



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:43 PM GMT

PDB ID : 4JAJ  
Title : Crystal Structure of Aurora Kinase A in complex with BENZO[C][1,8]NAPH  
THYRIDIN-6(5H)-ONE  
Authors : Jiang, X.; Josephson, K.; Huck, B.; Goutopoulos, A.; Karra, S.  
Deposited on : 2013-02-18  
Resolution : 2.70 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

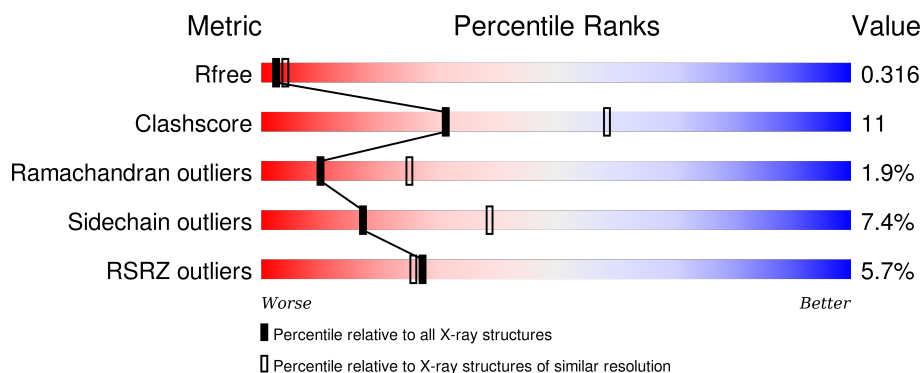
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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  $\geq 3$ , 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	284	<div> <div>5%</div> <div>69%</div> <div>22%</div> <div>• 7%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2189 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.

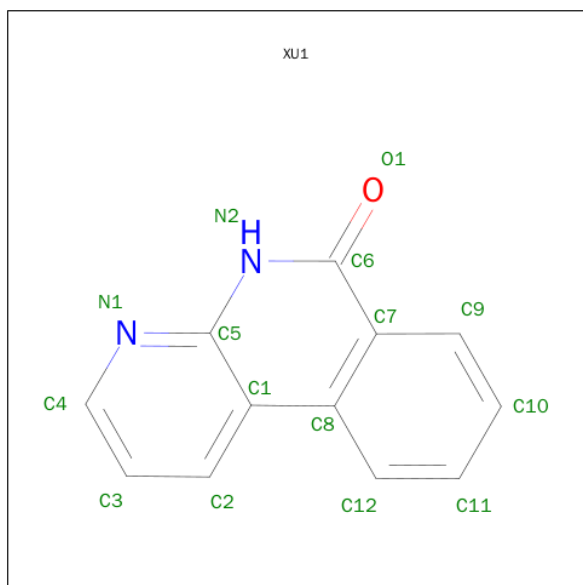
- Molecule 1 is a protein called Aurora kinase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	62	0	0
			2164	1391	382	385	6			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	MET	-	EXPRESSION TAG	UNP O14965
A	114	HIS	-	EXPRESSION TAG	UNP O14965
A	115	HIS	-	EXPRESSION TAG	UNP O14965
A	116	HIS	-	EXPRESSION TAG	UNP O14965
A	117	HIS	-	EXPRESSION TAG	UNP O14965
A	118	HIS	-	EXPRESSION TAG	UNP O14965
A	119	HIS	-	EXPRESSION TAG	UNP O14965
A	120	GLY	-	EXPRESSION TAG	UNP O14965
A	121	GLY	-	EXPRESSION TAG	UNP O14965

- Molecule 2 is BENZO[C][1,8]NAPHTHYRIDIN-6(5H)-ONE (three-letter code: XU1) (formula: C<sub>12</sub>H<sub>8</sub>N<sub>2</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	12	2	1		

