



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:20 PM GMT

PDB ID : 1OIR  
Title : IMIDAZOPYRIDINES: A POTENT AND SELECTIVE CLASS OF CYCLIN-DEPENDENT KINASE INHIBITORS IDENTIFIED THROUGH STRUCTURE-BASED HYBRIDISATION  
Authors : Beattie, J.F.; Breault, G.A.; Byth, K.F.; Culshaw, J.D.; Ellston, R.P.A.; Green, S.; Minshull, C.A.; Norman, R.A.; Pauptit, R.A.; Thomas, A.P.; Jewsbury, P.J.  
Deposited on : 2003-06-24  
Resolution : 1.91 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

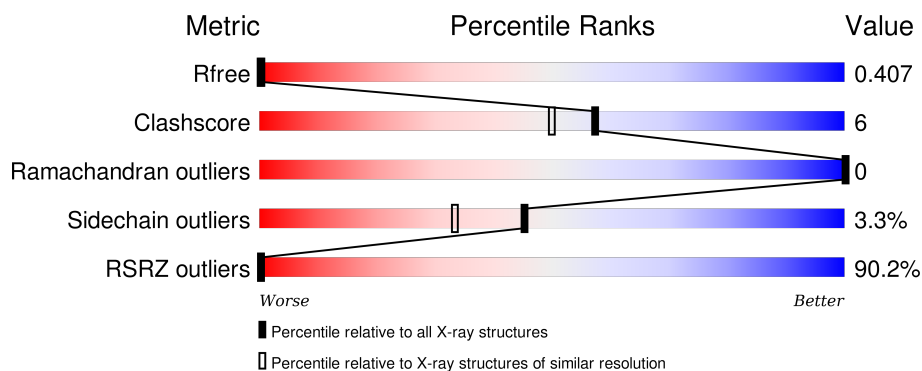
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.91 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	5832 (1.94-1.90)
Clashscore	102246	6540 (1.94-1.90)
Ramachandran outliers	100387	6464 (1.94-1.90)
Sidechain outliers	100360	6465 (1.94-1.90)
RSRZ outliers	91569	5846 (1.94-1.90)

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	299	

## 2 Entry composition [i](#)

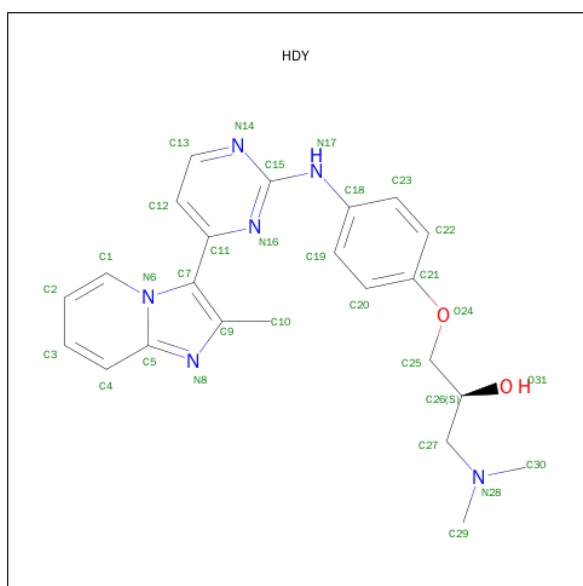
There are 3 unique types of molecules in this entry. The entry contains 2439 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2285	1490	383	404	8			

- Molecule 2 is 1-(DIMETHYLAMINO)-3-(4-{4-(2-METHYLIMIDAZO[1,2-A]PYRIDIN-3-YL)PYRIMIDIN-2-YL}AMINO}PHENOXY)PROPAN-2-OL (three-letter code: HDY) (formula: C<sub>23</sub>H<sub>26</sub>N<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	23	6	2		

