARG:HG3	2.08	0.54
1:A:1336:ARG:O	1:A:1340:ILE:HG13	2.08	0.53
1:A:1269:PHE:O	1:A:1272:LEU:HB3	2.07	0.53
1:A:1088:HIS:O	1:A:1230:TYR:CD1	2.63	0.52
1:A:1230:TYR:CG	1:A:1230:TYR:O	2.63	0.51
1:A:1171:ASN:HB3	2:A:719:HOH:O	2.11	0.50
1:A:1172:GLU:OE1	1:A:1174:HIS:ND1	2.45	0.49
1:A:1306:GLU:O	1:A:1307:TYR:HB2	2.12	0.49
1:A:1091:CYS:HB3	2:A:674:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1086:ARG:HH11	1:A:1167:ASN:ND2	2.11	0.48
1:A:1287:VAL:HG23	1:A:1291:ASP:HB2	1.93	0.48
1:A:1207:ALA:N	1:A:1272:LEU:HD22	2.29	0.48
1:A:1172:GLU:OE1	1:A:1174:HIS:HB2	2.13	0.48
1:A:1251:ALA:HA	1:A:1267:TRP:CD2	2.48	0.48
1:A:1086:ARG:NH1	1:A:1167:ASN:ND2	2.62	0.47
1:A:1304:GLN:HB2	1:A:1313:TYR:CG	2.50	0.47
1:A:1252:LEU:HD21	1:A:1297:LEU:CD1	2.44	0.47
1:A:1306:GLU:O	1:A:1307:TYR:CB	2.62	0.47
1:A:1312:LEU:HD23	1:A:1312:LEU:HA	1.81	0.47
1:A:1084:ILE:HD13	1:A:1094:HIS:CE1	2.52	0.45
1:A:1066:VAL:HG12	1:A:1129:ILE:CD1	2.48	0.44
1:A:1193:LYS:HD2	1:A:1334:VAL:HG11	1.98	0.44
1:A:1086:ARG:NH1	1:A:1167:ASN:CG	2.76	0.44
1:A:1344:PHE:CD2	1:A:1345:ILE:N	2.86	0.44
1:A:1066:VAL:HG13	1:A:1129:ILE:HD11	1.99	0.43
1:A:1344:PHE:CG	1:A:1345:ILE:N	2.86	0.43
1:A:1345:ILE:O	1:A:1346:GLY:C	2.63	0.42
1:A:1329:SER:O	1:A:1333:LEU:HD22	2.20	0.42
1:A:1214:GLU:H	1:A:1214:GLU:CD	2.27	0.42
1:A:1141:SER:HA	2:A:651:HOH:O	2.19	0.42
1:A:1127:GLU:OE1	1:A:1224:GLY:HA2	2.20	0.42
1:A:1325:GLU:H	1:A:1325:GLU:CD	2.27	0.42
1:A:1331:SER:O	1:A:1334:VAL:CG1	2.68	0.41
1:A:1092:VAL:HG21	1:A:1229:MET:HE2	2.02	0.41
1:A:1305:PRO:HG2	1:A:1308:CYS:CB	2.49	0.41
1:A:1272:LEU:C	1:A:1272:LEU:CD1	2.94	0.41
1:A:1152:SER:HA	1:A:1153:PRO:HD3	1.82	0.41
1:A:1304:GLN:HB2	1:A:1313:TYR:CD2	2.56	0.40
1:A:1240:LYS:HG2	1:A:1243: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	299/318 (94%)	280 (94%)	16 (5%)	3 (1%)	12 8

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1345	ILE
1	A	1103	LYS
1	A	1174	HIS

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	267/282 (95%)	246 (92%)	21 (8%)	11 7

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1046	LEU
1	A	1048	GLN
1	A	1067	GLN
1	A	1098	LEU
1	A	1105	ILE
1	A	1140	LEU
1	A	1154	LEU
1	A	1171	ASN
1	A	1172	GLU
1	A	1174	HIS
1	A	1181	LEU
1	A	1195	LEU
1	A	1215	LYS
1	A	1232	LYS
1	A	1272	LEU
1	A	1276	LEU

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Mol	Chain	Res	Type
1	A	1287	VAL
1	A	1297	LEU
1	A	1312	LEU
1	A	1333	LEU
1	A	1334	VAL

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	1081	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	301/318 (94%)	0.32	25 (8%) 17 19	21, 31, 56, 74	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1346	GLY	7.5
1	A	1345	ILE	6.1
1	A	1230	TYR	5.2
1	A	1173	THR	5.0
1	A	1086	ARG	4.3
1	A	1174	HIS	4.2
1	A	1102	GLY	4.0
1	A	1085	GLY	3.9
1	A	1344	PHE	3.9
1	A	1172	GLU	3.7
1	A	1101	ASP	3.4
1	A	1307	TYR	3.3
1	A	1091	CYS	2.9
1	A	1084	ILE	2.9
1	A	1046	LEU	2.8
1	A	1286	ASP	2.8
1	A	1098	LEU	2.8
1	A	1099	ASP	2.6
1	A	1104	LYS	2.6
1	A	1047	LEU	2.5
1	A	1148	ARG	2.4
1	A	1100	ASN	2.3
1	A	1103	LYS	2.3
1	A	1310	ASP	2.0
1	A	1088	HIS	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.