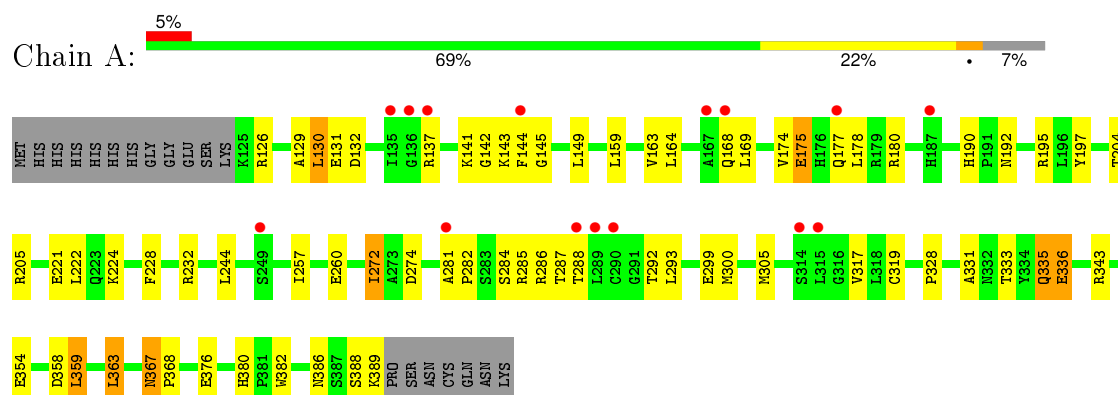
- Molecule 3 is water.

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

### 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 errors 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: Aurora kinase A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.84Å 81.84Å 169.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.43 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.70) 99.1 (29.43-2.70)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.232 , 0.323 0.235 , 0.316	Depositor DCC
$R_{free}$ test set	736 reflections (8.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.9	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 55.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 9727 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2189	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: XU1

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	1.13	4/2218 (0.2%)	1.07	3/2997 (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	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	336	GLU	CG-CD	7.46	1.63	1.51
1	A	319	CYS	CB-SG	-5.89	1.72	1.81
1	A	260	GLU	CD-OE2	5.59	1.31	1.25
1	A	175	GLU	CG-CD	5.28	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	ASP	CB-CG-OD1	6.45	124.10	118.30
1	A	386	ASN	OD1-CG-ND2	5.79	135.22	121.90
1	A	376	GLU	OE1-CD-OE2	-5.35	116.88	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	281	ALA	Peptide

## 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	2164	0	2165	44	1
2	A	15	0	8	1	0
3	A	10	0	0	1	0
All	All	2189	0	2173	45	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 11.

All (45) 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:284:SER:O	1:A:285:ARG:C	2.11	0.86
1:A:144:PHE:O	1:A:164:LEU:HA	1.85	0.77
1:A:335:GLN:H	1:A:335:GLN:HE21	1.33	0.76
1:A:358:ASP:OD2	1:A:380:HIS:HE1	1.74	0.70
1:A:284:SER:O	1:A:285:ARG:O	2.17	0.62
1:A:331:ALA:HB1	1:A:336:GLU:OE1	2.00	0.62
1:A:359:LEU:HD22	1:A:363:LEU:HD22	1.82	0.61
1:A:177:GLN:HG2	1:A:180:ARG:NH1	2.15	0.61
1:A:343:ARG:HG3	1:A:343:ARG:HH11	1.65	0.60
1:A:292:THR:HG23	3:A:1003:HOH:O	2.02	0.60
1:A:292:THR:HG23	1:A:292:THR:O	2.02	0.59
1:A:144:PHE:CD2	1:A:169:LEU:HD23	2.36	0.59
1:A:367:ASN:HD22	1:A:368:PRO:HD2	1.69	0.57
1:A:331:ALA:HB1	1:A:336:GLU:CD	2.25	0.56
1:A:190:HIS:HD2	1:A:192:ASN:H	1.51	0.56
1:A:333:THR:HG22	1:A:335:GLN:H	1.71	0.55
1:A:145:GLY:HA3	1:A:163:VAL:O	2.06	0.54
1:A:141:LYS:HG2	1:A:142:GLY:O	2.09	0.53
1:A:367:ASN:HD22	1:A:368:PRO:CD	2.21	0.53
1:A:317:VAL:HG13	1:A:328:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:THR:HG23	1:A:205:ARG:HD2	1.93	0.50
1:A:244:LEU:HD21	1:A:257:ILE:HD11	1.94	0.50
1:A:380:HIS:CD2	1:A:382:TRP:H	2.29	0.50
1:A:190:HIS:CD2	1:A:192:ASN:H	2.29	0.49
1:A:380:HIS:HD2	1:A:382:TRP:H	1.60	0.49
1:A:333:THR:HG22	1:A:335:GLN:N	2.28	0.48
1:A:388:SER:O	1:A:389:LYS:HB2	2.14	0.48
1:A:343:ARG:CG	1:A:343:ARG:HH11	2.27	0.47
1:A:292:THR:CG2	1:A:292:THR:O	2.61	0.47
1:A:335:GLN:N	1:A:335:GLN:HE21	2.06	0.47
1:A:284:SER:O	1:A:286:ARG:CB	2.65	0.45
1:A:284:SER:C	1:A:285:ARG:O	2.54	0.45
1:A:144:PHE:N	1:A:144:PHE:CD1	2.84	0.45
1:A:367:ASN:HD22	1:A:368:PRO:N	2.15	0.44
1:A:174:VAL:HB	1:A:177:GLN:HE21	1.82	0.44
2:A:900:XU1:H2	2:A:900:XU1:H8	1.67	0.44
1:A:299:GLU:O	1:A:300:MET:C	2.55	0.43
1:A:129:ALA:O	1:A:132:ASP:HB2	2.18	0.42
1:A:174:VAL:HB	1:A:177:GLN:NE2	2.35	0.42
1:A:228:PHE:CG	1:A:232:ARG:HD2	2.54	0.42
1:A:195:ARG:HG2	1:A:197:TYR:CE2	2.55	0.42
1:A:257:ILE:HG12	1:A:272:ILE:CD1	2.50	0.42
1:A:143:LYS:HB3	1:A:144:PHE:CD1	2.55	0.41
1:A:144:PHE:HD2	1:A:169:LEU:CD2	2.34	0.40
1:A:221:GLU:OE2	1:A:224:LYS:HE2	2.22	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:336:GLU:OE2	1:A:336:GLU:OE2[10_444]	1.79	0.41

