



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:45 pm BST

PDB ID : 3UQG  
Title : c-SRC kinase domain in complex with bumpless BKI analog UW1243  
Authors : Merritt, E.A.; Larson, E.T.  
Deposited on : 2011-11-20  
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

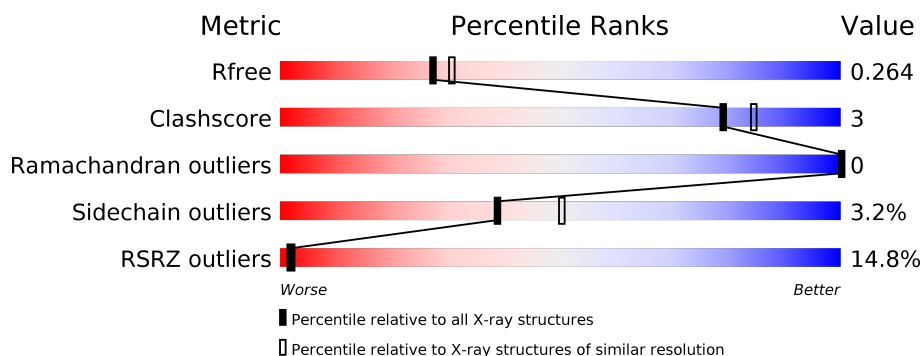
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	286	
1	B	286	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4194 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.

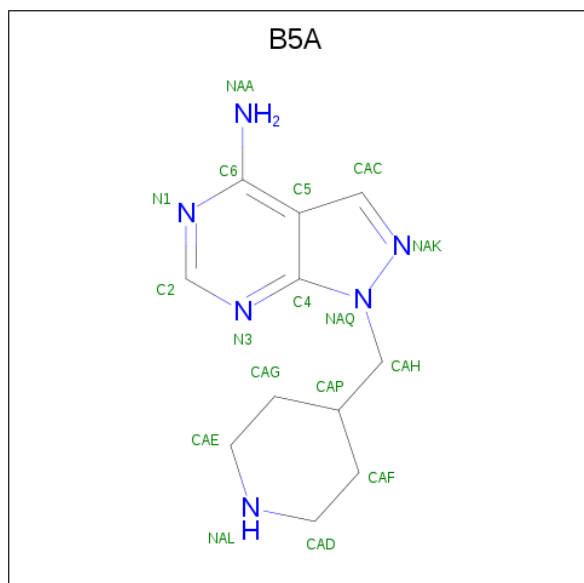
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	1	0
			2104	1351	351	385	17			
1	B	257	Total	C	N	O	S	0	0	0
			2028	1303	338	372	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLY	-	EXPRESSION TAG	UNP P00523
A	249	HIS	-	EXPRESSION TAG	UNP P00523
A	250	MET	-	EXPRESSION TAG	UNP P00523
B	248	GLY	-	EXPRESSION TAG	UNP P00523
B	249	HIS	-	EXPRESSION TAG	UNP P00523
B	250	MET	-	EXPRESSION TAG	UNP P00523

- Molecule 2 is 1-(piperidin-4-ylmethyl)-1H-pyrazolo[3,4-d]pyrimidin-4-amine (three-letter code: B5A) (formula: C<sub>11</sub>H<sub>16</sub>N<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			17	11	6		
2	B	1	Total	C	N	0	0
			17	11	6		

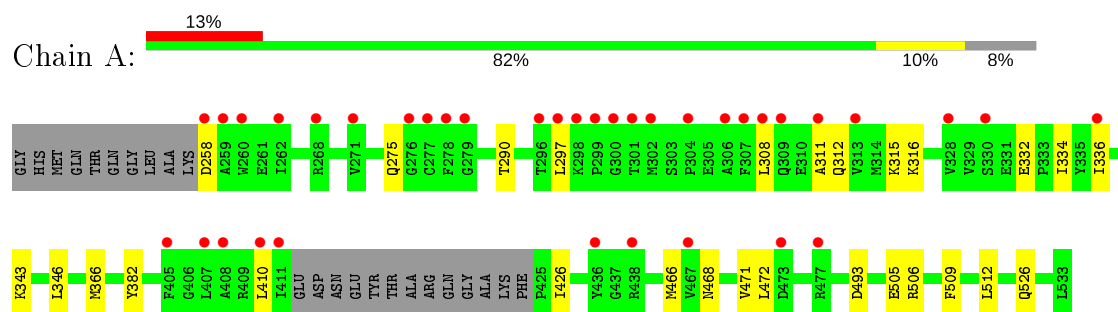
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		
3	B	11	Total	O	0	0
			11	11		

