



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:59 PM GMT

PDB ID : 4K6Z  
Title : The Jak1 kinase domain in complex with compound 37  
Authors : Fong, R.; Lupardus, P.J.  
Deposited on : 2013-04-16  
Resolution : 2.73 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

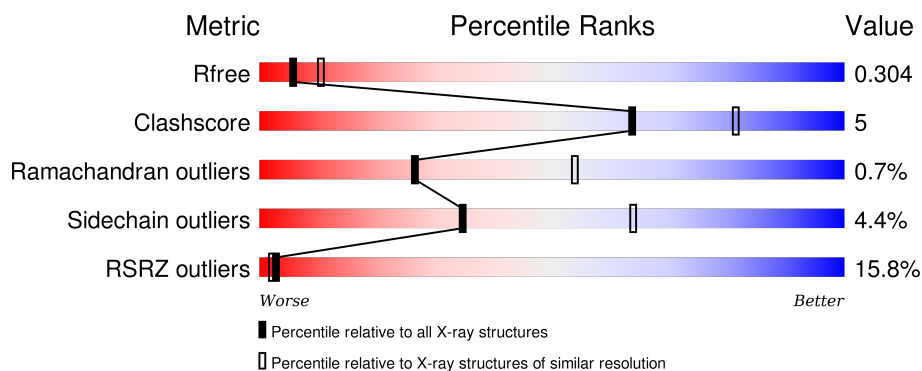
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.73 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	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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	302	<div> <div>15%</div> <div>78%</div> <div>14%</div> <div>7%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2343 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.

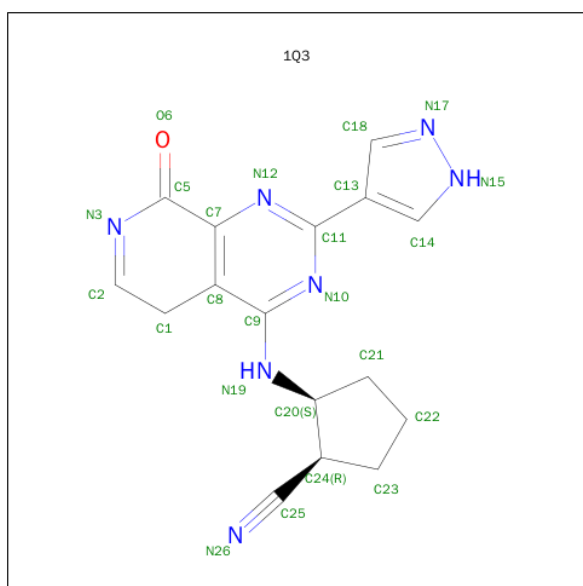
- Molecule 1 is a protein called Tyrosine-protein kinase JAK1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	281	2291	1461	388	425	2	15	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	853	GLY	-	EXPRESSION TAG	UNP P23458

- Molecule 2 is (1R,2S)-2-{[8-oxo-2-(1H-pyrazol-4-yl)-5,8-dihydropyrido[3,4-d]pyrimidin-4-yl]amino}cyclopentane carbonitrile (three-letter code: 1Q3) (formula: C<sub>16</sub>H<sub>15</sub>N<sub>7</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	24	16	7	1	0	0