## 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	263/284 (93%)	245 (93%)	13 (5%)	5 (2%)	10	25

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	PRO
1	A	287	THR
1	A	126	ARG
1	A	130	LEU
1	A	131	GLU

### 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	231/251 (92%)	214 (93%)	17 (7%)	17	39

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	LEU
1	A	137	ARG
1	A	149	LEU
1	A	159	LEU
1	A	168	GLN
1	A	175	GLU
1	A	178	LEU
1	A	222	LEU
1	A	272	ILE
1	A	288	THR
1	A	293	LEU
1	A	305	MET
1	A	335	GLN
1	A	354	GLU

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Mol	Chain	Res	Type
1	A	359	LEU
1	A	363	LEU
1	A	367	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	GLN
1	A	185	GLN
1	A	190	HIS
1	A	192	ASN
1	A	335	GLN
1	A	367	ASN
1	A	370	GLN
1	A	380	HIS

### 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](#)

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	XU1	A	900	-	17,17,17	1.88	4 (23%)	18,24,24	2.84	12 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XU1	A	900	-	-	0/0/0/0	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	XU1	C8-C7	-2.46	1.37	1.44
2	A	900	XU1	C12-C8	-2.36	1.36	1.41
2	A	900	XU1	C2-C1	-2.21	1.36	1.41
2	A	900	XU1	C6-C7	4.58	1.48	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	XU1	C6-C7-C8	-4.66	115.42	119.63
2	A	900	XU1	C11-C12-C8	-4.12	113.69	120.79
2	A	900	XU1	C12-C8-C1	-3.88	115.10	122.44
2	A	900	XU1	C10-C9-C7	-2.69	116.15	120.79
2	A	900	XU1	C3-C4-N1	-2.26	120.40	123.94
2	A	900	XU1	C2-C1-C8	-2.22	118.23	122.44
2	A	900	XU1	C3-C2-C1	-2.17	117.05	120.79
2	A	900	XU1	N1-C5-N2	2.05	118.95	115.84
2	A	900	XU1	C9-C7-C8	2.32	121.52	118.59
2	A	900	XU1	C2-C1-C5	2.81	120.66	116.93
2	A	900	XU1	C8-C1-C5	2.94	121.11	117.85
2	A	900	XU1	C12-C8-C7	5.64	125.71	118.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	XU1	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	265/284 (93%)	0.26	15 (5%)	27 26	52, 80, 127, 145	16 (6%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	288	THR	5.0
1	A	290	CYS	4.0
1	A	289	LEU	3.9
1	A	314	SER	3.6
1	A	136	GLY	3.1
1	A	281	ALA	3.0
1	A	168	GLN	3.0
1	A	137	ARG	2.6
1	A	177	GLN	2.5
1	A	167	ALA	2.3
1	A	135	ILE	2.3
1	A	315	LEU	2.1
1	A	144	PHE	2.1
1	A	187	HIS	2.1
1	A	249	SER	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	XU1	A	900	15/15	0.96	0.13	-0.87	53,69,94,96	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.