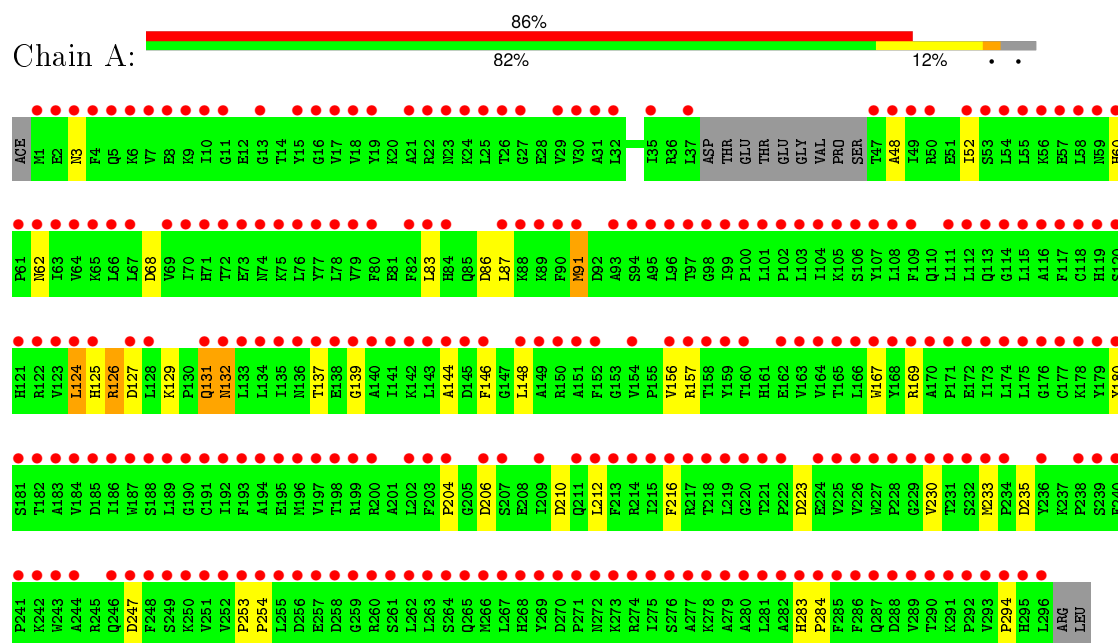
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	123	Total	O	0	0
			123	123		

### 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: CELL DIVISION PROTEIN KINASE 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.53Å 72.24Å 72.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.03 – 1.91 36.94 – 1.89	Depositor EDS
% Data completeness (in resolution range)	87.4 (43.03-1.91) 83.6 (36.94-1.89)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	10.76 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.204 , 0.241 0.396 , 0.407	Depositor DCC
$R_{free}$ test set	976 reflections (5.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.3	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 28.0	EDS
Estimated twinning fraction	0.025 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 19100 reflections	Xtriage
$F_o, F_c$ correlation	0.75	EDS
Total number of atoms	2439	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.86% 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: KCX, HDY

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	1/2332 (0.0%)	0.82	7/3169 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	MET	SD-CE	-7.16	1.37	1.77

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	ASP	CB-CG-OD2	7.71	125.24	118.30
1	A	68	ASP	CB-CG-OD2	5.95	123.65	118.30
1	A	235	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	86	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	247	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	210	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	206	ASP	CB-CG-OD2	5.04	122.84	118.30

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	2285	0	2295	26	0
2	A	31	0	26	2	0
3	A	123	0	0	4	0
All	All	2439	0	2321	28	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 6.