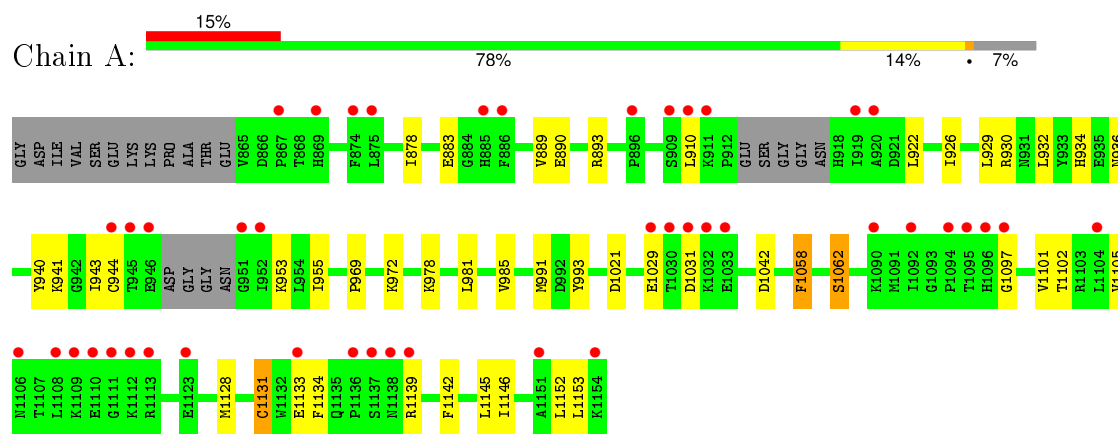
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total 28	O 28	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 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 ( $RSRZ > 2$ ). 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: Tyrosine-protein kinase JAK1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.57Å 42.70Å 44.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.85 – 2.73 42.85 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.2 (42.85-2.73) 98.6 (42.85-2.73)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.41 (at 2.73Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, $R_{free}$	0.238 , 0.297 0.240 , 0.304	Depositor DCC
$R_{free}$ test set	884 reflections (11.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.7	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 69.3	EDS
Estimated twinning fraction	0.066 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 8906 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	2343	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.22% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PTR, 1Q3

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	0.56	0/2306	0.72	0/3103

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	2291	0	2286	23	0
2	A	24	0	14	3	0
3	A	28	0	0	1	0
All	All	2343	0	2300	24	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 5.

All (24) 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:1021:ASP:HB2	2:A:1201:1Q3:H15	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:878:ILE:HD11	1:A:893:ARG:HB2	1.76	0.67
1:A:934:HIS:HD2	1:A:936:ASN:H	1.43	0.66
1:A:929:LEU:HA	1:A:932:LEU:HD12	1.83	0.59
1:A:934:HIS:CD2	1:A:936:ASN:H	2.22	0.58
1:A:944:CYS:HB3	1:A:953:LYS:HB2	1.86	0.57
2:A:1201:1Q3:H8	3:A:1305:HOH:O	2.06	0.56
1:A:978:LYS:HG2	1:A:1153:LEU:HD23	1.91	0.52
1:A:932:LEU:HD23	1:A:993:TYR:HE2	1.76	0.50
1:A:1128:MET:O	1:A:1131:CYS:HB2	2.12	0.50
1:A:1058:PHE:CE1	1:A:1062:SER:HB2	2.48	0.49
1:A:889:VAL:HG11	2:A:1201:1Q3:H1	1.95	0.47
1:A:969:PRO:HA	1:A:972:LYS:HE3	1.99	0.45
1:A:985:VAL:HG13	1:A:1146:ILE:HG23	1.99	0.45
1:A:930:ARG:HG3	1:A:940:TYR:CE2	2.52	0.45
1:A:926:ILE:HG21	1:A:943:ILE:CG2	2.46	0.45
1:A:1133:GLU:HB2	1:A:1139:ARG:HG3	1.97	0.45
1:A:991:MET:HB3	1:A:1142:PHE:CE2	2.52	0.44
1:A:1101:VAL:O	1:A:1105:VAL:HG23	2.18	0.43
1:A:941:LYS:HB2	1:A:955:ILE:HG22	2.01	0.43
1:A:910:LEU:HG	1:A:922:LEU:HD22	2.03	0.41
1:A:932:LEU:HD23	1:A:993:TYR:CE2	2.56	0.41
1:A:926:ILE:HG21	1:A:943:ILE:HG21	2.02	0.41
1:A:981:LEU:O	1:A:985:VAL:HG23	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	273/302 (90%)	253 (93%)	18 (7%)	2 (1%)	26 54

All (2) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	1097	GLY
1	A	1134	PHE

### 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	252/267 (94%)	241 (96%)	11 (4%)	35 64

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	883	GLU
1	A	890	GLU
1	A	1029	GLU
1	A	1031	ASP
1	A	1042	ASP
1	A	1058	PHE
1	A	1062	SER
1	A	1102	THR
1	A	1131	CYS
1	A	1145	LEU
1	A	1152	LEU

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](#)