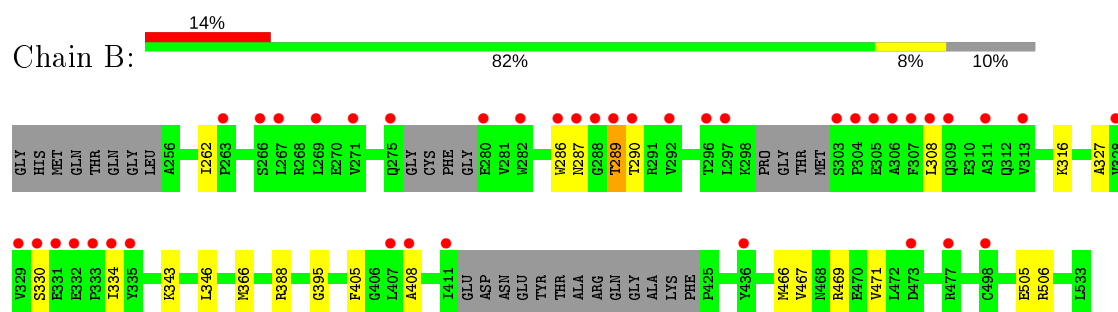
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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: Proto-oncogene tyrosine-protein kinase Src



- Molecule 1: Proto-oncogene tyrosine-protein kinase Src



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.54Å 63.72Å 74.98Å 78.17° 89.34° 90.08°	Depositor
Resolution (Å)	53.21 – 2.20 53.21 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.5 (53.21-2.20) 97.5 (53.21-2.20)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.229 , 0.259 0.237 , 0.264	Depositor DCC
$R_{free}$ test set	1905 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.65% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: B5A

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	0/2158	0.65	1/2923 (0.0%)
1	B	0.57	1/2075 (0.0%)	0.65	1/2814 (0.0%)
All	All	0.57	1/4233 (0.0%)	0.65	2/5737 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	286	TRP	CD2-CE2	5.07	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	506	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	A	506	ARG	NE-CZ-NH1	5.16	122.88	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2104	0	2086	13	0
1	B	2028	0	1981	10	0
2	A	17	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	17	0	16	0	0
3	A	17	0	0	1	0
3	B	11	0	0	0	0
All	All	4194	0	4099	23	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 3.

All (23) 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:297:LEU:HD23	1:A:334:ILE:HD13	1.47	0.97
1:B:466:MET:HE2	1:B:471:VAL:HG22	1.77	0.66
1:A:466:MET:HE2	1:A:471:VAL:HG22	1.78	0.63
1:A:382:TYR:CE1	1:A:410:LEU:HD13	2.34	0.62
1:A:308:LEU:HD23	1:A:312:GLN:HG2	1.82	0.61
1:B:343:LYS:HD3	1:B:395:GLY:O	2.06	0.56
1:A:526:GLN:HG2	3:A:17:HOH:O	2.07	0.54
1:A:258:ASP:OD1	1:A:315:LYS:NZ	2.27	0.53
1:B:346:LEU:CD1	1:B:366:MET:HE2	2.38	0.53
1:A:426:ILE:HG21	1:A:468:ASN:HB3	1.91	0.52
1:B:405:PHE:HB3	1:B:408:ALA:HB3	1.94	0.48
1:A:346:LEU:CD1	1:A:366:MET:HE2	2.44	0.47
1:B:346:LEU:CD1	1:B:366:MET:CE	2.94	0.45
1:A:410:LEU:O	1:A:410:LEU:HG	2.16	0.45
1:B:346:LEU:HD13	1:B:366:MET:HE2	1.98	0.44
1:A:334:ILE:H	1:A:334:ILE:HD12	1.83	0.44
1:B:287:ASN:O	1:B:289:THR:HG22	2.17	0.44
1:B:330:SER:O	1:B:334:ILE:HD12	2.18	0.43
1:A:426:ILE:HD11	1:A:472:LEU:CD2	2.49	0.43
1:A:311:ALA:HB2	1:A:336:ILE:HD13	2.01	0.43
1:B:467:VAL:O	1:B:471:VAL:HG23	2.20	0.42
1:A:509:PHE:HA	1:A:512:LEU:HD12	2.03	0.41
1:B:262:ILE:HG12	1:B:327:ALA:HB1	2.01	0.41

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	260/286 (91%)	253 (97%)	7 (3%)	0	100	100
1	B	249/286 (87%)	243 (98%)	6 (2%)	0	100	100
All	All	509/572 (89%)	496 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	225/245 (92%)	218 (97%)	7 (3%)	40	51
1	B	212/245 (86%)	205 (97%)	7 (3%)	38	49
All	All	437/490 (89%)	423 (97%)	14 (3%)	39	50

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	GLN
1	A	290	THR
1	A	316	LYS
1	A	332	GLU
1	A	343	LYS
1	A	493	ASP
1	A	505	GLU
1	B	289	THR