All (28) 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:126:ARG:O	3:A:2039:HOH:O	1.94	0.84
1:A:137:THR:O	3:A:2046:HOH:O	1.99	0.78
1:A:125:HIS:HD2	1:A:127:ASP:H	1.37	0.72
2:A:1298:HDY:H101	2:A:1298:HDY:H12	1.71	0.71
1:A:60:HIS:CD2	1:A:62:ASN:H	2.10	0.70
1:A:125:HIS:HE1	1:A:144:ALA:O	1.76	0.68
1:A:60:HIS:HD2	1:A:62:ASN:H	1.44	0.66
1:A:169:ARG:NH1	3:A:2067:HOH:O	2.34	0.58
1:A:129:LYS:H	1:A:132:ASN:HD21	1.53	0.57
1:A:131:GLN:H	1:A:131:GLN:NE2	2.04	0.56
1:A:253:PRO:HB2	1:A:254:PRO:HD3	1.89	0.55
1:A:127:ASP:HA	3:A:2039:HOH:O	2.09	0.53
1:A:52:ILE:HD12	1:A:148:LEU:HD23	1.91	0.51
1:A:156:VAL:O	1:A:157:ARG:HD3	2.10	0.51
1:A:124:LEU:HD23	1:A:124:LEU:N	2.26	0.50
1:A:87:LEU:HG	1:A:91:MET:HE2	1.93	0.48
1:A:87:LEU:HG	1:A:91:MET:CE	2.43	0.48
1:A:253:PRO:O	1:A:254:PRO:C	2.51	0.48
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.51	0.46
1:A:230:VAL:O	1:A:233:MET:HG3	2.17	0.44
1:A:48:ALA:O	1:A:52:ILE:HG12	2.18	0.43
1:A:139:GLY:HA2	1:A:294:PRO:HD3	2.00	0.43
1:A:125:HIS:CE1	1:A:144:ALA:O	2.65	0.42
1:A:132:ASN:HD22	1:A:132:ASN:C	2.23	0.41
1:A:157:ARG:HG3	1:A:157:ARG:HH11	1.85	0.41
2:A:1298:HDY:N16	2:A:1298:HDY:H1	2.36	0.41
1:A:283:HIS:HA	1:A:284:PRO:HD3	1.98	0.40
1:A:212:LEU:HG	1:A:216:PHE:CZ	2.56	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	282/299 (94%)	277 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	245/262 (94%)	237 (97%)	8 (3%)	45	33

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	83	LEU
1	A	124	LEU
1	A	126	ARG
1	A	131	GLN
1	A	132	ASN
1	A	146	PHE
1	A	180	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	59	ASN
1	A	60	HIS
1	A	125	HIS
1	A	131	GLN
1	A	132	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue 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
1	KCX	A	33	1	7,11,12	1.05	1 (14%)	7,12,14	0.77	0

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	KCX	A	33	1	-	0/6/10/12	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	KCX	CE-NZ	2.38	1.51	1.46

There are no bond angle outliers.

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	HDY	A	1298	-	30,34,34	1.88	4 (13%)	35,47,47	2.65	7 (20%)

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	HDY	A	1298	-	-	0/14/17/17	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1298	HDY	C1-N6	-2.70	1.34	1.38
2	A	1298	HDY	C1-C2	3.48	1.40	1.35
2	A	1298	HDY	C5-N8	4.20	1.37	1.33
2	A	1298	HDY	C7-C9	6.83	1.50	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1298	HDY	N14-C15-N16	-7.20	119.00	126.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1298	HDY	C12-C13-N14	-4.23	119.08	123.90
2	A	1298	HDY	C2-C1-N6	-2.70	116.85	120.41
2	A	1298	HDY	C3-C4-C5	-2.54	117.52	120.19
2	A	1298	HDY	C11-N16-C15	5.39	120.52	116.49
2	A	1298	HDY	C25-O24-C21	5.89	130.56	117.89
2	A	1298	HDY	C13-N14-C15	8.17	122.59	115.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1298	HDY	2	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	286/299 (95%)	3.88	258 (90%) 0 0	12, 17, 25, 30	0