2 non-standard protein/DNA/RNA residues are 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	$\# Z  > 2$
1	PTR	A	1034	1	14,16,17	1.61	3 (21%)	18,22,24	1.46	1 (5%)
1	PTR	A	1035	1	14,16,17	1.48	4 (28%)	18,22,24	1.20	3 (16%)

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
1	PTR	A	1034	1	-	0/9/11/13	0/1/1/1
1	PTR	A	1035	1	-	0/9/11/13	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1035	PTR	CE1-CZ	2.14	1.43	1.38
1	A	1035	PTR	CE2-CD2	2.20	1.42	1.38
1	A	1034	PTR	CE1-CZ	2.28	1.43	1.38
1	A	1035	PTR	CE1-CD1	2.30	1.42	1.38
1	A	1035	PTR	CE2-CZ	2.69	1.44	1.38
1	A	1034	PTR	CE2-CZ	2.78	1.44	1.38
1	A	1034	PTR	CD1-CG	2.85	1.44	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1035	PTR	O-C-CA	-2.17	119.84	125.49
1	A	1035	PTR	OH-CZ-CE2	2.21	126.02	119.22
1	A	1035	PTR	O3P-P-OH	2.38	113.77	105.22
1	A	1034	PTR	CG-CB-CA	4.55	124.49	114.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	1Q3	A	1201	-	24,27,27	2.02	4 (16%)	15,38,38	2.38	6 (40%)

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	1Q3	A	1201	-	-	0/4/30/30	0/3/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	1Q3	C1-C8	-2.24	1.46	1.51
2	A	1201	1Q3	C7-C8	2.12	1.46	1.41
2	A	1201	1Q3	C5-N3	2.55	1.45	1.39
2	A	1201	1Q3	C2-N3	8.00	1.36	1.27

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	1Q3	C5-C7-N12	-4.67	115.24	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	1Q3	C13-C11-N10	-3.64	110.89	117.26
2	A	1201	1Q3	C21-C20-N19	-3.56	107.22	112.76
2	A	1201	1Q3	C21-C20-C24	-3.04	99.74	104.22
2	A	1201	1Q3	C8-C1-C2	3.24	119.41	113.19
2	A	1201	1Q3	C13-C11-N12	3.38	123.17	117.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	1Q3	3	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 ⓘ

### 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, 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	279/302 (92%)	0.86	44 (15%) 3 2	17, 51, 85, 110	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1031	ASP	6.9
1	A	885	HIS	6.4
1	A	1032	LYS	5.8
1	A	1030	THR	5.5
1	A	1154	LYS	5.5
1	A	1095	THR	5.5
1	A	874	PHE	5.2
1	A	910	LEU	5.0
1	A	945	THR	4.7
1	A	867	PRO	4.6
1	A	952	ILE	4.2
1	A	1111	GLY	4.1
1	A	1123	GLU	3.7
1	A	869	HIS	3.6
1	A	1104	LEU	3.4
1	A	920	ALA	3.4
1	A	951	GLY	3.3
1	A	1108	LEU	3.3
1	A	1138	ASN	3.2
1	A	1092	ILE	3.1
1	A	1106	ASN	3.1
1	A	1137	SER	3.1
1	A	909	SER	2.9
1	A	1033	GLU	2.8
1	A	886	PHE	2.8
1	A	1097	GLY	2.8
1	A	1113	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1109	LYS	2.5
1	A	944	CYS	2.5
1	A	1094	PRO	2.5
1	A	1133	GLU	2.4
1	A	919	ILE	2.3
1	A	1139	ARG	2.3
1	A	946	GLU	2.2
1	A	1112	LYS	2.1
1	A	1136	PRO	2.1
1	A	1090	LYS	2.1
1	A	1029	GLU	2.1
1	A	1151	ALA	2.1
1	A	875	LEU	2.1
1	A	1096	HIS	2.1
1	A	1110	GLU	2.1
1	A	896	PRO	2.0
1	A	911	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	PTR	A	1035	16/17	0.88	0.20	-	69,70,73,73	0
1	PTR	A	1034	16/17	0.80	0.26	-	82,93,100,100	0

## 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	1Q3	A	1201	24/24	0.92	0.19	0.24	26,28,29,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.