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Mol	Chain	Res	Type
1	B	290	THR
1	B	308	LEU
1	B	316	LYS
1	B	388	ARG
1	B	469	ARG
1	B	505	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	397	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands 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	$\# Z  > 2$
2	B5A	B	1	-	17,19,19	1.59	2 (11%)	15,26,26	2.36	4 (26%)
2	B5A	A	1	-	17,19,19	1.55	2 (11%)	15,26,26	2.31	4 (26%)

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	B5A	B	1	-	-	2/2/12/12	0/3/3/3
2	B5A	A	1	-	-	2/2/12/12	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	B5A	C6-C5	-5.04	1.40	1.45
2	A	1	B5A	C6-C5	-4.72	1.40	1.45
2	A	1	B5A	CAC-C5	-3.48	1.33	1.40
2	B	1	B5A	CAC-C5	-3.36	1.33	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	B5A	CAC-NAK-NAQ	5.74	110.21	104.23
2	B	1	B5A	CAC-NAK-NAQ	5.43	109.88	104.23
2	B	1	B5A	N3-C2-N1	-4.41	121.78	128.68
2	A	1	B5A	N3-C2-N1	-4.11	122.25	128.68
2	B	1	B5A	CAH-NAQ-NAK	4.04	124.66	117.08
2	A	1	B5A	CAH-NAQ-NAK	3.49	123.63	117.08
2	A	1	B5A	C5-C6-N1	-3.39	118.41	121.93
2	B	1	B5A	C5-C6-N1	-3.37	118.42	121.93

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	B5A	NAQ-CAH-CAP-CAF
2	B	1	B5A	NAQ-CAH-CAP-CAG
2	A	1	B5A	NAQ-CAH-CAP-CAF
2	A	1	B5A	NAQ-CAH-CAP-CAG

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 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	263/286 (91%)	0.99	37 (14%) <b>2</b> <b>2</b>	39, 60, 115, 136	0
1	B	257/286 (89%)	1.12	40 (15%) <b>2</b> <b>1</b>	39, 58, 115, 127	0
All	All	520/572 (90%)	1.06	77 (14%) <b>2</b> <b>2</b>	39, 59, 115, 136	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	LEU	9.0
1	A	300	GLY	6.0
1	A	301	THR	5.9
1	A	306	ALA	5.9
1	A	278	PHE	5.7
1	B	307	PHE	5.6
1	B	308	LEU	5.5
1	B	331	GLU	5.4
1	B	311	ALA	5.4
1	A	407	LEU	5.4
1	A	313	VAL	5.3
1	A	408	ALA	5.3
1	B	306	ALA	5.2
1	B	334	ILE	5.0
1	B	333	PRO	5.0
1	A	307	PHE	4.8
1	B	271	VAL	4.7
1	B	329	VAL	4.7
1	A	299	PRO	4.7
1	A	411	ILE	4.6
1	B	407	LEU	4.5
1	A	304	PRO	4.5
1	A	298	LYS	4.5
1	B	335	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	309	GLN	4.3
1	B	269	LEU	4.3
1	B	288	GLY	4.3
1	B	267	LEU	4.3
1	B	297	LEU	4.2
1	A	308	LEU	4.1
1	B	305	GLU	4.0
1	B	309	GLN	4.0
1	A	277	CYS	3.9
1	B	330	SER	3.7
1	A	296	THR	3.7
1	B	286	TRP	3.7
1	B	292	VAL	3.7
1	B	304	PRO	3.6
1	B	313	VAL	3.6
1	A	279	GLY	3.4
1	A	311	ALA	3.4
1	B	289	THR	3.3
1	B	303	SER	3.3
1	A	328	VAL	3.2
1	B	328	VAL	3.2
1	B	408	ALA	3.2
1	B	411	ILE	3.1
1	B	332	GLU	3.1
1	A	268	ARG	3.1
1	B	477	ARG	3.1
1	A	276	GLY	3.1
1	B	473	ASP	2.9
1	B	280	GLU	2.9
1	B	287	ASN	2.9
1	B	282	TRP	2.9
1	A	302	MET	2.8
1	A	260	TRP	2.6
1	B	275	GLN	2.6
1	A	473	ASP	2.6
1	A	438[A]	ARG	2.5
1	A	271	VAL	2.5
1	A	330	SER	2.3
1	A	405	PHE	2.3
1	B	263	PRO	2.3
1	A	258	ASP	2.3
1	A	477	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	498	CYS	2.2
1	A	259	ALA	2.1
1	B	436	TYR	2.1
1	B	266	SER	2.1
1	A	336	ILE	2.1
1	B	290	THR	2.1
1	A	436	TYR	2.1
1	B	296	THR	2.1
1	A	467	VAL	2.1
1	A	410	LEU	2.0
1	A	262	ILE	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	B5A	B	1	17/17	0.82	0.25	76,83,101,102	0
2	B5A	A	1	17/17	0.86	0.19	58,62,92,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.