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	ALA	12.2
1	A	1	MET	10.5
1	A	225	VAL	10.3
1	A	275	ILE	10.1
1	A	72	THR	9.1
1	A	295	HIS	8.5
1	A	251	VAL	8.3
1	A	296	LEU	8.2
1	A	122	ARG	8.1
1	A	90	PHE	7.8
1	A	24	LYS	7.4
1	A	227	TRP	7.2
1	A	273	LYS	6.9
1	A	174	LEU	6.8
1	A	179	TYR	6.8
1	A	244	ALA	6.8
1	A	2	GLU	6.7
1	A	37	LEU	6.7
1	A	21	ALA	6.6
1	A	103	LEU	6.6
1	A	156	VAL	6.5
1	A	58	LEU	6.4
1	A	289	VAL	6.4
1	A	108	LEU	6.3
1	A	70	ILE	6.2
1	A	151	ALA	6.2
1	A	255	LEU	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	50	ARG	6.1
1	A	83	LEU	6.1
1	A	109	PHE	6.0
1	A	71	HIS	6.0
1	A	243	TRP	6.0
1	A	80	PHE	5.9
1	A	230	VAL	5.9
1	A	118	CYS	5.9
1	A	137	THR	5.8
1	A	99	ILE	5.8
1	A	240	PHE	5.7
1	A	78	LEU	5.7
1	A	218	THR	5.6
1	A	49	ILE	5.6
1	A	293	VAL	5.5
1	A	67	LEU	5.5
1	A	30	VAL	5.4
1	A	138	GLU	5.4
1	A	117	PHE	5.3
1	A	267	LEU	5.3
1	A	232	SER	5.3
1	A	59	ASN	5.3
1	A	10	ILE	5.2
1	A	112	LEU	5.2
1	A	262	LEU	5.2
1	A	175	LEU	5.2
1	A	52	ILE	5.1
1	A	285	PHE	5.1
1	A	25	LEU	5.0
1	A	152	PHE	5.0
1	A	219	LEU	5.0
1	A	47	THR	5.0
1	A	93	ALA	5.0
1	A	69	VAL	5.0
1	A	252	VAL	5.0
1	A	236	TYR	4.9
1	A	242	LYS	4.9
1	A	290	THR	4.9
1	A	3	ASN	4.9
1	A	146	PHE	4.8
1	A	228	PRO	4.8
1	A	123	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	177	CYS	4.7
1	A	253	PRO	4.7
1	A	96	LEU	4.7
1	A	180	TYR	4.7
1	A	261	SER	4.7
1	A	4	PHE	4.7
1	A	204	PRO	4.6
1	A	73	GLU	4.6
1	A	111	LEU	4.6
1	A	248	PHE	4.6
1	A	77	TYR	4.6
1	A	54	LEU	4.6
1	A	148	LEU	4.6
1	A	217	ARG	4.5
1	A	60	HIS	4.5
1	A	74	ASN	4.5
1	A	139	GLY	4.5
1	A	66	LEU	4.5
1	A	114	GLY	4.4
1	A	247	ASP	4.4
1	A	226	VAL	4.4
1	A	233	MET	4.4
1	A	281	LEU	4.4
1	A	6	LYS	4.4
1	A	283	HIS	4.3
1	A	19	TYR	4.3
1	A	279	ALA	4.3
1	A	7	VAL	4.3
1	A	287	GLN	4.3
1	A	26	THR	4.3
1	A	286	PHE	4.2
1	A	190	GLY	4.2
1	A	276	SER	4.2
1	A	107	TYR	4.2
1	A	120	SER	4.2
1	A	288	ASP	4.2
1	A	32	LEU	4.2
1	A	121	HIS	4.1
1	A	55	LEU	4.1
1	A	194	ALA	4.1
1	A	284	PRO	4.1
1	A	278	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	203	PHE	4.1
1	A	31	ALA	4.1
1	A	256	ASP	4.1
1	A	213	PHE	4.1
1	A	5	GLN	4.0
1	A	198	THR	4.0
1	A	216	PHE	4.0
1	A	191	CYS	4.0
1	A	163	VAL	4.0
1	A	269	TYR	4.0
1	A	178	LYS	4.0
1	A	35	ILE	3.9
1	A	215	ILE	3.9
1	A	158	THR	3.9
1	A	212	LEU	3.9
1	A	165	THR	3.9
1	A	140	ALA	3.9
1	A	241	PRO	3.9
1	A	48	ALA	3.9
1	A	197	VAL	3.9
1	A	105	LYS	3.8
1	A	116	ALA	3.8
1	A	64	VAL	3.8
1	A	292	PRO	3.8
1	A	193	PHE	3.7
1	A	11	GLY	3.7
1	A	27	GLY	3.7
1	A	168	TYR	3.7
1	A	184	VAL	3.7
1	A	254	PRO	3.7
1	A	294	PRO	3.6
1	A	207	SER	3.6
1	A	134	LEU	3.6
1	A	159	TYR	3.6
1	A	270	ASP	3.6
1	A	128	LEU	3.6
1	A	82	PHE	3.6
1	A	176	GLY	3.6
1	A	101	LEU	3.6
1	A	57	GLU	3.6
1	A	258	ASP	3.6
1	A	22	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	61	PRO	3.5
1	A	124	LEU	3.5
1	A	173	ILE	3.5
1	A	260	ARG	3.5
1	A	170	ALA	3.5
1	A	56	LYS	3.5
1	A	239	SER	3.4
1	A	79	VAL	3.4
1	A	53	SER	3.4
1	A	17	VAL	3.4
1	A	102	PRO	3.3
1	A	234	PRO	3.3
1	A	246	GLN	3.3
1	A	271	PRO	3.3
1	A	62	ASN	3.3
1	A	29	VAL	3.3
1	A	186	ILE	3.3
1	A	189	LEU	3.3
1	A	166	LEU	3.2
1	A	95	ALA	3.2
1	A	154	VAL	3.2
1	A	200	ARG	3.2
1	A	265	GLN	3.2
1	A	222	PRO	3.2
1	A	91	MET	3.2
1	A	231	THR	3.2
1	A	133	LEU	3.2
1	A	149	ALA	3.1
1	A	164	VAL	3.1
1	A	141	ILE	3.1
1	A	263	LEU	3.1
1	A	135	ILE	3.0
1	A	277	ALA	3.0
1	A	94	SER	3.0
1	A	87	LEU	2.9
1	A	272	ASN	2.9
1	A	104	ILE	2.9
1	A	291	LYS	2.9
1	A	127	ASP	2.8
1	A	84	HIS	2.8
1	A	131	GLN	2.8
1	A	182	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	268	HIS	2.8
1	A	145	ASP	2.8
1	A	16	GLY	2.8
1	A	249	SER	2.8
1	A	119	HIS	2.8
1	A	97	THR	2.7
1	A	65	LYS	2.7
1	A	15	TYR	2.7
1	A	23	ASN	2.7
1	A	196	MET	2.7
1	A	98	GLY	2.7
1	A	143	LEU	2.7
1	A	274	ARG	2.7
1	A	209	ILE	2.7
1	A	220	GLY	2.7
1	A	183	ALA	2.7
1	A	63	ILE	2.7
1	A	229	GLY	2.7
1	A	238	PRO	2.7
1	A	142	LYS	2.6
1	A	199	ARG	2.6
1	A	76	LEU	2.6
1	A	202	LEU	2.6
1	A	9	LYS	2.6
1	A	8	GLU	2.6
1	A	132	ASN	2.6
1	A	89	LYS	2.6
1	A	169	ARG	2.6
1	A	18	VAL	2.5
1	A	115	LEU	2.5
1	A	214	ARG	2.5
1	A	88	LYS	2.5
1	A	162	GLU	2.5
1	A	167	TRP	2.5
1	A	160	THR	2.5
1	A	136	ASN	2.4
1	A	259	GLY	2.4
1	A	13	GLY	2.4
1	A	282	ALA	2.4
1	A	264	SER	2.4
1	A	150	ARG	2.3
1	A	192	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	144	ALA	2.3
1	A	75	LYS	2.3
1	A	157	ARG	2.2
1	A	206	ASP	2.2
1	A	113	GLN	2.2
1	A	266	MET	2.2
1	A	181	SER	2.2
1	A	185	ASP	2.1
1	A	125	HIS	2.1
1	A	106	SER	2.1
1	A	172	GLU	2.1
1	A	187	TRP	2.1
1	A	171	PRO	2.1
1	A	224	GLU	2.1
1	A	195	GLU	2.1
1	A	257	GLU	2.1
1	A	100	PRO	2.1
1	A	250	LYS	2.0
1	A	221	THR	2.0
1	A	211	GLN	2.0
1	A	188	SER	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( $\text{\AA}^2$ )	Q<0.9
1	KCX	A	33	12/13	0.80	0.23	-	14,14,17,17	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	HDY	A	1298	31/31	0.69	0.27	0.03	17,19,28,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.